Fakultät für Mathematik
Lehrstuhl für wissenschaftliches Rechnen

Non-Hermitian Schrödinger dynamics with Hagedorn's wave packets

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Vollständiger Abdruck der von der Fakultät für Mathematik der Technischen Universität München zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften (Dr. rer. nat.)

genehmigten Dissertation.

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Die Dissertation wurde am 02. Mai 2017 bei der Technischen Universität München eingereicht und durch die Fakultät für Mathematik am 29. Juni 2017 angenommen.

Abstract

Hagedorn wave packets form an orthonormal basis of the L^2-functions and are known solutions of the semiclassical Schrödinger equation with quadratic Hamiltonians. In this thesis we analyse their structure, in particular the polynomial part, their connection to the Hermite functions and their representation in phase space.

Based on these findings we utilise them to investigate the time evolution generated by the Schrödinger equation with a non-Hermitian, quadratic Hamiltonian. Operators of this type appear for example in the context of diffusion models and absorbing potentials and are thus of interest in physics and chemistry. We provide explicit formulas for the propagated wave packets and thereby show that the non-unitary evolution activates lower excited states.

At last we apply our results to the Lindblad master equation with quadratic internal Hamiltonian and linear Lindblad terms.

Zusammenfassung

Hagedornsche Wellenpakete sind eine bekannte Orthonormalbasis des Hilbertraums der L^2-Funktionen und Lösungen der semiklassischen Schrödinger Gleichung mit quadratischem Hamiltonoperator. In dieser Dissertations analysieren wir ihre Form, insbesondere ihren polynomiellen Anteil, sowie ihre Verbindungen zu den Hermite Funktionen und ihre Darstellung im Phasenraum.

Darauf aufbauend verwenden wir die Wellenpakete um die Zeitentwicklung der Schrödinger Gleichung unter einem nicht-Hermiteschen, quadratischen Hamiltonoperator zu untersuchen. Solche Operatoren spielen beispielsweise bei der Modellierung von Diffusion oder auch absorbierenden Potentialen eine Rolle und sind somit in der Physik und der Chemie relevant. Wir geben eine explizite Formel für die zeitentwickelten Wellenpakete an und zeigen, dass die nicht-unitäre Entwicklung dazu führt, dass auch niedrigere angeregte Zustände aktiviert werden.

Zuletzt übertragen wir unsere Ergebnisse auf die Lindblad Mastergleichung mit quadratischem Hamiltonoperator und linearen Lindbladtermen.

Contents

1. Introduction

Hagedorn's wave packets are a family of semiclassical wave packets Hagedorn constructed in the 1980s to approximate solutions of the Schrödinger equation. They appear as a product of a multivariate polynomial and a scaled Gaussian and form a basis of the Hilbert space of square integrable functions $L^2(\mathbb{R}^n)$. Due to their form and properties these wave packets are often seen as multi-dimensional Hermite functions, this is however a simplification as they may attain a more complex structures involving also Laguerre polynomials.

For a quadratic potential Hagedorn's wave packets provide exact solutions to the Schrödinger equation, for more general potentials they have favourable approximation properties: the evolution of the wave packets is fully described by the dynamics of the centre and the linearisation of the flow around it, solutions to the Schrödinger can be approximated by the wave packets up to an exponentially small error. Hence, studying the time evolution of these wave packets gives a significant insight into Schrödinger dynamics and yields an efficient numerical tool.

So far, these investigations were restricted to Hermitian Hamiltonians, this means for a real potential and a unitary time evolution. The main contribution of this thesis is the expansion of Hagedorn's approach to non-Hermitian Hamiltonians. Operators of this type model diffusion and dissipation, i.e. an interaction of the quantum system with its environment. Since in all practical situation such an interaction occurs to some extent, the importance of non-Hermitian Hamiltonians can not be dismissed. Usual applications in physics and chemistry are potentials that absorb particles or light, models of resonance phenomena, lasers in quantum optics or a heat bath.

We follow the idea of Graefe and Schubert in their work "Complexified coherent states and quantum evolution with non-Hermitian Hamiltonians" and exploit the underlying geometry of the wave packets to determine their dynamics. Thereby, we establish a new notation for the semiclassical wave packets emphasising their close relation to Lagrangian subspaces.

In this manner we find that in contrast to Hagedorn's results for the Hermitian case, the wave packets are not invariant under a non-Hermitian Hamiltonian but can be expressed as a linear combination of lower excited states. The explicit formulas we derive furthermore allow us to calculate the propagation of the wave packets for some well-known physical examples such as the damped harmonic oscillator, the heat equation and the Fokker-Planck equation.

1.1. Reader's guide

This thesis is partitioned in two parts: The first part contains an analysis of Hagedorn's wave packets as an orthonormal set of L^2-functions that is essentially based on the publications [LT14], [DKT16] and Chapter 2 and 3 in the preprint [LST15].

Our main contributions in the first part are Theorem 4.2, where we trace back the ladders constructing the wave packets to a recursion relation only for the polynomial part and Theorem 6.1, where we show that the Wigner transform of two Hagedorn wave packets is a wave packet on phase space.

Part I is divided in six chapters.

- In Chapter 2 we introduce the linear algebra fundamentals that we need to construct Hagedorn's wave packets in Chapter 4 and we will fall back on this in many proofs and calculations in this thesis. This chapter can be seen as a reproduction of [LST15, Chapter 2] augmented with basic definitions and results of symplectic geometry from [Sil06, Chapter 1,3 and 12]. The central task of this chapter is to establish a one-to-one correspondence of Lagrangian frames, symplectic matrices and the upper Siegel half space. This bridge between the theory of Hagedorn's wave packets and symplectic geometry turns out to be useful in a lot of computations.

- Chapter 3 provides an overview over the definition and familiar properties of Hermite functions. Hagedorn's wave packets can in some sense be interpreted as a generalisation of Hermite functions to multi-dimensions and we will obtain similar results for the wave packets and the Hermite functions. However, we want to clearly point out that Hagedorn's wave packets are not simple tensor products of Hermite functions and will specify this case in Chapter 4.

  Our repetition is based on the introductions in [Tha93, Chapter 1] and [Fol09, Chapter 1]. Furthermore, we use this preliminary chapter to establish basic definitions such as function spaces and integral transforms we require in the remaining thesis. We give short proofs also for well-known results whenever our definitions differ from the one in the quoted literature.

- After we set the basis, Hagedorn's wave packets are finally discussed in Chapter 4. We use the ladder-based approach of [Hag98] rewritten by means of the Lagrangian frames from Chapter 2. We follow thereby the outline in [LST15, Chapter 3], but also regard the generalised wave packets discussed in [DKT16, Chapter 2]. The main result of this chapter is that Hagedorn's wave packets and also their generalisations can always be written as product of a multivariate polynomial and a Gaussian, where the polynomials are all generated in an equivalent way.

- Motivated by this observation Chapter 5 presents a closer study of polynomials of this type. We reproduce our results from [DKT16, Chapter 3] and the generating function deduced in [Hag15]. Of particular interest is the Laguerre connection stated in Proposition 5.2 since it provides an explanation for the factorisation of the symmetric Wigner function of Hagedorn's wave packets.

- In Chapter 6 we determine the phase space representation of Hagedorn's wave packets. As we consider the Wigner transform of two arbitrary Hagedorn wave packets we extend our findings from [LT14, Chapter 4] and [DKT16, Chapter 4], where we only allowed for wave packets parametrised by the same Lagrangian frame. However, the main statement, the Wigner transform of Hagedorn's wave packets can be written as a Hagedorn wave packet on phase space, also holds true in the general setting. These results are part of a joint work with C. Lasser and R. Schubert that has not been published yet.

- To close the analysis of the wave packets we summarise in Chapter 7 alternative definitions that are widely-spread in literature and show their equivalence to Hagedorn's wave packets.

  Our investigation comprises the squeezed states from [CR12] and [Gos10] as well as the metaplectic approach from [Ohs15] and the Bogoliubov transformation used in [BFG16]. The relation to the squeezed states of [CR12] was already discussed in [LT14, Chapter 5], the remaining equivalences are unpublished so far.

The second part of this thesis treats the time evolution of Hagedorn's wave packets under a quadratic, non-Hermitian Hamiltonian. We carry on Hagedorn's approach from the 80's in [Hag81] resp. [Hag85] where he utilised the wave packets to approximate solutions of the semiclassical Schrödinger equation with a Hermitian Hamiltonian and showed that if the Hamiltonian is quadratic, the propagation of the wave packets can be described by the dynamics of the centre and the linearisation of the classical flow around it. We merge his ansatz with the techniques developed by Graefe and Schubert in [GS12] resp. [GS11], where they investigated non-Hermitian, quadratic Hamiltonians with coherent states.

This study incorporates [LST15, Chapter 4 and 5], the remaining parts are unpublished results prepared as joint work with Caroline Lasser and Roman Schubert.

The main result of the second part is Theorem 9.2 where we formulate that in contrast to the Hermitian case, the form of the wave packets is not directly preserved under a non-unitary time evolution. Lower excited states are activated, the propagated state must be expanded into states of lower order.

Part II is divided in three chapters.

- Chapter 8 gives a review of the findings for Hermitian Hamiltonians in the language of Lagrangian frames. We state basic principles of quantum dynamics based on [Tes09] and [EN00] and derive the propagation of the multi-dimensional wave packets originally found in [Hag85]. We then show the equivalence of our notion to the one given in [Hag81] resp. [HJ00]. Finally, we briefly recap the evolution under the harmonic oscillator since one can read the Swanson-Davies oscillator executed as example in the next chapter as harmonic oscillator with complex potential.

- The main chapter of the second part is Chapter 9 where we derive explicit formulas for the time evolution of the wave packets under a non-Hermitian propagation. This part basically follows [LST15, Chapter 4] and restates the main findings of this work. The results in the special case of coherent states are equivalent to the ones in [GS12]. The first section treating the existence of the time evolution operator is unpublished so far. The given example, the one-dimensional Davies-Swanson oscillator is resumed from [LST15, Chapter 5].

- In the Chapter 10 we then transfer our results to the Lindblad master equation that describes the evolution of open quantum systems. We use the Wigner transform of Hagedorn's wave packets, that are wave packets on phase space, as ansatz functions, similar ideas with coherent states are carried out in [Alm02] and [AB10]. The given findings here are yet unpublished.

- To complete this thesis Chapter 11 presents further areas of applications for our findings. We thereby stay in the physical field and briefly recap the connection between the diffusion equation, Brownian motion and the Fokker-Planck equation. All three models can under certain conditions be written as Schrödinger equation with quadratic, complex Hamiltonian. For each equation we study an explicit example. The introduction of the diffusion equation follows [Eva98, §2.3], the theory of Brownian motion and its connection to the Fokker-Planck equation is adopted from [BH02, §5.2]. For a more general form of Fokker-Planck we moreover draw back on [Ris84].

Furthermore, this thesis contains three appendices, discussing computation tools and proofs that are shortened in the main part to focus on the central theme.

- Weyl-operators are utilised in a lot of proofs throughout this thesis. Hence, Appendix A summarises basic calculation formulas and symbol classes given in [Zwo11, §4] and [Fol89, §2.1].

- Appendix B is dedicated to the metaplectic group. The theory of squeezed states we investigate in Chapter 7 heavily relies on metaplectic operators and we thus provide for the reader's convenience a summary of their construction based on [Gos10]. The results here vary from the one in the literature as we choose our phase space variable differently.

- Since the existence of a time evolution operator is not self-evident, we require a closer study of dynamical semigroups. Appendix C follows the outline in [EN00] and [Vra03] and contains a full proof of Proposition 9.1.

1.2. Quantum dynamics on potential energy surfaces

Due to the significant overlap with the thesis "Quantum dynamics on potential energy surfaces" from J. Keller we list similarities and distinctions of both works. [Kel15] treats several approximation methods for unitary time evolution problems. In this context also Hagedorn's wave packets and their Wigner functions are discussed. Although the focus of this thesis is non-selfadjoint Hamiltonians, the analysis of the static wave packets is similar. The authors also published a joint work, [DKT16], dealing with the polynomial part of the wave packets. This publication is moreover a cooperation with Helge Dietert from the University of Cambridge. Hence, similarities are mainly found in the Chapter 4 resp. [Kel15, §7] stating the analysis of the wave packets, Chapter 5 resp. [Kel15, §6] handling the polynomial part of the wave packets and Chapter 6 resp. [Kel15, §8] where the Wigner transform of the wave packets is expressed as a wave packet on phase space.

In [Kel15] the wave packets and their relation to the Hermite functions are introduced via the polynomial part. Thus, the analysis of the polynomials in [Kel15] starts from their three-term recurrence relation, while here the wave packets are characterised via a raising and lowering operator what yields a ladder operator for the polynomial factor. These differences in the approach result in a different line of argumentation throughout most proofs of [Kel15, §6] and Chapter 5.

In more detail, [Kel15, §6.1] and Section 5.1 discuss the polynomial factor of Hagedorn's wave packets in one-dimension as scaled Hermite polynomials. However, [Kel15, Proposition 7] provides a growth bound for the polynomials to ensure the convergence of the generating function, that we neglect, since we use an ansatz via an exponential series in Proposition 5.1. Besides that we present a formula for polynomials as a determinant in the univariate case, see 5.2 that is not part of [Kel15, §6.1].

The polynomials in the general case can be defined via a ladder operator, their generating function or a three-term recurrence relation. All of them are named in [Kel15, §6.2] and Section 5.2. In particular, the result for the generating functions in [Kel15, Proposition 8] is equivalent to Proposition 5.1, and the Rodrigues formula [Kel15, Eq. (6.18)] can be found in Lemma 5.3. The ladder operators derived in [Kel15, Proposition 9] are the same we obtain from the definition of the wave packets in Theorem 4.2, but we additionally need to verify the equivalence of the ladder operators to the recurrence relation in Corollary 5.4.

The part [Kel15, §6.3] gives a profound characteristic when the polynomials factorise, in this thesis in contrast we only highlight two special cases for the factorisation we encounter in applications, see Corollary 5.6.

The connection to the Laguerre polynomials stated in Section 5.3 is equivalent to [Kel15, §6.4]. The main result, Proposition 5.2, can analogously be found as [Kel15, Proposition 11]. Also Corollary 5.5 that explicitly writes out the Laguerre connection for two-dimensional polynomials coincides with [Kel15, Corollary 1]. We point out that also the proofs in this section are obtained similarly and quoted from [DKT16, §3.3].

The tensor product representation of the polynomials from [Kel15, §6.5] then again is not in particularly discussed here, we only mention the special case of two-dimensional polynomials. The examples M_1, M_2 and M_3 chosen in Section 5.3 for the nodal sets of the polynomials are the canonical examples and also used in [Kel15, §6.5] resp. [DKT16, §5]. However, the more general example M_4 differs in both works.

Chapter 7 of [Kel15] then analyses Hagedorn's wave packets and thus resembles Chapter 4 of this thesis. Both definitions are based on the notion of Lagrangian frames, see [Kel15, Definition 3] and Definition 2.1.

Since many proofs and arguments in this thesis, especially in the second part, are based on Lagrangian subspaces, our repetition of symplectic geometry in Chapter 2 is more extensive than [Kel15]. [Kel15, §7.1] gives a brief summary including the definition of a symplectic metric and a compatible complex structure in [Kel15, Lemma 9], we introduce in Definition 2.4 and generalise in Proposition 2.3. The projection of a complex phase space centre to a real centre by means of the complex structure, that was originally found in [GS12, Theorem 2.1], is noted in [Kel15, Remark 10]. Since this projection is crucial when we investigate wave packets under a non-unitary time evolution we present it in more detail in Theorem 4.4.

The definition of the wave packets in [Kel15, §7.2] is a small generalisation of Hagedorn's original definition via ladder operators in [Hag98]. We start in Section 4.3 from the standard definition and then allow for the same generalisations in Corollary 4.2 and Section 4.5. The commutator relations for the ladder operators given in [Kel15, Lemma 10] can be found as Lemma 4.1 here.

The spectral properties of the wave packets in [Kel15, §7.3] are in the current work shorten to Lemma 4.3, the orthogonality of non-normalised wave packets, see [Kel15, Proposition 12], is not investigated. The number operator used in both theses goes back to notes of Caroline Lasser.

In [Kel15, §7.4] Hagedorn's wave packets are then characterised as a product of a Gaussian and the multivariate polynomials discussed in [Kel15, §6]. This representation is also a fundamental conclusion of this thesis and a continuation of [LT14, Proposition 2]. In particular, [Kel15, Lemma 11] coincides with Theorem 4.2 and [Kel15, Proposition 13] with Proposition 4.2, while the techniques of proofs are varying. [Kel15, Corollary 2] that restates the three term recurrence relation for the wave packets from [Lub08, Eq.(2.7)] is here explicitly quoted as implication of the polynomial recurrence at the end of Section 5.2.

As in this manuscript after investigating Hagedorn's wave packets and their polynomial part, [Kel15, §8] comprises a formula for the Wigner function of two wave packets parametrised by the same Lagrangian frame. The generalised metric we introduce in Section 2.6 allows us to go beyond and also investigate the Wigner transform of two arbitrary wave packets.

Thereby, both arguments are based on a lift of Lagrangian frames to phase space. This lift is for two different Lagrangian frames Z_1 and Z_2 elaborated in Definition 6.1, the special case $Z_1 = Z_2$ is determined in [Kel15, Lemma 12]. Consequently, [Kel15, Theorem 3] can be obtained from Theorem 6.1 for the standard wave packets or, equivalently from Proposition 6.4 for generalised wave packets, by taking $Z_1 = Z_2$.

The remaining parts of the phase space analysis are developed differently. Both theses use the polynomial representation to provide an explanation for factorisation of the Wigner function, see [Kel15, §8.3] and Corollary 6.1. This observation as well as [Kel15, Corollary 3] are reformulations of [LT14, Theorem 1]. In addition [Kel15, Remark 11, Corollary 4] uses the findings for the factorisation of the polynomials to give more informations about the tensor product structure of the Wigner function. In [Kel15, §8.4] the Wigner function is expanded in lower symmetric Wigner functions based on a recurrence relation for the Wigner transforms, see [Kel15, Proposition 15]. The same recurrence is obtained at the end of Section 6.2 showing that the results here are equivalent to the ones in [LT14].

The focus of the phase space chapter of this thesis is the lift of the Lagrangian frames and its equivalence to the standard lift, see for example [SA16, §2]. Furthermore, we deduce formulas for the FBI and the Husimi transform in Section 6.3.

Part I.

Stationary wave packets

2. Lagrangian subspaces

In this chapter we restate some basic principles of symplectic geometry to set the fundamentals we will need later to construct Hagedorn's wave packets.

We focus on the definitions for vector spaces here. Analogously one could also define a symplectic structure on manifolds but since we are handling vectors in $\mathbb{R}^n$ resp. $\mathbb{C}^n$ we restrict the repetition to symplectic vector spaces.

The results and definitions given in the first section and in the general discussion at the beginning of Section 2.4 are adopted from the lecture notes [Sil06, §1, §12, §13]. We then extend the standard setting and introduce Lagrangian frames that are spanning the Lagrangian subspaces defined in the first section. These frames will parametrise the ladder operators for the wave packets, what is a difference to Hagedorn's original notation in [Hag85] and [Hag98]. However, we can show that both approaches are equivalent. By means of the Lagrangian frames we can moreover equip each Lagrangian subspaces with a symplectic metric and a complex structure. These characteristics will become crucial when we lift the wave packets to phase space.

The basic outline of this chapter follows the one given in [LST15, §2], but we will add two more points and investigate non-normalised Lagrangian frames and the mixed metric of two Lagrangian frames. In general, we need the normalisation of a Lagrangian frame to ensure that the corresponding subspace is positive, but under a non-unitary time evolution, as we will investigate in the second part of this work, a Lagrangian frame can become non-normalised. In this case we need the tools developed in Section 2.5. The generalised metric will play a role when we determine the Wigner function of two Hagedorn wave packets parametrised by different Lagrangian frames.

2.1. Symplectic vector spaces

In general, one obtains a symplectic vector space by equipping a finite dimensional K-vector space V, $K \in \{\mathbb{R}, \mathbb{C}\}$ with a bilinear, skew-symmetric form $\omega : V \times V \to K$, such that

$$\tilde{\omega} : V \mapsto V^*, \quad v \to \omega(v, \cdot)$$

is bijective, where V^* denotes the dual space of V. The last condition is equivalent to $\omega(v, u) = 0$ for all $u \in V$ implies $v = 0$. In this case, we call ω a *symplectic structure* and (V, ω) a *symplectic vector space*. The following result for symplectic vector spaces is more or less standard and can be found as [Sil06, Theorem 1.1].

Theorem 2.1 — Symplectic basis. If (V, ω) is a symplectic vector space, the dimension of V is even, i.e. $\dim(V) = 2n$ for $n \in \mathbb{N}$. Moreover, there exists a basis $e_1, \dots, e_n$,

$f_1, \dots, f_n$ of V such that

$$\omega(e_i, f_j) = \delta_{i,j} \quad \text{and} \quad \omega(e_i, e_j) = \omega(f_i, f_j) = 0 \tag{2.1}$$

for $i, j = 1, \dots, n$.

Similarly one can define symplecticity not only for vector spaces V, but also for subspaces of V. We call $Y \subseteq V$ *symplectic* if $\omega\ |_{Y\times Y}$ is non-degenerate and *isotropic* if $\omega\ |_{Y\times Y} \equiv 0$. Using the orthogonal complement

$$Y^\omega = \{v \in V\,;\, \omega(u, v) = 0\ \forall u \in Y\} \tag{2.2}$$

we can show that

$$\dim(Y) \leq \frac{1}{2}\dim(V) \tag{2.3}$$

for any isotropic subspace Y.

Lemma 2.1 Let (V, ω) be a symplectic vector space and Y a linear subspace of V. Then,

$$\dim(Y) + \dim(Y^\omega) = \dim(V).$$

Proof. The claim follows as a consequence of the rank-nullity theorem for the linear map

$$\tilde{\omega}_Y : V \to Y^*, \quad v \mapsto \omega(v, \cdot)\ |_Y\ .$$

It is clear from the definition that $\mathrm{kern}(\tilde{\omega}_Y) = Y^\omega$. Since $\dim(Y) = \dim(Y^*)$ it remains to show that $\mathrm{im}(\tilde{\omega}_Y) = Y^\omega$. But since $\tilde{\omega}$ is a bijective mapping, $\tilde{\omega}_Y$ has to be surjective. ■

If Y is isotropic, $Y \subseteq Y^\omega$ and Inequality (2.3) follows. If the identity

$$\dim(Y) = \tfrac{1}{2}\dim(V)$$

holds, we call Y a *Lagrangian subspace*.

We can illustrate these definitions with the basis in Theorem 2.1: $\mathrm{span}(e_1, f_1)$ for example forms a symplectic subspace, while $\mathrm{span}(e_1, \dots, e_n)$ and $\mathrm{span}(f_1, \dots, f_n)$ both define Lagrangian subspaces of V.

Thus, Lagrangian subspaces, that are the basis for our construction of wave packets later on, are defined via a vector space and a symplectic structure. In this work, it suffices to observe a simple standard case: Let $V = \mathbb{C}^{2n}$ and

$$\Omega = \begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix} \in \mathbb{R}^{2n\times 2n}. \tag{2.4}$$

denote the standard skew-symmetric matrix. Then, one can easily verify that

$$\omega : \mathbb{C}^{2n} \times \mathbb{C}^{2n} \to \mathbb{C}, \quad \omega(v, u) = v^T \Omega u. \tag{2.5}$$

defines a symplectic form and we will refer to ω in the following as *standard symplectic form*. To simplify the notation we write Id for the $n \times n$- identity matrix and only specify the dimension in other cases, for example Id_{2n}.

We call a matrix $S \in \mathbb{C}^{2n\times 2n}$ that respects the symplectic form in the sense that $\omega(Su, Sv) = \omega(u, v)$ a *symplectic matrix*. For our special choice of ω, this means that S satisfies

$$S^T \Omega S = \Omega. \tag{2.6}$$

We refer to the set of all real or complex-valued symplectic $2n \times 2n$- matrices as $\mathrm{Sp}(n, \mathbb{R})$ resp. $\mathrm{Sp}(n, \mathbb{C})$. The following corollary gives some useful properties for symplectic matrices that follow directly from the definition.

Corollary 2.1 Every symplectic matrix S is invertible and satisfies

$$S^{-1} = \Omega^T S^T \Omega. \tag{2.7}$$

In particular, $\det(S) = 1$.

Proof. Taking the determinant in (2.6) shows

$$1 = \det(S)\det(S^T) = \det(S)^2.$$

Thus, S is invertible and the formula for the inverse follows from (2.6) by multiplying with S^{-1} from the right. ■

In the next section we will parametrise a Lagrangian subspace $L \subset \mathbb{C}^{2n}$ with a complex matrix $Z \in \mathbb{C}^{2n\times n}$, i.e.

$$L = \mathrm{range}(Z),$$

and find a direct link between symplectic matrices and Lagrangian subspaces.

2.2. Lagrangian frames

In the following we will always assume that $V = \mathbb{C}^{2n}$ and ω is the standard symplectic form on $\mathbb{C}^{2n}$.

Let $L \subset \mathbb{C}^{2n}$ be a Lagrangian subspace. Then, $\dim(L) = n$ and there are basis vectors $l_1, \dots, l_n \in \mathbb{C}^{2n}$ such that

$$L = \mathrm{span}(l_1, \dots, l_n).$$

Since L is isotropic $\omega(l_j, l_k) = l_j^T \Omega l_k = 0$ for all $j, k = 1, \dots, n$. To shorten the notation, we summarise the vectors $l_1, \dots, l_n$ in a matrix,

$$Z = \begin{pmatrix} | & & | \\ l_1 & \cdots & l_n \\ | & & | \end{pmatrix} \in \mathbb{C}^{2n\times n}$$

and find $L = \mathrm{range}(Z)$.

The following definition can also be found as [LST15, Definition 2.2].

Definition 2.1 — Lagrangian frame. We say that a matrix $Z \in \mathbb{C}^{2n\times n}$ is *isotropic* if

$$Z^T \Omega Z = 0 \tag{2.8}$$

and *normalised* if

$$Z^* \Omega Z = 2\mathrm{iId}. \tag{2.9}$$

We call an isotropic matrix of rank n a *Lagrangian frame*.

The first condition reflects the isotropy of L. If additionally an isotropic matrix has full rank, then its columns are linearly independent and thus form a basis of a Lagrangian subspace. This means, if Z is a Lagrangian frame, then

$$L_Z := \{Zx\,;\, x \in \mathbb{C}^n\} \subset \mathbb{C}^{2n}$$

is a Lagrangian subspace. Vice versa, if L is a Lagrangian subspace we can construct a Lagrangian frame Z by taking basis vectors of L as columns of Z. Note that as the choice of the basis of L, also the choice of a Lagrangian frame Z is not unique. We define by

$$F_n(L) = \{Z \in \mathbb{C}^{2n\times n}\,;\, \mathrm{range}(Z) = L, Z^*\Omega Z = 2\mathrm{iId}\}$$

the set of all normalised Lagrangian frames spanning a Lagrangian subspace L.

The second condition first of all ensures that the quadratic form

$$h(v, u) = \tfrac{1}{2\mathrm{i}} v^* \Omega u \quad \text{for } v, u \in \mathbb{C}^{2n} \tag{2.10}$$

is positive on L. We call such a Lagrangian subspace *positive*. A *negative* Lagrangian subspace is accordingly a Lagrangian subspace L with $h(l, l) < 0$ for all $l \in L\backslash\{0\}$.

Besides that a normalised Lagrangian frame not only yields a basis for a Lagrangian subspaces but for the symplectic vector space $(\mathbb{R}^{2n}, \omega)$.

Corollary 2.2 Let $Z \in \mathbb{C}^{2n\times n}$ denote a normalised Lagrangian frame and $l_1, \dots, l_n$ the columns of Z. Then,

$$\mathrm{Re}(l_1), \dots, \mathrm{Re}(l_n), \mathrm{Im}(l_1), \dots, \mathrm{Im}(l_n)$$

form a basis of $\mathbb{R}^{2n}$ that satisfies (2.1).

Proof. If we rewrite the isotropy condition (2.8) and the normalisation condition (2.9) in terms of real and imaginary part of Z, we find

$$\mathrm{Re}(Z)^T \Omega \mathrm{Re}(Z) = \mathrm{Im}(Z)^T \Omega \mathrm{Im}(Z) = 0$$

and

$$\mathrm{Re}(Z)^T \Omega \mathrm{Im}(Z) = -\mathrm{Im}(Z)^T \Omega \mathrm{Re}(Z) = \mathrm{Id},$$

what is equivalent to (2.1). ■

The two equations for the real and imaginary part of a normalised Lagrangian frame Z in the above proof furthermore yield the approached connection to symplectic matrices, see also [LST15, §2].

Remark 2.1 If Z is a normalised Lagrangian frame, then

$$S = \begin{pmatrix} \mathrm{Re}(Z) & -\mathrm{Im}(Z) \end{pmatrix} \in \mathbb{R}^{2n\times 2n}$$

is symplectic. On the other hand, if $S = \begin{pmatrix} U & V \end{pmatrix} \in \mathbb{R}^{2n\times 2n}$ is a symplectic matrix, then $Z = U - \mathrm{i}V$ defines a normalised Lagrangian frame.

The ansatz to formulate (2.8) and (2.9) as a symplecticity condition on matrices was already introduced in [Lub08, Chapter V.I] using a different representation, which we will discuss next.

2.3. Hagedorn's parametrisation

If we write $Z = \begin{pmatrix} P \\ Q \end{pmatrix}$ as a block matrix with $P, Q \in \mathbb{C}^{n\times n}$, or, $Z = (P; Q)$ as a short notation, then Z is isotropic if

$$Q^T P - P^T Q = 0 \tag{2.11}$$

and normalised if

$$Q^* P - P^* Q = 2\mathrm{i}\mathrm{Id}. \tag{2.12}$$

These conditions coincide with the requirements in [Lub08, Chapter V.I] or, for $Q = A^T$ and $P = \mathrm{i}B^T$ with Hagedorn's original definition given in [Hag98, Chapter 3]. Thus, we can adopt the following lemma for Lagrangian frames.

Lemma 2.2 Let $Z = (P; Q) \in \mathbb{C}^{2n\times n}$ be a normalised Lagrangian frame. Then, P and Q are invertible, and

$$B = PQ^{-1} \in \mathbb{C}^{n\times n} \tag{2.13}$$

is complex symmetric with positive imaginary part

$$\mathrm{Im}(B) = (QQ^*)^{-1}. \tag{2.14}$$

Conversely, every complex symmetric matrix B with positive definite imaginary part can be written as $B = PQ^{-1}$ with $Z = (P; Q)$ being a normalised Lagrangian frame.

Proof. This result can be found as [Lub08, Chapter V.I, Lemma 1.1]. The matrices P and Q are invertible if $\mathrm{kern}(P) = \mathrm{kern}(Q) = \{0\}$, but this follows from Equation (2.12), since

$$(Qy)^*(Py) - (Py)^*(Qy) = 2\mathrm{i}\|y\|^2$$

for all $y \in \mathbb{C}^n$. For the symmetry of B we note that

$$B - B^T = Q^{-T}(Q^T P - P^T Q)Q^{-1} = 0$$

and, analogously, for the imaginary part,

$$B - B^* = Q^{-*}(Q^*P - P^*Q)Q^{-1} = 2\mathrm{i}Q^{-*}Q^{-1}.$$

For the inversion, assume that $B \in \mathbb{C}^{n\times n}$ is symmetric and $\mathrm{Im}(B) > 0$. Then, we can construct a normalised Lagrangian frame $Z = (P;Q)$ by taking $Q = \mathrm{Im}(B)^{-1/2}$ and $P = BQ$. This choice satisfies

$$Q^TP - P^TQ = Q^T(B - B^T)Q = 0,$$

and

$$Q^*P - P^*Q = Q^*(B - B^*)Q = 2\mathrm{i}\mathrm{Im}(B)^{-1/2}\mathrm{Im}(B)\mathrm{Im}(B)^{-1/2} = 2\mathrm{i}\mathrm{Id}.$$

■

With this lemma we can identify the set of normalised Lagrangian frames with the Siegel upper half-space

$$\Sigma_n = \{W \in \mathbb{C}^{n\times n}\,;\, W = W^T, \mathrm{Im}(W) > 0\}.$$

Moreover, with [LST15, Lemma 2.4], we find that a large set of Lagrangian subspaces can be naturally parametrised by complex symmetric matrices.

Lemma 2.3 — Siegel half space. Assume that $L \subset \mathbb{C}^{2n}$ is a Lagrangian subspace so that the projection $\mathbb{C}^{2n} \mapsto \mathbb{C}^n$, $(p,q) \to p$ is non-singular on L. Then there exists a unique symmetric $B \in \mathbb{C}^{n\times n}$ such that

$$L = \{(Bx, x)\,;\, x \in \mathbb{C}^n\}\ .$$

The matrix B can be written as $B = PQ^{-1}$, where $P, Q \in \mathbb{C}^{n\times n}$ are the components of any Lagrangian frame $Z \in \mathbb{C}^{2n\times n}$ spanning L. Furthermore, L is positive (negative) if and only if $\mathrm{Im}(B)$ is positive (negative) definite.

Proof. That the projection of L to $\mathbb{C}^n$ is non-singular means that there exists a function f such that

$$L = \{(f(x), x)\,;\, x \in \mathbb{C}^n\}$$

and since L is linear f also has to be linear. Thus f is of the form $f(x) = Bx$ for a uniquely determined matrix $B \in \mathbb{C}^{n\times n}$.

Now let us denote elements of L as $l_B(x) = (Bx, x) \in \mathbb{C}^{2n}$ for $x \in \mathbb{C}^n$. Since L is isotropic, we need

$$0 = l_B^T(x)\Omega l_B(x') = x \cdot (B - B^T)x'$$

for all $x, x' \in \mathbb{C}^n$. This implies $B = B^T$. The matrix B can be defined via any Lagrangian frame since for any two Lagrangian frames $Z = (P;Q)$ and $Z_1 = (P_1;Q_1)$ spanning L, there is an unitary matrix $U \in \mathbb{C}^{n\times n}$ with $Z_1 = ZU$, so that

$$P_1Q_1^{-1} = PQ^{-1} = B.$$

Moreover, we find for the quadratic form

$$h(l_B(x), l_B(x)) = \frac{1}{2\mathrm{i}} l_B(x)^* \Omega l_B(x) = \frac{1}{2\mathrm{i}} x^*(B - \overline{B})x = x^*(\mathrm{Im}B)x$$

for all $x \in \mathbb{C}^n$. Hence L is positive (negative) if and only if $\mathrm{Im}(B)$ is positive (negative). ■

The observations in this chapter yet mainly focus on the imaginary part of B, but we need to add a short remark on $\mathrm{Re}(B)$ here as well, since the real part gives us a criterion to classify pure states, i.e. symmetric Wigner functions, later on.

■ **Remark 2.2** The matrix B is purely imaginary if

$$\mathrm{Re}(PQ^{-1}) = PQ^{-1} - \mathrm{i}(QQ^*)^{-1} = (P - iQ^{-*})Q^{-1} = 0,$$

i.e. if the normalisation condition (2.9) is fulfilled with $Q^*P = -P^*Q = \mathrm{iId}$.

All in all, we stated a one-to-one correspondence between positive Lagrangian subspaces, symplectic matrices and the upper Siegel half space.

As a next step, we will equip the symplectic vector space $(\mathbb{C}^{2n}, \omega)$ with an ω- compatible complex structure J and a metric G. These characteristics will become crucial when we lift the wave packets to phase space.

2.4. Metric and complex structure

Let us briefly consider the general case first. Let (V, ω) be a symplectic vector space.

Definition 2.2 A *complex structure* on V is a linear map

$$j : V \mapsto V \quad \text{with} \quad j^2 = -\mathrm{id},$$

where $\mathrm{id} : V \mapsto V, \mathrm{id}(u) = u$ denotes the identity map. If additionally

$$\omega(j(u), j(v)) = \omega(u, v) \quad \forall u, v \in V \quad \text{and} \quad \omega(u, j(u)) > 0 \quad \forall u \in V \backslash \{0\}$$

the map j is called an *ω-compatible* complex structure.

This definition is taken from [Sil06, Definition 12.2]. For a better intuition one can identify the complex structure j with the multiplication by i on a $\mathbb{C}$-vector space.

It can be shown that every symplectic vector space possesses such a ω-compatible structure, see [Sil06, Proposition 12.3]. Moreover, from a symplectic form and a compatible complex structure one can deduce a *Riemannian metric* $g : V \times V \to K$ via

$$g(u, v) = \omega(u, j(v)).$$

The three maps (ω, g, j) form a compatible triple, each two of the forms uniquely determine the third, see [Sil06, §12.3] for more details. However, there may be several complex structures compatible with one symplectic form ω.

Please note that we slightly stretched the definition of a Riemannian metric here. Since we also allow for symplectic forms that map to $\mathbb{C}$, the metric g might yield complex values as well, but we find that g is only a positive inner product on $\mathbb{R}$. We will still refer to g as a metric, since the description is more a formal one.

In the special case, where we choose $V = \mathbb{C}^{2n}$ and ω to be the standard symplectic structure, we can equivalently transfer these definitions to matrices.

Definition 2.3 A matrix $J \in \mathbb{C}^{2n\times 2n}$ is an ω-compatible complex structure if

$$J^T\Omega J = \Omega, \quad \Omega J > 0 \quad \text{and} \quad J^2 = -\mathrm{Id}_{2n}.$$

Furthermore, if J is an ω-compatible complex structure, then $G := \Omega J$ defines a metric on $\mathbb{R}^{2d}$.

Starting from a positive Lagrangian subspace L, our goal is now to construct a metric G and a complex structure J from a Lagrangian frame $Z \in F_n(L)$. We first note that although the choice of a Lagrangian frame spanning L might not be unique, all frames $Z, Z_1 \in F_n(L)$ are related by a unitary matrix $U \in U(n)$:
Since $\mathrm{range}(Z) = \mathrm{range}(Z_1)$, there exists an invertible $U \in \mathbb{C}^{n\times n}$ such that $Z_1 = ZU$. Moreover, since Z_1 is normalised,

$$2\mathrm{i}\mathrm{Id} = Z_1^*\Omega Z_1 = U^*Z^*\Omega ZU = 2\mathrm{i}U^*U$$

and U is unitary. So, all normalised frames $Z \in F_n(L)$ not only define the same matrix $B \in \Sigma_n$, but also the same Hermitian square ZZ^*. The next result that can also be found in [LST15, Proposition 2.3] will characterise L based on this Hermitian square.

Proposition 2.1 — Projections. Let $L \subset \mathbb{C}^{2n}$ be a positive Lagrangian and $Z \in F_n(L)$. Then, the complex conjugate $\overline{L}$ is a negative Lagrangian and

$$h(\bar{l}, l') = 0 \quad \text{for all} \quad \bar{l} \in \overline{L}, l' \in L.$$

The orthogonal projections onto L and $\overline{L}$, respectively, are given by

$$\pi_L = \tfrac{\mathrm{i}}{2}ZZ^*\Omega^T \quad \text{and} \quad \pi_{\overline{L}} = -\tfrac{\mathrm{i}}{2}\overline{Z}Z^T\Omega^T, \tag{2.15}$$

that is,

(i) $\pi_L \mid_L = \mathrm{Id}_{2n}$, $\pi_L \mid_{\overline{L}} = 0$ and $\pi_{\overline{L}} \mid_{\overline{L}} = \mathrm{Id}_{2n}$, $\pi_{\overline{L}} \mid_L = 0$,

(ii) $\pi_L^2 = \pi_L$ and $\pi_{\overline{L}}^2 = \pi_{\overline{L}}$,

(iii) $h(\pi_L v, u) = h(v, \pi_L u)$ and $h(\pi_{\overline{L}} v, u) = h(v, \pi_{\overline{L}} u)$ for all $v, u \in \mathbb{C}^{2n}$.

Proof. Let $l_1, \ldots, l_n$ be a basis of L. Then, $\bar{l}_1, \ldots, \bar{l}_n$ is a basis of $\overline{L}$, i.e. $\dim(\overline{L}) = n$ and

$$\bar{l}^T\Omega\bar{l}' = \overline{l^T\Omega l'} = 0$$

for all $\bar{l}, \bar{l}' \in \overline{L}$. Thus $\overline{L}$ is a Lagrangian subspace and since

$$h(\bar{l},\bar{l}) = \tfrac{1}{2\mathrm{i}} l^T \Omega \bar{l} = \tfrac{1}{2\mathrm{i}} l^* \Omega^T l = -h(l,l) < 0$$

for all $\bar{l} \in \overline{L}$, $\overline{L}$ is negative. In addition, $h(\bar{l}, l') = \frac{1}{2\mathrm{i}} l^T \Omega l' = 0$ for all $\bar{l} \in \overline{L}$, $l' \in L$ and we can interpret L and $\overline{L}$ as an orthogonal decomposition of $\mathbb{C}^{2n}$, $L \oplus \overline{L} = \mathbb{C}^{2n}$, with respect to h. To prove $\pi_L \mid_L = \mathrm{Id}_{2n}$ and $\pi_L \mid_{\overline{L}} = 0$, we observe

$$\pi_L Z = \tfrac{\mathrm{i}}{2} Z Z^* \Omega^T Z = Z, \qquad \pi_L \overline{Z} = \tfrac{\mathrm{i}}{2} Z Z^* \Omega^T \overline{Z} = 0.$$

Furthermore,

$$\pi_L^2 = (\tfrac{\mathrm{i}}{2})^2 Z Z^* \Omega Z Z^* \Omega = \tfrac{\mathrm{i}}{2} Z Z^* \Omega^T = \pi_L$$

and

$$h(\pi_L v, u) = \tfrac{1}{2\mathrm{i}} v^* (\tfrac{\mathrm{i}}{2} Z Z^* \Omega^T)^* \Omega u = \tfrac{1}{2\mathrm{i}} v^* \Omega (-\tfrac{\mathrm{i}}{2} Z Z^* \Omega) u = h(v, \pi_L u).$$

The properties of $\pi_{\overline{L}}$ are also proved by short calculations using that Z is isotropic and normalised. ■

We now examine the real and imaginary parts of Hermitian squares ZZ^* to see more of their geometric information unfolding, see [LST15, Proposition 2.5].

Proposition 2.2 — Hermitian square. Let $Z \in \mathbb{C}^{2n \times n}$ be a normalised Lagrangian frame. Then,

$$Z Z^* = \mathrm{Re}(Z Z^*) - \mathrm{i}\Omega,$$

where $\mathrm{Re}(ZZ^*) \in \mathrm{Sp}(n, \mathbb{R})$ is a real symmetric and positive definite. In particular, $\mathrm{Re}(ZZ^*)^{-1} = \Omega^T \mathrm{Re}(ZZ^*)\Omega$. Moreover,

$$\mathrm{Re}(ZZ^*)\Omega Z = \mathrm{i}Z, \qquad \mathrm{Re}(ZZ^*)\Omega \overline{Z} = -\mathrm{i}\overline{Z},$$

so that $(\mathrm{Re}(ZZ^*)\Omega)^2 = -\mathrm{Id}_{2n}$.

Proof. Writing $\pi_L + \pi_{\overline{L}} = \mathrm{Id}_{2n}$ in terms of Z, we obtain

$$\tfrac{\mathrm{i}}{2} Z Z^* \Omega^T - \tfrac{\mathrm{i}}{2} \overline{Z} Z^T \Omega^T = -\tfrac{\mathrm{i}}{2} (Z Z^* - \overline{Z} Z^T)\Omega = \mathrm{Im}(ZZ^*)\Omega = \mathrm{Id}_{2n}.$$

Hence, $\mathrm{Im}(ZZ^*) = -\Omega$. This implies symplecticity of the real part, since

$$\begin{aligned} \mathrm{Re}(ZZ^*)^T \Omega \mathrm{Re}(ZZ^*) &= \tfrac{1}{4}(\overline{Z} Z^T + Z Z^*)\Omega(\overline{Z} Z^T + Z Z^*) \\ &= \tfrac{1}{4}(-2\mathrm{i}\, \overline{Z} Z^T + 2\mathrm{i}\, Z Z^*) = -\mathrm{Im}(ZZ^*) = \Omega. \end{aligned}$$

Checking positive definiteness, we see

$$z^* \mathrm{Re}(ZZ^*) z = \tfrac{1}{2} z^* (Z Z^* z + \overline{Z} Z^T z) = |Z^* z|^2 \geq 0$$

for all $z \in \mathbb{R}^{2n}$. If $Z^* z = 0$, then $Z Z^* z = 0$ and $\mathrm{Im}(ZZ^*) z = 0$, which means $z = 0$. Finally we compute $\mathrm{Re}(ZZ^*)\Omega Z = \frac{1}{2}(Z Z^* + \overline{Z} Z^T)\Omega Z = \mathrm{i}Z$. ■

These properties of the Hermitian square ZZ^* motivate our next definitions, see [LST15, Definition 2.6].

Definition 2.4 — Symplectic metric and complex structure. Let $L \subset \mathbb{C}^{2n}$ be a positive Lagrangian subspace and $Z \in F_n(L)$.

(i) We call the symmetric, positive definite, symplectic matrix

$$G = \Omega^T \mathrm{Re}(ZZ^*)\Omega$$

the *symplectic metric* of L.

(ii) We call the symplectic matrix

$$J = -\Omega G$$

with $J^2 = -\mathrm{Id}_{2n}$ the *complex structure* of L.

With Hagedorn's parametrisation $Z = (P;Q)$ we can write G in terms of the real and imaginary part of $B = PQ^{-1}$ and show that our definition is equivalent to the one given in [GS11, Eq. (3)] resp. [GS12].

Corollary 2.3 Let $L \subset \mathbb{C}^{2n}$ be a positive Lagrangian subspace, $Z = (P;Q) \in F_n(L)$ and $B = PQ^{-1}$. We can write the symplectic metric G of L as

$$G = \begin{pmatrix} QQ^* & -QP^* - \mathrm{iId} \\ -PQ^* + \mathrm{iId} & PP^* \end{pmatrix}$$

or, equivalently,

$$G = \begin{pmatrix} \mathrm{Im}(B)^{-1} & -\mathrm{Im}(B)^{-1}\mathrm{Re}(B) \\ -\mathrm{Re}(B)\mathrm{Im}(B)^{-1} & \mathrm{Re}(B)\mathrm{Im}(B)^{-1}\mathrm{Re}(B) + \mathrm{Im}(B) \end{pmatrix}. \tag{2.16}$$

Proof. The first expression for G follows by a direct calculation, $G = \Omega^T ZZ^*\Omega + \mathrm{i}\Omega$. For the second form, we use that $\mathrm{Im}(B)^{-1} = QQ^*$. So,

$$\begin{aligned} -PQ^* + \mathrm{iId} &= -B \cdot QQ^* + \mathrm{iId} = -(\mathrm{Re}(B) + \mathrm{iIm}(B))\mathrm{Im}(B)^{-1} + \mathrm{iId} = -\mathrm{Re}(B)\mathrm{Im}(B)^{-1}, \\ -QP^* - \mathrm{iId} &= -QQ^* \cdot B^* - \mathrm{iId} = -\mathrm{Im}(B)^{-1}(\mathrm{Re}(B) - \mathrm{iIm}(B)) - \mathrm{iId} = -\mathrm{Im}(B)^{-1}\mathrm{Re}(B), \end{aligned}$$

and

$$\begin{aligned} PP^* = BQQ^*B^* &= (\mathrm{Re}(B) + \mathrm{iIm}(B))\mathrm{Im}(B)^{-1}(\mathrm{Re}(B) - \mathrm{iIm}(B)) \\ &= \mathrm{Re}(B)\mathrm{Im}(B)^{-1}\mathrm{Re}(B) + \mathrm{Im}(B). \end{aligned}$$

■

The correspondence

$$J = -\mathrm{Re}(ZZ^*)\Omega = -(ZZ^* + i\Omega)\Omega = ZZ^*\Omega^T + \mathrm{iId}$$

suggest a closer study of the relation between the complex structure J and the projection π_L, see [LST15, Corollary 2.7].

Corollary 2.4 — Orthogonal projections. Let $L \subset \mathbb{C}^{2n}$ be a positive Lagrangian and $J \in \mathrm{Sp}(n, \mathbb{R})$ its complex structure. Then, the orthogonal projections on L and $\overline{L}$ can be written as

$$\pi_L = \tfrac{1}{2}(\mathrm{Id}_{2n} + \mathrm{i}J), \qquad \pi_{\overline{L}} = \tfrac{1}{2}(\mathrm{Id}_{2n} - \mathrm{i}J).$$

Proof. We have

$$\pi_L = \tfrac{\mathrm{i}}{2} Z Z^* \Omega^T = \frac{\mathrm{i}}{2}(J - \mathrm{i}\mathrm{Id}) = \frac{1}{2}(\mathrm{Id} + \mathrm{i}J)$$

and $\pi_{\overline{L}} = \overline{\pi_L}$. ■

So far, we stated that every positive Lagrangian subspace possesses a symplectic metric G, that is a real-valued, symmetric and positive definite matrix. Conversely, we can also show that for every symmetric $G \in \mathrm{Sp}(n, \mathbb{R})$ with $G > 0$ there exists a positive Lagrangian subspace whose symplectic metric is given by G:

The eigenvalues of any symmetric, positive definite matrix $G \in \mathrm{Sp}(n, \mathbb{R})$ occur in pairs, there exist $\lambda_1, \dots, \lambda_n \geq 1$ so that

$$\sigma(G) = \left\{\lambda_1, \dots, \lambda_n, \lambda_1^{-1}, \dots, \lambda_n^{-1}\right\} .$$

In particular, if $u_1, \dots, u_n \in \mathbb{R}^{2n}$ are orthonormal eigenvectors of G associated with the eigenvalues $\lambda_1, \dots, \lambda_n$, that is,

$$G u_k = \lambda_k u_k \,, \qquad u_j \cdot u_k = \delta_{jk} \,, \qquad j, k = 1, \dots, n \,,$$

then the vectors $v_k := \Omega u_k$ are eigenvectors of G so that

$$G v_k = \lambda_k^{-1} v_k \,, \qquad k = 1, \dots, n \,,$$

since $G\Omega = \Omega G^{-1}$. This special spectral structure allows to extract a normalised Lagrangian frame from a symplectic metric.

Lemma 2.4 Let $G \in \mathrm{Sp}(n, \mathbb{R})$ be symmetric and positive definite. Consider an eigenbasis $u_1, \dots, u_n, v_1, \dots, v_n \in \mathbb{R}^{2n}$ of G as described above and denote

$$l_k := \tfrac{1}{\sqrt{\lambda_k}} u_k - \mathrm{i}\sqrt{\lambda_k} v_k \,, \qquad k = 1, \dots, n \,.$$

Then, the matrix $Z \in \mathbb{C}^{2n \times n}$ with column vectors $l_1, \dots, l_n$ is a normalised Lagrangian frame so that $G = \Omega^T \mathrm{Re}(Z Z^*) \Omega$.

Proof. This result can also be found as [LST15, Lemma 2.8]. The vectors $l_1, \dots, l_n$ are normalised, since

$$\begin{aligned} l_j^* \Omega l_k &= \left(\tfrac{1}{\sqrt{\lambda_j}} u_j + \mathrm{i}\sqrt{\lambda_j} v_j\right) \cdot \Omega \left(\tfrac{1}{\sqrt{\lambda_k}} u_k - \mathrm{i}\sqrt{\lambda_k} v_k\right) \\ &= \delta_{jk} \left(\mathrm{i} v_k \cdot \Omega u_k - \mathrm{i} u_k \cdot \Omega v_k\right) = 2\mathrm{i}\delta_{jk} \,. \end{aligned}$$

Isotropy is seen by an analogous calculation. Furthermore,

$$\mathrm{Re}(ZZ^*) = \sum_{k=1}^{n} \mathrm{Re}(l_k l_k^*) = \sum_{k=1}^{n} \left(\tfrac{1}{\lambda_k} u_k u_k^T + \lambda_k v_k v_k^T \right) = G^{-1} ,$$

where we have used that $\mathrm{Re}(l_k l_k^*) u_k = \frac{1}{\lambda_k} u_k$ and $\mathrm{Re}(l_k l_k^*) v_k = \lambda_k v_k$ for all $k = 1, \ldots, n$. ■

This section completes the part of symplectic linear algebra we will need to construct Hagedorn's wave packets. Beyond that we allow for two generalisations we will make use of when we specify the non-symmetric Wigner function or, when we propagate our Lagrangian subspaces with a non-unitary time evolution. These two extensions are discussed in the next sections.

2.5. Non-normalised Lagrangian frames

First we want to review the construction of Lagrangian subspaces via non-normalised Lagrangian frames, i.e. Lagrangian frames that do not satisfy (2.9). By definition such frames still span a Lagrangian subspace $L = \mathrm{range}(Z)$, but its characterisation is encoded in the matrix $Z^*\Omega Z$. We will encounter frames of this type in Chapter 9, when we discuss the effects of non-Hermitian Schrödinger dynamics.

Definition 2.5 — Normalisation. Let $Z \in \mathbb{C}^{2n\times n}$ be a Lagrangian frame. We define its *normalisation* $N \in \mathbb{C}^{n\times n}$ as

$$Z^*\Omega Z = 2\mathrm{i}N,$$

with N being a Hermitian, invertible matrix.

The invertibility of N follows since for all $v \in \mathbb{C}^{2n}\backslash\{0\}$, $Z^*\Omega Z v = 0$ implies that each column of $\overline{Z}$ is an element of Z. But this is a contradiction since L is a positive Lagrangian frame, while $\overline{L}$ is negative, see Proposition 2.1.

In §2.2 we stated that the normalisation condition (2.9) ensures that the quadratic form h defined in (2.10) is positive on L. We can generalise this result here in terms of the normalisation N.

Lemma 2.5 Let $Z \in \mathbb{C}^{2n\times n}$ be a Lagrangian frame and N the normalisation of Z. Then, the Lagrangian subspace $L := \mathrm{range}(Z)$ is positive (negative) if and only if N is positive (negative) definite.

Proof. Let $l_1, \ldots, l_n \in \mathbb{C}^{2n}$ denote the columns of Z. Then, L is positive, if

$$h\left(\sum_{j=1}^{n} \alpha_j l_j, \sum_{j=1}^{n} \alpha_j l_j \right) > 0$$

for all $\alpha_j \in \mathbb{C}$, $j = 1, \ldots, n$. But by the definitions of h and N,

$$h\left(\sum_{j=1}^{n} \alpha_j l_j, \sum_{j=1}^{n} \alpha_j l_j \right) = \sum_{j,k=1}^{n} \frac{1}{2\mathrm{i}} \overline{\alpha}_i l_i^* \Omega l_j \alpha_j = \alpha^* N \alpha$$

with the vector notation $\alpha = \begin{pmatrix}\alpha_1 & \dots & \alpha_n\end{pmatrix}^T$. ■

With this lemma we can also argue that if N is a positive definite matrix, the Lagrangian subspace L is positive and can thus be parametrised by a normalised Lagrangian frame $Z' \in F_n(L)$. We find such a frame Z' by taking $Z' = ZN^{-1/2}$, since

$$Z'^T \Omega Z' = (N^{-1/2})^T Z^T \Omega Z N^{-1/2} = 0$$

and

$$Z'^* \Omega Z' = (N^{-1/2})^* Z^* \Omega Z N^{-1/2} = 2\mathrm{i} N^{-1/2} N N^{-1/2} = 2\mathrm{i}\mathrm{Id}.$$

This construction is well-defined as N is positive definite, Hermitian and invertible.

■ **Remark 2.3** Both frames, Z' and Z, define the same Lagrangian subspace L, because $N^{-1/2}$ is invertible, the same metric G, because $N^{-1/2}$ is Hermitian, and the same complex symmetric matrix B, see Section 2.3.

Moreover, we can also rewrite the parametrisation of Hagedorn discussed in Section 2.3 in terms of the normalisation N.

Lemma 2.6 Let $Z = (P; Q) \in \mathbb{C}^{2n\times n}$ be a Lagrangian frame with normalisation N. Then, the matrices P and Q are invertible and the matrix $B = PQ^{-1}$ is symmetric and satisfies

$$\mathrm{Im}(B)^{-1} = QN^{-1}Q^*.$$

In particular, the imaginary part of B is positive definite if and only if N is positive definite.

Proof. The invertibility of P and Q follows since N is invertible and

$$(Qy)^*(Py) - (Py)^*(Qy) = 2\mathrm{i} y^* N y.$$

The symmetry B is a consequence of the isotropy of Z, see Lemma 2.2, and is thus preserved. For the imaginary part of B we can calculate

$$\mathrm{Im}(B) = \tfrac{1}{2\mathrm{i}}\left(B - B^*\right) = \tfrac{1}{2\mathrm{i}} Q^{-*}\left(Q^*P - P^*Q\right)Q^{-1} = Q^{-*}NQ^{-1}.$$

■

2.6. Generalised metric

Let $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ be two normalised Lagrangian frames. In the following we will construct a joined metric of Z_1 and Z_2 and give a criterion for the case in which Z_1 and Z_2 define the same Lagrangian subspace L. This joined metric becomes important when we deduce the Wigner function of two Hagedorn wave packets, one parametrised by Z_1 and one by Z_2.

We start with defining a mixed isotropy $C \in \mathbb{C}^{n\times n}$ via

$$Z_1^T \Omega Z_2 = 2\mathrm{i} C \tag{2.17}$$

and, accordingly, a mixed normalisation $D \in \mathbb{C}^{n\times n}$ satisfying

$$Z_1^* \Omega Z_2 = 2\mathrm{i}D. \tag{2.18}$$

If $Z_1 = Z_2$, we find $C = 0$ and $D = \mathrm{Id}$. In general, we can only be sure that D is invertible with the same argument as for the normalisation N.

Following further the idea from the previous section, we could normalise Z_1 and Z_2 by multiplying with $D^{-1/2}$,

$$(Z_1 D^{-1/2})^* \Omega Z_2 D^{-1/2} = 2\mathrm{i}\mathrm{Id},$$

if the matrix D would be Hermitian and positive definite. Unfortunately, taking the square root of D is in general not well-defined. However, for the symplectic metric of a Lagrangian frame, see Definition 2.4, we only used the Hermitian square

$$K := Z_2 D^{-\frac{1}{2}} (Z_1 D^{-\frac{1}{2}*})^* = Z_2 D^{-1} Z_1^*, \tag{2.19}$$

which can be defined in any case. This motivates our next result.

Proposition 2.3 — Joined metric. Let Z_1 and Z_2 be two normalised Lagrangian frames, D their mixed normalisation and K as in (2.19). Then, the matrix

$$G = \frac{1}{2}\Omega^T (K + K^T)\Omega. \tag{2.20}$$

is symmetric, symplectic and has a positive definite real part.

Proof. The symmetry of G follows directly from the definition. For the symplecticity we calculate

$$(K + K^T)\Omega(K + K^T) = K\Omega K - (K\Omega K)^T + K^T\Omega K + K^T \Omega K$$

where

$$K\Omega K = Z_2 D^{-1} Z_1^* \Omega Z_2 D^{-1} Z_1^* = 2\mathrm{i} Z_2 D^{-1} Z_1^* = 2\mathrm{i}\mathrm{Id}$$

and

$$K^T \Omega K = \overline{Z}_1 D^{-T} Z_2^T \Omega Z_2 D^{-1} Z_1^* = 0.$$

Therefore, $G\Omega G = \frac{\mathrm{i}}{2}\Omega(K - K^T)\Omega$ and it remains to show that $K - K^T = 2\mathrm{i}\Omega$. But this holds true since

$$(K^T - K)\Omega^T \overline{Z}_1 = \overline{Z}_1 D^{-T} Z_2^T \Omega^T \overline{Z}_1 = \overline{Z}_1 D^{-T}(2\mathrm{i}D^T) = 2\mathrm{i}\overline{Z}_1.$$

Equivalently, we could also multiply by ΩZ_2. Positive definiteness of the real part follows by the next corollary. ■

The construction above can be seen as a generalisation of the symplectic metric. In particular, both constructions are consistent as for $Z = Z_1 = Z_2$, we find $D = \mathrm{Id}$ and

$$G = \frac{1}{2}\Omega^T (ZZ^* + (ZZ^*)^T)\Omega = \frac{1}{2}\Omega^T (ZZ^* + \overline{ZZ^*})\Omega = \Omega^T \mathrm{Re}(ZZ^*)\Omega.$$

This also raises the question how the joined metric G of two normalised Lagrangian frames Z_1 and Z_2 is related to their single symplectic metrics.

Corollary 2.5 Let $Z_1 \in \mathbb{C}^{2n\times n}$ and $Z_2 \in \mathbb{C}^{2n\times n}$ be two normalised Lagrangian frames,

$$G_1 = \Omega^T \mathrm{Re}(Z_1 Z_1^*)\Omega \quad \text{and} \quad G_2 = \Omega^T \mathrm{Re}(Z_2 Z_2^*)\Omega.$$

Then, the joined metric G of Z_1 and Z_2 can be written as

$$G = 2(G_1^{-1} + G_2^{-1})^{-1} + \mathrm{i}(G_1 - G_2)(G_1 + G_2)\Omega. \tag{2.21}$$

Proof. A direct calculation yields

$$\begin{aligned} G(G_1^{-1} + G_2^{-1}) &= \frac{1}{2}\Omega^T (Z_2 D^{-1} Z_1^* + \overline{Z}_1 D^{-T} Z_2^T)\Omega(\overline{Z}_1 Z_1^T + Z_2 Z_2^*) \\ &= \frac{1}{2}\Omega^T (Z_2 D^{-1} Z_1^* \Omega Z_2 Z_2^* + \overline{Z}_1 D^{-T} Z_2^T \Omega \overline{Z}_1 Z_1^T) \\ &= \mathrm{i}\Omega^T (Z_2 Z_2^* - \overline{Z}_1 Z_1^T) \end{aligned}$$

Using that $G_j^{-1} = Z_j Z_j^* + i\Omega$ is real symmetric and the fact that symplecticity implies $\Omega G_j^{-1} = G_j \Omega$ for $j = 1, 2$, we find

$$\begin{aligned} G(G_1^{-1} + G_2^{-1}) &= \mathrm{i}\Omega^T (G_2^{-1} - G_1^{-1} - 2\mathrm{i}\Omega) \\ &= 2\mathrm{Id} + \Omega(G_1^{-1} - G_2^{-1}) = 2\mathrm{Id} + (G_2 - G_1)\Omega \end{aligned}$$

Multiplying with $(G_1^{-1} + G_2^{-1})^{-1}$ and using the symplecticity once more to rewrite the inverse of G_1 resp. G_2 proves the claim. ∎

With Equation (2.21), we can complete the proof of Proposition 2.3:

$$\mathrm{Re}(G)^{-1} = \frac{1}{2}(G_1^{-1} + G_2^{-1})$$

is positive definite since G_1 and G_2 are positive definite matrices. In particular, we mention that G is real if and only if $G_1 = G_2$.

Although the relation between G and G_1, G_2 appears very complex, the matrix G differs from G_1 and G_2 only by a singular matrix.

Corollary 2.6 Let $Z_1 \in \mathbb{C}^{2n\times n}$ and $Z_2 \in \mathbb{C}^{2n\times n}$ denote two normalised Lagrangian frames, G_1 and G_2 their symplectic metrics and G their joined metric. Then, the matrices $G - G_1$ and $G - G_2$ are singular.

Proof. We only present the proof for $G - G_1$ here, an analogous computation can be executed for $G - G_2$. With Corollary 2.5

$$\begin{aligned} G - G_1 &= (2\mathrm{Id} + i(G_1 - G_2)\Omega)\,(G_1^{-1} + G_2^{-1})^{-1} - G_1 \\ &= \left(\mathrm{Id} + i(G_1 - G_2)\Omega - G_1 G_2^{-1}\right)(G_1^{-1} + G_2^{-1})^{-1} \\ &= \left((-\Omega + iG_1)\Omega - (i\Omega + G_1)G_2^{-1}\right)(G_1^{-1} + G_2^{-1})^{-1} \\ &= -(G_1 + i\Omega)(G_2^{-1} - i\Omega)(G_1^{-1} + G_2^{-1})^{-1} \end{aligned}$$

Thus, the difference $G - G_1$ is singular for all G_2 if $G_1 + i\Omega$ is singular. But this holds true due to Proposition 2.1 and Definition 2.4:

$$G_1 + i\Omega = \Omega^T \overline{Z}_1 Z_1^T \Omega$$

is singular, since the projection $\pi_{\overline{L}_1} = \frac{\mathrm{i}}{2}\overline{Z}_1 Z_1^T \Omega$ has a non-trivial kernel. ■

Rewriting the difference $G - G_1$ also allows us to give a more profound characteristic of the mixed isotropy C. Using that $G_1 + \mathrm{i}\Omega = \Omega^T \overline{Z}_1 Z_1^T \Omega$ and $G_2^{-1} - \mathrm{i}\Omega = Z_2 Z_2^*$, we find

$$G - G_1 = \Omega \overline{Z}_1 Z_1^T \Omega Z_2 Z_2^* (G_1^{-1} + G_2^{-1})^{-1}$$

and we can read off that $G = G_1$ if and only if $C = 0$.

■ **Remark 2.4** Two normalised Lagrangian frames Z_1 and Z_2 span the same Lagrangian subspace if they satisfy

$$Z_1^T \Omega Z_2 = 0.$$

This is the only case where the generalised metric G of Z_1 and Z_2 is a real matrix.

3. Hermite functions

In this chapter we want to review basic definitions and properties of Hermite functions that are Hermite polynomials times a Gaussian,

$$\varphi_k(x) = \frac{\pi^{-1/4}}{\sqrt{2^k k!}} h_k(x) e^{-x^2/2}, \quad x \in \mathbb{R}.$$

Hagedorn's wave packets can be seen as a generalisation of Hermite functions to several dimensions and with varying width of the Gaussian. In the one-dimensional setting they appear as scaled Hermite functions, while in multi-dimensions most characteristics of Hermite functions can be logically extended to Hagedorn wave packets. We will also present the proofs of some well-known results for the Hermite functions here in order to introduce techniques that we will use for the wave packets in the next chapter. There are several equivalent ways to define Hermite functions, for example via a Rodriguez-formula, a generating function or a differential equation. We will start here with the approach via ladder operators, what is a common approach in quantum mechanics, and derive more formulations in §3.3. Still, we could start with any of these definition and obtain the same results.

3.1. Dirac's ladder operators

To be precise we start with introducing some well-known function spaces we will work on later. Our basic setting is the Hilbert space $L^2(\mathbb{R}^n)$ of square integrable functions with the scalar product

$$\langle \varphi, \psi \rangle = \int_{\mathbb{R}^n} \varphi(x) \overline{\psi}(x)\, dx, \quad \text{for all} \quad \varphi, \psi \in L^2(\mathbb{R}^n)$$

and the induced norm $\|\varphi\|^2 = \langle \varphi, \varphi \rangle$. Furthermore, we will consider two subsets of $L^2(\mathbb{R}^n)$, the Schwartz space

$$\mathcal{S}(\mathbb{R}^n) = \{ f \in C^\infty(\mathbb{R}^n)\,;\, \forall \alpha, \beta \in \mathbb{N}^n\, \exists C > 0 : |x^\alpha \partial_x^\beta f| < C \}$$

of all rapidly decaying smooth functions and $\mathcal{D}(\mathbb{R}^n) = C_0^\infty(\mathbb{R}^n)$, the set of all smooth functions with compact support. We have $\mathcal{D}(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$. The Dirac ladder operators appear as operators on $L^2(\mathbb{R}^n)$. In particular, they can be written as *Weyl-quantisation*

$$(\mathrm{op}[a]\varphi)(x) = (2\pi)^{-n} \int_{\mathbb{R}^{2n}} a(\xi, \tfrac{1}{2}(x+y)) e^{\mathrm{i}\xi^T(x-y)} \varphi(y)\, d\xi dy, \quad \forall \varphi \in \mathcal{S}(\mathbb{R}^n) \tag{3.1}$$

of a function $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$, see [Gos10, §10.1] for a detailed discussion of the Weyl-correspondence and Appendix A for a formal introduction of Weyl-operators. In quantum mechanics, see [Zwo11, §1.2], such an $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$ is called a *classical observable* and its Weyl-quantised operator $\mathrm{op}[a]$ a *quantum observable*. We also refer to a as *symbol* of $\mathrm{op}[a]$.

Two typical important examples for observables are position and momentum. We consider a phase space variable $z = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$, where q denotes the position and p the momentum. For the position operator, we find with $a(p, q) = q_j$, $1 \leq j \leq n$, that

$$\begin{aligned}(\mathrm{op}[a]\varphi)(x) &= (2\pi)^{-n} \int_{\mathbb{R}^{2n}} \tfrac{1}{2}(x_j + y_j)e^{\mathrm{i}\xi^T(x-y)}\varphi(y)\,d\xi dy = \tfrac{1}{2}\int_{\mathbb{R}^{2n}} \delta(x-y)(x_j+y_j)\varphi(y)\,dy \\ &= x_j\varphi(x),\end{aligned}$$

i.e. $(\hat{q}_j\varphi)(x) = x_j\varphi(x)$ for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$ with the short notation $\hat{q}_j = \mathrm{op}[q_j]$. Moreover, for $a(p, q) = p_j$, $1 \leq j \leq n$, it follows by partial integration that

$$\begin{aligned}(\mathrm{op}[a]\varphi)(x) &= (2\pi)^{-n} \int_{\mathbb{R}^{2n}} \xi_j e^{\mathrm{i}\xi^T(x-y)}\varphi(y)\,d\xi dy = (2\pi)^{-n}\int_{\mathbb{R}^{2n}} (\mathrm{i}\partial_{y_j} e^{\mathrm{i}\xi^T(x-y)})\varphi(y)\,d\xi dy \\ &= (2\pi)^{-n}\int_{\mathbb{R}^{2n}} -\mathrm{i}e^{\mathrm{i}\xi^T(x-y)}\partial_{y_j}\varphi(y)\,d\xi dy = -\mathrm{i}\int_{\mathbb{R}^{2n}} \delta(x-y)\partial_{y_j}\varphi(y)\,dy \\ &= -\mathrm{i}\partial_{x_j}\varphi(x),\end{aligned}$$

i.e. $(\hat{p}_j\varphi)(x) = -\mathrm{i}\partial_{x_j}\varphi(x)$, since boundary values vanish for $\varphi \in \mathcal{S}(\mathbb{R}^n)$. In the following we will use the vector-valued notation $\hat{z} = (\hat{p}, \hat{q})$ where

$$(\hat{q}\varphi)(x) = x\varphi(x) \quad \text{and} \quad (\hat{p}\varphi)(x) = -\mathrm{i}\nabla_x\varphi(x) \tag{3.2}$$

for $\varphi \in \mathcal{S}(\mathbb{R}^n)$. The position and momentum operator satisfy the following important property.

Lemma 3.1 — Canonical commutator relation. The position operator $\hat{q}$ and the momentum operator $\hat{p}$ as defined in (3.2) are canonically conjugates, this means

$$[\hat{q}_j, \hat{p}_k] = \mathrm{i}\delta_{jk}, \quad \text{for all } 1 \leq j, k \leq n \tag{3.3}$$

with the commutator bracket $[\hat{a}, \hat{b}] = \hat{a}\hat{b} - \hat{b}\hat{a}$.

Proof. Due to the standard differentiation rules, we have

$$(\hat{q}_j(\hat{p}_k\varphi))(x) = -\mathrm{i}x_j\partial_{x_k}\varphi(x)$$

and

$$(\hat{p}_k(\hat{q}_j\varphi))(x) = -\mathrm{i}(\delta_{jk}\varphi(x) + x_j\partial_{x_k}\varphi(x))$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$. Taking the difference yields the result. ∎

A more general view on canonical commutator relations is given in [Ohs15, §2.1], we will take up on this again in Section 7.3.

Based on the position and momentum operator we are now able to introduce the ladder operators for the Hermite functions.

Definition 3.1 — Dirac's ladder operators. We call the operator

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - \mathrm{i}\hat{p}) \tag{3.4}$$

the creation or *raising operator* of the Hermite functions and

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + \mathrm{i}\hat{p}) \tag{3.5}$$

the annihilation or *lowering operator*.

By their definition these operators inherit three useful characteristics from the position and momentum operator

Lemma 3.2 Dirac's ladder operators have to following properties:

a, $\hat{a}$ and $\hat{a}^\dagger$ map Schwartz functions to Schwartz functions, i.e. $\hat{a}_j\varphi, \hat{a}_j^\dagger\varphi \in \mathcal{S}(\mathbb{R}^n)$ for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$ and $1 \leq j \leq n$.

b, $\hat{a}$ and $\hat{a}^\dagger$ are formal adjoints on $\mathcal{S}(\mathbb{R}^n)$, i.e.$\langle \hat{a}_j^\dagger\varphi, \psi\rangle = \langle \varphi, \hat{a}_j\psi\rangle$ for all $\varphi, \psi \in \mathcal{S}(\mathbb{R})$ and $1 \leq j \leq n$.

c, $\hat{a}$ and $\hat{a}^\dagger$ satisfy the commutator relation $[\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}$ for $1 \leq j, k \leq n$.

Proof. Let $\varphi \in \mathcal{S}(\mathbb{R}^n)$. Then, for all multiindices $\alpha, \beta \in \mathbb{N}^n$ there exists by definition a $C > 0$ such that $|x^\alpha \partial_x^\beta \varphi| > 0$. The same obviously holds true for $x_j\varphi(x)$ and $\partial_{x_j}\varphi(x)$, $1 \leq j \leq n$, and thus $\hat{q}_j\varphi, \hat{p}_j\varphi \in \mathcal{S}(\mathbb{R}^n)$ what proves a.

For b, we find with partial integration for $j = 1, \ldots, n$

$$\langle \hat{a}_j^\dagger\varphi, \psi\rangle = \frac{1}{\sqrt{2}}\int_{\mathbb{R}^n} (x_j - \partial_{x_j})\varphi(x)\overline{\psi}(x)\, dx = \frac{1}{\sqrt{2}}\int_{\mathbb{R}^n} \varphi(x)(x_j + \partial_{x_j})\overline{\psi}(x)\, dx = \langle \varphi, \hat{a}_j\psi\rangle$$

since $\varphi(x)\overline{\psi}(x) \mid_{\mathbb{R}^n} = 0$ for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$.

Claim c, follows from the canonical commutator relations (3.3)

$$[\hat{a}_j, \hat{a}_k^\dagger] = \frac{1}{2}[\hat{q}_j + \mathrm{i}\hat{p}_j, \hat{q}_k - \mathrm{i}\hat{p}_k] = \frac{-\mathrm{i}}{2}\left([\hat{q}_j, \hat{p}_k] - [\hat{p}_j, \hat{q}_k]\right) = \frac{-\mathrm{i}}{2}(2\mathrm{i}\delta_{jk}) = \delta_{jk}.$$

■

As a last remark in this section we want to add the relation of Dirac's ladder operators to the harmonic oscillator $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{q}^2)$, In the one-dimensional case it is clear from the definition that

$$\hat{a}^\dagger\hat{a} = \frac{1}{2}(\hat{q} - \mathrm{i}\hat{p})(\hat{q} + \mathrm{i}\hat{p}) = \frac{1}{2}(\hat{p}^2 + \hat{q}^2 + \mathrm{i}(\hat{q}\hat{p} - \hat{p}\hat{q})) = \frac{1}{2}(\hat{p}^2 + \hat{q}^2) - \frac{1}{2}$$

and, analogously, $\hat{a}\hat{a}^\dagger = \frac{1}{2}(\hat{p}^2 + \hat{q}^2) + \frac{1}{2}$. So, the harmonic oscillator and $\hat{a}^\dagger\hat{a}$ resp. $\hat{a}\hat{a}^\dagger$ have the same eigenfunctions.

3.2. Coherent and excited states

In this section we derive Hermite functions as eigenfunctions of the one-dimensional harmonic oscillator. From the previous section we know that eigenfunctions of $\hat{H}$ with eigenvalue $k + \frac{1}{2}$, $k \in \mathbb{N}$, are eigenfunctions of $\hat{a}^\dagger \hat{a}$ with eigenvalue k.

First, we note that all eigenfunctions of $\hat{a}^\dagger \hat{a}$ with eigenvalue 0 are elements of the kernel of $\hat{a}$,

$$I = \{\varphi \in \mathcal{S}(\mathbb{R})\,;\, \hat{a}\varphi = 0\}.$$

as it follows from $\hat{a}^\dagger \hat{a}\varphi = 0$ that

$$0 = \langle \hat{a}^\dagger \hat{a}\varphi, \varphi\rangle = \langle \hat{a}\varphi, \hat{a}\varphi\rangle = \|\hat{a}\varphi\|^2.$$

Lemma 3.3 — Coherent state. Every element $\varphi \in I$ is of the form

$$\varphi(x) = c \cdot e^{-x^2/2}$$

where $c \in \mathbb{C}$.

Proof. Let $\varphi \in I$. Then,

$$\nabla_x(e^{x^2/2}\varphi(x)) = xe^{x^2/2}\varphi(x) + e^{x^2/2}\nabla_x\varphi(x) = e^{x^2/2}\hat{a}\varphi = 0$$

and φ is a constant multiple of $e^{-x^2/2}$. ■

So, we found that eigenfunctions of the harmonic oscillator with eigenvalue $\frac{1}{2}$ are constant multiples of $e^{-x^2/2}$. However, in quantum mechanics wave functions are used to describe the state of quantum systems, i.e. they provide a probability distribution for an observable a. Hence, to be physically meaningful, we consider only normalised L^2-functions and denote as *coherent ground state*

$$\varphi_0(x) = \pi^{-1/4}e^{-x^2/2} \tag{3.6}$$

with $\|\varphi_0\| = 1$, see [Fol09, §1.1]. The expression coherent states for eigenstates of the harmonic oscillator was introduced in [Gla63] and later generalised, see for example [CR12, §1, §2].

From the ground state φ_0 we can now construct eigenfunctions of $\hat{a}^\dagger \hat{a}$ with higher eigenvalues. Since

$$\langle \hat{a}^\dagger \varphi_0, \varphi_0\rangle = \langle \varphi_0, \hat{a}\varphi_0\rangle = 0$$

we find that the iterative application of $\hat{a}^\dagger$ to φ_0 generates a family of orthogonal functions. To preserve the normalisation of the eigenfunctions, we calculate for $k \in \mathbb{N}$

$$\langle (\hat{a}^\dagger)^k\varphi_0, (\hat{a}^\dagger)^k\varphi_0\rangle = \langle (\hat{a}^\dagger)^{k-1}\varphi_0, \hat{a}(\hat{a}^\dagger)^k\varphi_0\rangle = k\langle (\hat{a}^\dagger)^{k-1}\varphi_0, (\hat{a}^\dagger)^{k-1}\varphi_0\rangle$$

where we used the commutator relation from Lemma 3.2 and $\hat{a}\varphi_0 = 0$. With an inductive argument, we can conclude that $\|(\hat{a}^\dagger)^k\varphi_0\|^2 = k!$, this motivates our following definition of the Hermite functions.

Definition 3.2 — Hermite functions. Let $k \in \mathbb{N}$ and φ_0 denote the coherent ground state given in (3.6). Then, we define the k-th Hermite function via

$$\varphi_k = \frac{1}{\sqrt{k!}}(\hat{a}^\dagger)^k\varphi_0$$

or, equivalently, $\varphi_k = \frac{1}{\sqrt{k}}\hat{a}^\dagger\varphi_{k-1}$.

The above definition also explains the name raising or creation operator for $\hat{a}^\dagger$. For $\hat{a}$, it holds

$$\hat{a}\varphi_k = \frac{1}{\sqrt{k!}}\hat{a}(\hat{a}^\dagger)^k\varphi_0 = \frac{k}{\sqrt{k!}}(\hat{a}^\dagger)^{k-1}\varphi_0 = \sqrt{k}\varphi_{k-1},$$

i.e. $\varphi_{k-1} = \frac{1}{\sqrt{k}}\hat{a}\varphi_k$ for $k \geq 1$ and $\hat{a}$ lowers or annihilates the eigenstates φ_k. Moreover,

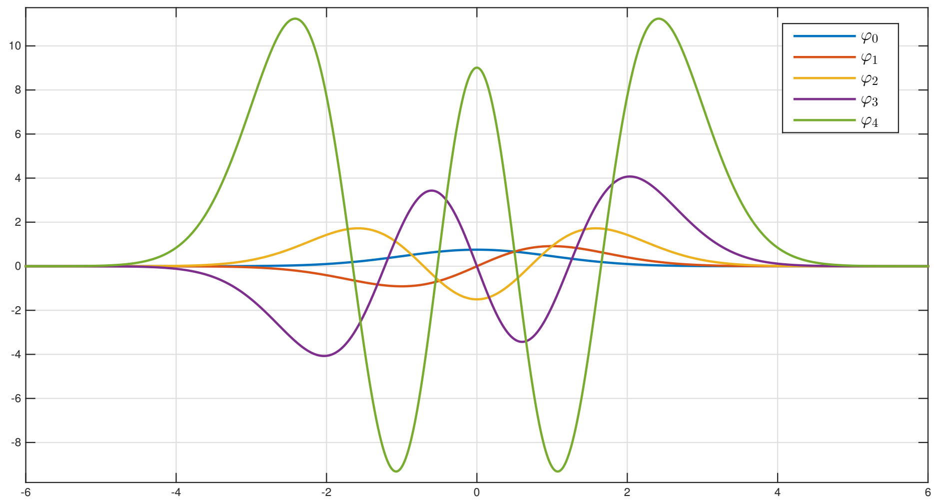

Figure 1.: Hermite functions φ_k for $k = 0, \dots, 4$.

this relation shows that the Hermite functions are indeed eigenfunctions of $\hat{a}^\dagger\hat{a}$ as

$$\hat{a}^\dagger\hat{a}\varphi_k = \sqrt{k}\hat{a}^\dagger\varphi_{k-1} = k\varphi_k$$

for all $k \in \mathbb{N}$. Thus, the k-th Hermite function φ_k is an eigenstate of $\hat{a}^\dagger\hat{a}$ with eigenvalue k and an eigenstate of the harmonic oscillator with eigenvalue $k + \frac{1}{2}$. From the construction it is also clear that the next result holds true.

Theorem 3.1 — Orthonormal set. The Hermite functions $(\varphi_k)_{k\in\mathbb{N}}$ form an orthonormal basis of $L^2(\mathbb{R})$.

Detailed proofs of this result can easily be found, see for example [Tha93, Lemma 1.1.2] or [Fol09, Theorem 6.11].

Another well-known property of the Hermite functions is that they are not only eigenfunctions of the harmonic oscillator but also of the one-dimensional Fourier transform

$$\mathcal{F}\varphi(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \varphi(x) e^{-\mathrm{i}x\xi}\, dx \tag{3.7}$$

for all $\varphi \in L^2(\mathbb{R})$. This seems logical as $\hat{H}$ is invariant under the Fourier transform, see [Tha93, §1.1]. We will present a proof here that is based on the Dirac ladder operators since we can use a similar approach later for the generalised wave packets.

Lemma 3.4 — Fourier transform. Let $k \in \mathbb{N}$ and φ_k denote the k-th Hermite function. Then,

$$\mathcal{F}\varphi_k = (-\mathrm{i})^k \varphi_k.$$

Proof. We denote by

$$\mathcal{F}^{-1}\varphi(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \varphi(\xi) e^{\mathrm{i}x\xi}\, d\xi$$

the inverse of the Fourier transform. Then, $\mathcal{F}\varphi_0$ satisfies

$$0 = \mathcal{F}\hat{a}\varphi_0 = \mathcal{F}\hat{a}\mathcal{F}^{-1}\mathcal{F}\varphi_0$$

and is thus an element of the kernel of $\hat{a}_{\mathcal{F}} := \mathcal{F}\hat{a}\mathcal{F}^{-1}$. In particular, $\mathcal{F}\varphi_0$ is the normalised element of $\mathrm{kern}(\hat{a}_{\mathcal{F}})$, since $\mathcal{F}$ and $\mathcal{F}^{-1}$ are adjoints on $L^2(\mathbb{R})$, i.e.

$$\|\mathcal{F}\varphi\|^2 = \langle \mathcal{F}\varphi, \mathcal{F}\varphi\rangle = \langle \varphi, \mathcal{F}^{-1}\mathcal{F}\varphi\rangle = \|\varphi\|^2$$

for all $\varphi \in L^2(\mathbb{R})$. For the excited states φ_k, $k \geq 1$, we moreover have

$$\mathcal{F}\varphi_k = \frac{1}{\sqrt{k}} \mathcal{F}\hat{a}^\dagger \varphi_{k-1} = \frac{1}{\sqrt{k}} \mathcal{F}\hat{a}^\dagger \mathcal{F}^{-1}\mathcal{F}\varphi_{k-1} := \frac{1}{\sqrt{k}} \hat{a}^\dagger_{\mathcal{F}} \mathcal{F}\varphi_{k-1}.$$

This means, we can construct the Fourier transforms analogously to the Hermite functions using the ladder operators $\hat{a}_{\mathcal{F}}$ and $\hat{a}^\dagger_{\mathcal{F}}$.

Let $\varphi \in \mathcal{S}(\mathbb{R})$. By partial integration

$$\begin{aligned}
(\mathcal{F}\hat{q}\mathcal{F}^{-1}\varphi)(\xi) &= \frac{1}{2\pi} \int_{\mathbb{R}^2} x\varphi(\xi') e^{\mathrm{i}x(\xi'-\xi)}\, d\xi' dx = \frac{-\mathrm{i}}{2\pi} \int_{\mathbb{R}^2} \varphi(\xi') \partial_{\xi'} e^{\mathrm{i}x(\xi'-\xi)}\, d\xi' dx \\
&= \frac{\mathrm{i}}{2\pi} \int_{\mathbb{R}^2} \partial_{\xi'}\varphi(\xi') e^{\mathrm{i}x(\xi'-\xi)}\, dx d\xi' = \mathrm{i} \int_{\mathbb{R}^2} \delta(\xi'-\xi) \partial_{\xi'}\varphi(\xi')\, d\xi' \\
&= \mathrm{i}\partial_\xi \varphi(\xi) = -(\hat{p}\varphi)(\xi)
\end{aligned}$$

and

$$\begin{aligned}
(\mathcal{F}\hat{p}\mathcal{F}^{-1}\varphi)(\xi) &= \frac{-\mathrm{i}}{\sqrt{2\pi}} \int_{\mathbb{R}} \partial_x (\mathcal{F}^{-1}\varphi)(x) e^{-\mathrm{i}x\xi}\, dx = \frac{\mathrm{i}}{\sqrt{2\pi}} \int_{\mathbb{R}} (\mathcal{F}^{-1}\varphi)(x) \partial_x e^{-\mathrm{i}x\xi}\, dx \\
&= \frac{\xi}{\sqrt{2\pi}} \int_{\mathbb{R}} (\mathcal{F}^{-1}\varphi)(x) e^{-\mathrm{i}x\xi}\, dx = \xi \mathcal{F}(\mathcal{F}^{-1}\varphi)(\xi) \\
&= \xi\varphi(\xi) = (\hat{q}\varphi)(\xi).
\end{aligned}$$

Thus, $\hat{a}_{\mathcal{F}} = \frac{1}{\sqrt{2}}(-\hat{p} + \mathrm{i}\hat{q}) = \mathrm{i}\hat{a}$ and $\hat{a}^\dagger_{\mathcal{F}} = \frac{1}{\sqrt{2}}(-\hat{p} - \mathrm{i}\hat{q}) = -\mathrm{i}\hat{a}^\dagger$ what finishes the proof.

The strategy of using the ladder operators to prove the Fourier result is adapted from [Hag98, §2]. ■

From the definition of the raising operator $\hat{a}^\dagger = \frac{1}{\sqrt{2}}(x - \nabla_x)$ and the ground state $\varphi_0(x) = \pi^{-1/4}e^{-x^2/2}$, one can already deduce that the Hermite functions attain the form

$$\varphi_k(x) = \frac{1}{\sqrt{2^k k!}} h_k(x)\varphi_0(x) \tag{3.8}$$

where h_k is a one-dimensional polynomial of degree k. This polynomial part is generally known as *Hermite polynomials* and includes most of the characteristics of the Hermite functions. The next section is an analysis of this part including some equivalent definitions for the Hermite functions.

3.3. Hermite polynomials

With Ansatz (3.8) for the Hermite functions, we can trace back $\hat{a}^\dagger$ resp. $\hat{a}$ to operators $\hat{b}^\dagger$ and $\hat{b}$ that act only on the polynomials. We have for $k \geq 0$

$$\begin{aligned}\varphi_{k+1}(x) = \frac{1}{\sqrt{k+1}}\hat{a}^\dagger\varphi_k(x) &= \frac{1}{\sqrt{2^k(k+1)!}}\hat{a}^\dagger(h_k(x)\varphi_0(x)) \\ &= \frac{1}{\sqrt{2^{k+1}(k+1)!}}(2xh_k(x) - \nabla_x h_k(x))\varphi_0(x).\end{aligned}$$

So, the Hermite polynomials can be generated as

$$h_{k+1} = \hat{b}^\dagger h_k(x), \quad \text{where} \quad \hat{b}^\dagger = 2x - \nabla_x = 2\hat{q} - i\hat{p}$$

starting from the initial value $h_0(x) = 1$. In Figure 2 we present for a better illustration the first few Hermite polynomials, $k = 0, \ldots, 4$.

Figure 2.: Hermite polynomials h_k for $k = 0, \ldots, 4$.

The same approach for the lowering operator yields

$$\varphi_{k-1}(x) = \frac{1}{\sqrt{k}}\hat{a}\varphi_k(x) = \frac{1}{\sqrt{k \cdot 2^{k+1}k!}}\nabla_x h_k(x)\varphi_0(x),$$

which means

$$\nabla_x h_k(x) = 2k \cdot h_{k-1}(x), \quad k \geq 1 \tag{3.9}$$

and differentiation can be seen as lowering operator on the polynomial level. A sequence of polynomials satisfying this condition is called an *Appell sequence*, see [App80].

Starting from the polynomial ladder operators we can now deduce several equivalent definitions for Hermite polynomials. Please note that we could have started with any of these definitions and maintain the same results.

In [CDG06, §4] the authors showed that polynomials that form an Appell sequence can also be characterised via their generating function or a determinant. We add two more points here: From the ladder operator $\hat{b}^\dagger$ and using that the Hermite polynomials form an Appell sequence we can clearly follow a recurrence relation and since

$$\hat{b}^\dagger h_k(x) = 2xh_k(x) - \nabla_x h_k(x) = e^{x^2}\nabla_x(h_k(x)e^{-x^2})$$

also a type of Rodrigues' formula.

Theorem 3.2 Let $(h_k)_{k\in\mathbb{N}}$ denote the Hermite polynomials as defined in (3.8).Then, also the following three statements hold true:

a, The Hermite polynomials $(h_k)_{k\in\mathbb{N}}$ satisfy the three-term recurrence relation

$$h_{k+1}(x) = 2xh_k(x) - 2kh_{k-1}(x) \tag{3.10}$$

for $k \geq 0$ with $h_0(x) = 1$ and $h_k(x) = 0$ for $k < 0$. We will shorty refer to this definition as TTRR.

b, The generating function of the Hermite polynomials is given by

$$g(x,t) = \sum_{k=0}^{\infty} \frac{t^k}{k!} h_k(x) = e^{2xt-t^2}, \tag{3.11}$$

i.e. $h_k(x) = \partial_t^k g(x,t) \mid_{t=0}$.

c, The Hermite polynomials $(h_k)_{k\in\mathbb{N}}$ fulfil the Rodrigues' type formula

$$h_k(x) = e^{x^2}(-\nabla_x)^k e^{-x^2} \tag{3.12}$$

for $k \geq 0$.

Proof. The TTRR follows directly from the raising operator $\hat{b}^\dagger$ and (3.9). For the Rodrigues' formula in c, we calculate

$$\nabla_x h_k(x) = \nabla_x \left((-1)^k (\nabla_x^k e^{-x^2}) e^{x^2}\right) = (-1)^k \left((\nabla_x^{k+1} e^{-x^2}) e^{x^2} + 2x(\nabla_x^k e^{-x^2}) e^{x^2}\right)$$
$$= 2x h_k(x) - h_{k+1}(x)$$

what matches with the recurrence relation in (3.10). At last, for the generating function we note that with the Rodrigues' formula

$$\partial_t^k e^{-(x-t)^2} \mid_{t=0} = (-1)^k \partial_u^k e^{-u^2} \mid_{u=x} = h_k(x) e^{-x^2}$$

where we substituted $u = x - t$. The exponential function $e^{-(x-t)^2}$ can be written exactly as its Taylor expansion around $t = 0$,

$$e^{-(x-t)^2} = \sum_{k=0}^{\infty} \frac{t^k}{k!} \left(\partial_t^k e^{-(x-t)^2} \mid_{t=0}\right) = \sum_{k=0}^{\infty} \frac{t^k}{k!} h_k(x) e^{-x^2}$$

and the result follows from $e^{-(x-t)^2} e^{x^2} = e^{2xt-t^2}$. ■

These properties of the Hermite polynomials are widely known and can be found in the literature, see for example [Fol09, §1.7] or [Tha93, §1.1]. However, we could not find an established representation of the Hermite polynomials via a determinant and will thus deduce one in the following.

As it was shown in [CDG06, §1] the Bernoulli polynomials are closely related to the power sums

$$S_k(m) = \sum_{j=1}^{k} j^m,$$

with $m \geq 0$. For the Hermite polynomials we have to adapt this sums slightly and introduce a recursive definition.

Definition 3.3 Let $S_k^1 = S_k(1) = \sum_{j=1}^{k} j$ denote the first power sum. We set

$$S_k^{m+1} = \sum_{j=1}^{k} S_{j+1}^m j$$

for all $k, m \geq 1$.

The sum notation here shall emphasise the relation to the Bernoulli polynomials. However, we can also give an explicit formula for the numbers S_k^m that is more familiar in the context of Hermite polynomials.

Lemma 3.5 Let $k, m \geq 1$. We can calculate the numbers S_k^m via

$$S_k^m = 2^{-m} \frac{(2m+k-1)!}{m!(k-1)!}. \tag{3.13}$$

Proof. We prove this statement by induction over m. For $m = 1$ we find

$$S_k^1 = \frac{k(k+1)}{2} = \frac{1}{2}\frac{(k+1)!}{(k-1)!},$$

and Equation (3.13) holds true for $m = 1$ and all $k \geq 1$. If we further assume (3.13) is true for $k, m \geq 1$, we moreover find

$$\begin{aligned} S_k^{m+1} &= 2^{-m}\sum_{j=1}^{k}\frac{(2m+j)!}{m!(j-1)!} = 2^{-m}\frac{(2m+1)!}{m!}\sum_{j=1}^{k}\binom{2m+j}{2m+1} \\ &= 2^{-m}\frac{(2m+1)!}{m!}\sum_{j=0}^{k-1}\binom{2m+1+j}{2m+1} = 2^{-m}\frac{(2m+1)!}{m!}\binom{2m+k+1}{2m+2} \\ &= 2^{-(m+1)}\frac{(2m+k+1)!}{(m+1)!(k-1)!} \end{aligned}$$

since $\sum_{j=0}^{k}\binom{m+j}{m} = \binom{m+k+1}{m+1}$. ∎

From Formula (3.13) we can also deduce the initial values $S_k^0 = 1$ for all $k \geq 1$ and to be well-defined we set $S_k^m = 0$ whenever $k \leq 0$ or $m < 0$.

The coefficients S_k^m in the form (3.13) appear if one writes an arbitrary polynomial as linear combination of Hermite polynomials. From their definition it is clear that the polynomials $(h_j)_{j\leq k}$ form a basis of the set P_k of all polynomials with degree at most k. Thus, one can expand every polynomial of degree k in terms of Hermite polynomials $(h_j)_{j\leq k}$. The next lemma gives an explicit formula of this expansion for monomials.

Lemma 3.6 Let $(h_k)_{k\in\mathbb{N}}$ denote the Hermite polynomials as defined in (3.8). Then, we can write

$$(2x)^{2k} = \sum_{j=0}^{k} 2^{k-j} S_{2j+1}^{k-j} h_{2j}(x),$$

for even degrees and for odd degrees

$$(2x)^{2k+1} = \sum_{j=0}^{k} 2^{k-j} S_{2(j+1)}^{k-j} h_{2j+1}(x),$$

with $k \geq 0$.

Proof. Both formulas can easily be verified for $k = 0$,

$$(2x)^0 = h_0(x) = 1, \quad (2x)^1 = h_1(x) = 2x.$$

Also, by induction using the recurrence relation (3.10) and the initial values $S_0^{k+1} =$

$S_{2(k+2)}^{-1} = 0$

$$\begin{aligned}(2x)^{2(k+1)} &= \sum_{j=0}^{k} 2^{k-j} S_{2(j+1)}^{k-j} (2x) h_{2j+1}(x) = \sum_{j=0}^{k} 2^{k-j} S_{2(j+1)}^{k-j} \left(h_{2j+2}(x) + 2(2j+1)h_{2j}(x)\right) \\ &= \sum_{j=1}^{k+1} 2^{k+1-j} S_{2j}^{k+1-j} h_{2j}(x) + \sum_{j=0}^{k} 2^{k+1-j}(2j+1) S_{2(j+1)}^{k-j} h_{2j}(x) \\ &= \sum_{j=0}^{k+1} 2^{k+1-j} \left(S_{2j}^{k+1-j} + (2j+1) S_{2(j+1)}^{k-j}\right) h_{2j}(x)\end{aligned}$$

and it remains to show that $S_{2j}^{k+1-j} + (2j+1)S_{2(j+1)}^{k-j} = S_{2j+1}^{k+1-j}$. But this holds true since with Lemma 3.5

$$\begin{aligned}S_{2j}^{k+1-j} + (2j+1)S_{2(j+1)}^{k-j} &= 2^{-(k-j+1)} \frac{(2k+1)!}{(k-j+1)!(2j-1)!} + 2^{-(k-j)} \frac{(2k+1)!}{(k-j)!(2j)!} \\ &= 2^{-(k-j+1)} \frac{(2k+1)!}{(k-j+1)!(2j)!} \left(2j + 2(k-j+1)\right) \\ &= 2^{-(k-j+1)} \frac{(2k+2)!}{(k-j+1)!(2j)!} = S_{2j+1}^{k+1-j}.\end{aligned}$$

The proof for $(2x)^{2(k+1)+1}$ works analogously. ■

With this lemma we are now able to give a determinant representation of the one-dimensional Hermite polynomials.

Proposition 3.1 Let $k \in \mathbb{N}$. Then, the k-th Hermite polynomial h_k as defined in (3.8) can be written as determinant of a $(k+1) \times (k+1)$- matrix that is constructed in the following way:

$$h_k(x) = (-1)^k \det \begin{pmatrix} 1 & x & x^2 & x^3 & x^4 & x^5 & \dots & x^k \\ 2 & 0 & S_1^1 & 0 & \frac{1}{2}S_1^2 & 0 & & \vdots \\ 0 & 2 & 0 & S_2^1 & 0 & \frac{1}{2}S_2^2 & \ddots & \\ \vdots & 0 & 2 & 0 & S_3^1 & 0 & \ddots & 0 \\ & \vdots & 0 & 2 & 0 & S_4^1 & \ddots & \frac{1}{2}S_{k-3}^2 \\ & & & 0 & 2 & 0 & \ddots & 0 \\ & & & \dots & 0 & 2 & \ddots & S_{k-1}^1 \\ 0 & & & & \dots & 0 & 2 & 0 \end{pmatrix}. \tag{3.14}$$

Proof. The proof follows again by induction. We first state that the determinant of an upper Hessenberg matrix $M_k = (m_{i,j})_{1 \le i,j \le k}$, i.e. a matrix that has only zero-entries below the first subdiagonal, can be written as

$$\det(M_k) = m_{k,k} \det(M_{k-1}) + \sum_{j=1}^{k-1} (-1)^{k-j} m_{j,k} \det(M_{j-1}) \prod_{l=j}^{k-1} m_{l+1,l}$$

where $\det(M_0) = 1$, see [CDG06, Lemma 3]. Assuming that the claim is true for all polynomials $h_{k'}$, $k' < k$, we find

$$\begin{aligned} h_k(x) &= (-1)^k \sum_{j=1}^{k} (-1)^{k-j+1} m_{j,k+1} \det(M_{j-1}) 2^{k+1-j} \\ &= 2^k m_{1,k+1} + \sum_{j=2}^{k} (-1)^{-j+1} 2^{k+1-j} m_{j,k+1} (-1)^{j-2} h_{j-2}(x) \\ &= (2x)^k - \sum_{j=2}^{k} 2^{k+1-j} m_{j,k+1} h_{j-2}(x). \end{aligned}$$

Next, we have to insert the entries of the last column. For an even index h_{2k}, we find

$$(x^{2k}, \frac{1}{2^{k-1}} S_1^k, 0, \frac{1}{2^{k-2}} S_3^{k-1}, 0, \dots, S_{2k-1}^1, 0)^T$$

and therefore

$$h_{2k}(x) = (2x)^{2k} - \sum_{j=1}^{k} 2^{2(k-j)+1} \frac{1}{2^{k-j}} S_{2j-1}^{k+1-j} h_{2j-2}(x) = (2x)^{2k} - \sum_{j=0}^{k-1} 2^{k-j} S_{2j+1}^{k-j} h_{2j}(x)$$

what is consistent with the expansion formula in Lemma 3.6. A similar argument yields the claim in the odd case h_{2k+1}. ■

So far, we were following the outline for the analysis of the Bernoulli polynomials given in [CDG06]. But besides that, the Hermite polynomials are also closely related to the Laguerre polynomials. This relation will come to the fore when we investigate the Hermite functions in phase space in the next section.

3.4. Hermite functions in phase space

The Wigner transform

$$\mathcal{W}(\varphi, \psi)(\xi, x) = (2\pi)^{-n} \int_{\mathbb{R}^n} \overline{\varphi}(x + \tfrac{y}{2}) \psi(x - \tfrac{y}{2}) e^{\mathrm{i} y^T \xi} \, dy, \quad (\xi, x) \in \mathbb{R}^n \oplus \mathbb{R}^n \tag{3.15}$$

of two Schwartz functions $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$ is the Fourier transform of their correlation function and, again, a Schwartz function on phase space. It is a quasi-probability distribution as it might also attain negative values, that measures both, position and momentum, simultaneously, see [LT14, §1]. However, the symmetric Wigner function $\mathcal{W}(\varphi) := \mathcal{W}(\varphi, \varphi)$ is a real-valued function since by definition $\mathcal{W}(\varphi, \psi) = \overline{\mathcal{W}(\psi, \varphi)}$ and thus provides a pure density operator, see [Gos10, §13.1.1] or [LST15, §3, §4].

In order to calculate the Wigner transform of two Hermite functions φ_k and φ_l, $k, l \in \mathbb{N}$, we first have to state some basic properties of $\mathcal{W}$.

Lemma 3.7 For the Wigner transform $\mathcal{W}$ the following three statements hold:

a, Let $\varphi_1, \varphi_2, \psi_1, \psi_2 \in \mathcal{S}(\mathbb{R}^n)$. Then, $\mathcal{W}(\varphi_1, \psi_1)$ and $\mathcal{W}(\varphi_2, \psi_2)$ are elements of $\mathcal{S}(\mathbb{R}^n \oplus$

$\mathbb{R}^n$) and satisfy *Moyal's identity*,

$$\langle \mathcal{W}(\varphi_1,\psi_1), \mathcal{W}(\varphi_2,\psi_2)\rangle_{L^2(\mathbb{R}^{2n})} = (2\pi)^{-n} \langle \varphi_1,\varphi_2\rangle_{L^2(\mathbb{R}^n)} \overline{\langle \psi_1,\psi_2\rangle}_{L^2(\mathbb{R}^n)} \tag{3.16}$$

b, Let $\varphi \in \mathcal{S}(\mathbb{R}^n)$. Then, the marginal distributions of $\mathcal{W}(\varphi)$ give the position and momentum distribution of φ,

$$\int_{\mathbb{R}^n} \mathcal{W}(\varphi)(\xi,x)\, d\xi = |\varphi(x)|^2, \quad \int_{\mathbb{R}^n} \mathcal{W}(\varphi)(\xi,x)\, dx = |(\mathcal{F}\varphi)(\xi)|^2. \tag{3.17}$$

c, Let $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$ be an observable and $\hat{a}$ its Weyl-quantisation. Then,

$$\int_{\mathbb{R}^{2n}} \mathcal{W}(\varphi,\psi)(z) a(z)\, d(z) = \langle \varphi, \hat{a}\psi\rangle, \quad z = (\xi,x) \in \mathbb{R}^n \oplus \mathbb{R}^n \tag{3.18}$$

for all $\varphi,\psi \in \mathcal{S}(\mathbb{R}^n)$.

Proof. For Moyal's identity we find

$$\begin{aligned}
&\langle \mathcal{W}(\varphi_1,\psi_1), \mathcal{W}(\varphi_2,\psi_2)\rangle_{L^2(\mathbb{R}^{2n})} = \\
&\quad = (2\pi)^{-2n} \int_{\mathbb{R}^{4n}} \varphi_1(x+\tfrac{y}{2})\overline{\varphi}_2(x+\tfrac{y'}{2})\overline{\psi}_1(x-\tfrac{y}{2})\psi_2(x-\tfrac{y'}{2}) e^{\mathrm{i}\xi^T(y-y')}\, d(y,y')d(\xi,x) \\
&\quad = (2\pi)^{-n} \int_{\mathbb{R}^{2n}} \varphi_1(x+\tfrac{y}{2})\overline{\varphi}_2(x+\tfrac{y}{2})\overline{\psi}_1(x-\tfrac{y}{2})\psi_2(x-\tfrac{y}{2})\, d(x,y)
\end{aligned}$$

where we again made use of the delta-distribution relation

$$\int_{\mathbb{R}^n} e^{\mathrm{i}\xi^T(y-y')}\, d\xi = (2\pi)^n \delta(y-y') \quad \text{and} \quad \int_{\mathbb{R}^n} \delta(y-y') f(y')\, dy' = f(y).$$

By substituting $x' = x - \frac{y}{2}$, we find the stated equality,

$$\begin{aligned}
\langle \mathcal{W}(\varphi_1,\psi_1), \mathcal{W}(\varphi_2,\psi_2)\rangle_{L^2(\mathbb{R}^{2n})} &= (2\pi)^{-n} \int_{\mathbb{R}^n} \overline{\psi}_1(x')\psi_2(x') \int_{\mathbb{R}^n} \varphi_1(x'+y)\overline{\varphi}_2(x'+y)\, dy dx' \\
&= (2\pi)^{-n} \langle \varphi_1,\varphi_2\rangle_{L^2(\mathbb{R}^n)} \overline{\langle \psi_1,\psi_2\rangle}_{L^2(\mathbb{R}^n)}.
\end{aligned}$$

Let $\varphi \in \mathcal{S}(\mathbb{R}^n)$. The marginal distributions of $\mathcal{W}(\varphi)$ are given by

$$\begin{aligned}
\int_{\mathbb{R}^n} \mathcal{W}(\varphi)(\xi,x)\, d\xi &= (2\pi)^{-n} \int_{\mathbb{R}^{2n}} \overline{\varphi}(x+\tfrac{y}{2})\varphi(x-\tfrac{y}{2}) e^{\mathrm{i}y^T\xi}\, d\xi dy \\
&= \int_{\mathbb{R}^n} \overline{\varphi}(x+\tfrac{y}{2})\varphi(x-\tfrac{y}{2})\delta(y)\, d\xi dy = |\varphi(x)|^2
\end{aligned}$$

and

$$\begin{aligned}
\int_{\mathbb{R}^n} \mathcal{W}(\varphi)(\xi,x)\, dx &= (2\pi)^{-n} \int_{\mathbb{R}^{2n}} \overline{\varphi}(x+\tfrac{y}{2})\varphi(x-\tfrac{y}{2}) e^{\mathrm{i}y^T\xi}\, dx dy \\
&= (2\pi)^{-n} \int_{\mathbb{R}^{2n}} \overline{\varphi}(y')\varphi(x') e^{\mathrm{i}\xi^T(y'-x')}\, dy' dx' = |(\mathcal{F}\varphi)(\xi)|^2
\end{aligned}$$

where we substituted $x' = x - \frac{y}{2}$ and $y' = y + x'$, see also [Fol09, Proposition 1.96]. The proof of the last claim can also be found in [Gos10, Proposition 200]. For $\varphi,\psi \in \mathcal{S}(\mathbb{R}^n)$

and $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$, we have

$$\begin{aligned}\langle \varphi, \hat{a}\psi \rangle &= (2\pi)^{-n} \int_{\mathbb{R}^{3n}} \overline{\varphi}(x)\varphi(y) e^{\mathrm{i}\xi^T(x-y)} a(\xi, \tfrac{1}{2}(x+y))\, d(\xi, x) dy \\ &= (2\pi)^{-n} \int_{\mathbb{R}^{3n}} \overline{\varphi}(x' + \tfrac{y'}{2})\varphi(x' - \tfrac{y'}{2}) e^{\mathrm{i}\xi^T y'} a(\xi, x')\, d(\xi, x') dy' \\ &= \int_{\mathbb{R}^{2n}} \mathcal{W}(\varphi, \psi)(\xi, x') a(\xi, x')\, d(\xi, x')\end{aligned}$$

and again, a suitable substitution, $y' = x - y$ and $x' = y + \frac{y'}{2}$ yielded the result. ■

Equation (3.18) in the previous lemma already displays the close relation between the Wigner transform and the Weyl-quantisation that was originally examined in [Gro46]. For any quantum observable $\hat{a} : \mathcal{S}(\mathbb{R}^n) \mapsto \mathcal{S}(\mathbb{R}^n)$ the expectation value in a state $\psi \in L^2(\mathbb{R}^n)$ is given by

$$\langle \hat{a} \rangle_\psi = \frac{\langle \psi, \hat{a}\psi \rangle}{\langle \psi, \psi \rangle}$$

and can thus be calculated using the Wigner function, see for example [Gos10, Definition 204] or [Lub08, §I.4.1].

With the Weyl calculus from Appendix A we are able to compute the Wigner transform of two Hermite functions φ_k and φ_l. Our aim is to write Dirac's ladder operators as equivalent operators acting on the Wigner function $\mathcal{W}$, i.e. to find operators $\hat{A}_1, \hat{A}_2$ resp. $\hat{A}_1^\dagger, \hat{A}_2^\dagger$ such that

$$\begin{aligned}\hat{A}_1 \mathcal{W}(\varphi, \psi) &= \mathcal{W}(\hat{a}\varphi, \psi), \quad & \hat{A}_2 \mathcal{W}(\varphi, \psi) &= \mathcal{W}(\varphi, \hat{a}\psi), \\ \hat{A}_1^\dagger \mathcal{W}(\varphi, \psi) &= \mathcal{W}(\hat{a}^\dagger\varphi, \psi), \quad & \hat{A}_2^\dagger \mathcal{W}(\varphi, \psi) &= \mathcal{W}(\varphi, \hat{a}^\dagger\psi),\end{aligned}$$

for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$. Thereby, we can analogously to the calculation of the Fourier transform define the Wigner transform $\mathcal{W}(\varphi_0)$ of the coherent ground state as element of the kernels of $\hat{A}_1$ and $\hat{A}_2$ and produce Wigner transform of the form $\mathcal{W}(\varphi_k, \varphi_l)$ by iteratively applying $\hat{A}_1^\dagger$ and $\hat{A}_2^\dagger$.

Lemma 3.8 — Phase space ladders. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$ and set $y = \mathrm{i}\xi + x$ for $\xi, x \in \mathbb{R}^n$. Then, we find for the lowering operator $\hat{a}$

$$\begin{aligned}\mathcal{W}(\hat{a}\varphi, \psi)(\xi, x) &= \tfrac{1}{\sqrt{2}}(\overline{y} + \nabla_y)\mathcal{W}(\varphi, \psi)(\xi, x), \\ \mathcal{W}(\varphi, \hat{a}\psi)(\xi, x) &= \tfrac{1}{\sqrt{2}}(y + \nabla_{\overline{y}})\mathcal{W}(\varphi, \psi)(\xi, x),\end{aligned}$$

and for the raising operator $\hat{a}^\dagger$,

$$\begin{aligned}\mathcal{W}(\hat{a}^\dagger\varphi, \psi)(\xi, x) &= \tfrac{1}{\sqrt{2}}(y - \nabla_{\overline{y}})\mathcal{W}(\varphi, \psi)(\xi, x), \\ \mathcal{W}(\varphi, \hat{a}^\dagger\psi)(\xi, x) &= \tfrac{1}{\sqrt{2}}(\overline{y} - \nabla_y)\mathcal{W}(\varphi, \psi)(\xi, x).\end{aligned}$$

Proof. We will exhibit the proof only for the annihilator $\hat{a}$ here, the proof for the creator $\hat{a}^\dagger$ works analogously. From Lemma 3.7 c, we know that for $z = (\xi, x)$ and any $w \in$

$\mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$,

$$\int_{\mathbb{R}^{2n}} \mathcal{W}(\hat{a}\varphi, \psi)(z) w(z)\, dz = \langle \hat{a}\varphi, \hat{w}\psi \rangle = \langle \varphi, \hat{a}^\dagger \hat{w}\psi \rangle = \int_{\mathbb{R}^{2n}} \mathcal{W}(\varphi, \psi)(z)(a^\dagger \# w)(z)\, dz$$

and

$$\int_{\mathbb{R}^{2n}} \mathcal{W}(\varphi, \hat{a}\psi)(z) w(z)\, dz = \langle \varphi, \hat{w}\hat{a}\psi \rangle = \int_{\mathbb{R}^{2n}} \mathcal{W}(\varphi, \psi)(z)(w \# a)(z)\, dz$$

where $a(\xi, x) = \frac{1}{\sqrt{2}}(x + \mathrm{i}\xi) = \frac{1}{\sqrt{2}} y$ and $a^\dagger(\xi, x) = \frac{1}{\sqrt{2}}(x - \mathrm{i}\xi) = \frac{1}{\sqrt{2}}\overline{y}$. The Moyal product can be calculated with the formula given in Corollary A.1,

$$\begin{aligned} (a^\dagger \# w)(z) &= \tfrac{1}{\sqrt{2}}(\overline{y} w(z) + \tfrac{\mathrm{i}}{2}(\partial_\xi w(z) + \mathrm{i}\partial_x w(z))), \\ (w \# a)(z) &= \tfrac{1}{\sqrt{2}}(y w(z) + \tfrac{\mathrm{i}}{2}(-\partial_\xi w(z) + \mathrm{i}\partial_x w(z))), \end{aligned}$$

and with partial integration

$$\begin{aligned} \int_{\mathbb{R}^{2n}} \mathcal{W}(\hat{a}\varphi, \psi)(z) w(z)\, dz &= \frac{1}{\sqrt{2}} \int_{\mathbb{R}^{2n}} (\overline{y} + \tfrac{1}{2}(-\mathrm{i}\partial_\xi + \partial_x)) \mathcal{W}(\varphi, \psi)(z) w(z)\, dz \\ \int_{\mathbb{R}^{2n}} \mathcal{W}(\varphi, \hat{a}\psi)(z) w(z)\, dz &= \frac{1}{\sqrt{2}} \int_{\mathbb{R}^{2n}} (y + \tfrac{1}{2}(\mathrm{i}\partial_\xi + \partial_x)) \mathcal{W}(\varphi, \psi)(z) w(z)\, dz. \end{aligned}$$

■

Using these phase space ladders, we can now identify the ground state of the Wigner transform of the Hermite functions. We stress here that all results stated above are valid in multi-dimensions, although we will only investigate the one-dimensional case in the remaining section.

Lemma 3.9 Let φ_0 denote the coherent state (3.6). The symmetric Wigner function of φ_0 reads

$$\mathcal{W}(\varphi_0)(\xi, x) = \tfrac{1}{\pi} e^{-(\xi^2 + x^2)} = \tfrac{1}{\pi} e^{-|y|^2}$$

where $y = \mathrm{i}\xi + x$.

Proof. We will in the following use the short-notation $\mathcal{W}_0 := \mathcal{W}(\varphi_0)$. Since $\hat{a}\varphi_0 = 0$ it follows from the previous lemma that

$$(\overline{y} + \nabla_y)\mathcal{W}_0(y) = 0 \quad \text{and} \quad (y + \nabla_{\overline{y}})\mathcal{W}_0(y) = 0.$$

Every function satisfying those two conditions is of the form $ce^{-|y|^2}$ since

$$\nabla_y (W(y) e^{|y|^2}) = (\overline{y} W(y) + \nabla_y W(y)) e^{|y|^2} = 0$$

for all functions W satisfying $(\overline{y} + \nabla_y)W(y) = 0$. Lemma 3.7 a, implies $\|W_0\|^2 = (2\pi)^{-1}$ and the result follows from $\int_{\mathbb{R}^2} e^{-2(\xi^2 + x^2)}\, d\xi dx = \frac{\pi}{2}$. ■

The form of the Wigner ground state $\mathcal{W}(\varphi_0)$ is not suprising, it seems as the logical expansion of φ_0 to two dimensions. Proceeding further, the application of the phase space ladders $\frac{1}{\sqrt{2}}(y-\nabla_{\overline{y}})$ and $\frac{1}{\sqrt{2}}(\overline{y}-\nabla_y)$ will again create a polynomial prefactor and it is a well-known fact, see for example [Fol09, Theorem 1.105] or [Tha93, Theorem 1.3.4 and 1.3.5], that this factor can be written in terms of the *associated Laguerre polynomials*

$$L_k^{(\alpha)}(x)=\sum_{j=0}^{k}(-1)^j\binom{k+\alpha}{k-j}\frac{x^j}{j!}$$

with $k\in\mathbb{N}$ and $\alpha\in\mathbb{R}$. The following proposition can also be found in [LT14, Corollary 1] using a different technique of proof based on a integral formula for the Hermite polynomials. Here we will use the phase space ladders similar to [Tha93, §1.3].

Proposition 3.2 If φ_k,φ_l are the k-th and l-th Hermite function, $k,l\in\mathbb{N}$, then their Wigner transform is

$$\mathcal{W}(\varphi_k,\varphi_l)(\xi,x)=\begin{cases}(-1)^k\sqrt{2^{l-k}}\sqrt{\frac{k!}{l!}}\,\overline{y}^{l-k}L_k^{(l-k)}(2|y|^2)\mathcal{W}_0(\xi,x), & k\le l\\ (-1)^l\sqrt{2^{k-l}}\sqrt{\frac{l!}{k!}}\,y^{k-l}L_l^{(k-l)}(2|y|^2)\mathcal{W}_0(\xi,x), & l\le k\end{cases}\tag{3.19}$$

with $y=\mathrm{i}\xi+x$. In particular,

$$\mathcal{W}(\varphi_k)(\xi,x)=(-1)^kL_k^{(0)}(2|y|^2)\mathcal{W}_0(\xi,x).$$

Proof. We present here a proof by induction for the case $k<l$. Suppose that (3.19) holds true for $\mathcal{W}(\varphi_k,\varphi_l)$. Then,

$$\begin{aligned}&\mathcal{W}(\varphi_{k+1},\varphi_l)(\xi,x)=\tfrac{1}{\sqrt{k+1}}\mathcal{W}(\hat{a}^\dagger\varphi_k,\varphi_l)(\xi,x)=\tfrac{(-1)^k}{\sqrt{k+1}}\sqrt{2^{l-(k+1)}}\sqrt{\tfrac{k!}{l!}}\mathcal{W}_0(\xi,x)\\&\quad\Big(2y\overline{y}^{l-k}L_k^{(l-k)}(2|y|^2)-(l-k)\overline{y}^{l-(k+1)}L_k^{(l-k)}(2|y|^2)-2y\overline{y}^{l-k}L_k'^{(l-k)}(2|y|^2)\Big)\\&=\tfrac{(-1)^k}{\sqrt{k+1}}\sqrt{2^{l-(k+1)}}\sqrt{\tfrac{k!}{l!}}\mathcal{W}_0(\xi,x)\overline{y}^{l-(k+1)}\Big((2|y|^2-(l-k))L_k^{(l-k)}(2|y|^2)-2|y|^2L_k'^{(l-k)}(2|y|^2)\Big)\end{aligned}$$

and since the associated Laguerre polynomials satisfy $\nabla_x^jL_k^{(\alpha)}(x)=(-1)^jL_{k-j}^{(\alpha+j)}(x)$, see [Tha93, Eq.(1.1.49)], we can rewrite the expression in the brackets as

$$(l-k-2|y|^2)L_{k+1}'^{(l-(k+1))}(2|y|^2)+2|y|^2L_{k+1}''^{(l-(k+1))}(2|y|^2).$$

The claim follows from Laguerre's equation: $xL_k''^{(\alpha)}(x)+(\alpha+1-x)L_k'^{(\alpha)}(x)+kL_k^{(\alpha)}(x)=0$, see [Tha93, Eq.(1.1.48)]. Moreover,

$$\begin{aligned}\mathcal{W}(\varphi_k,\varphi_{l+1})(\xi,x)&=\tfrac{1}{\sqrt{l+1}}\mathcal{W}(\varphi_k,\hat{a}^\dagger\varphi_l)(\xi,x)\\&=(-1)^k\sqrt{2^{l-k-1}}\sqrt{\tfrac{k!}{(l+1)!}}\mathcal{W}_0(\xi,x)\Big(2\overline{y}^{l-k+1}L_k^{(l-k)}(2|y|^2)-2\overline{y}^{l-k+1}L_k'^{(l-k)}(2|y|^2)\Big)\\&=(-1)^k\sqrt{2^{l-k+1}}\sqrt{\tfrac{k!}{(l+1)!}}\mathcal{W}_0(\xi,x)\overline{y}^{l+1-k}\Big(L_k^{(l-k)}(2|y|^2)+L_{k-1}^{(l-k+1)}(2|y|^2)\Big)\end{aligned}$$

and the claim in this case follows from the identity

$$L_k^{(\alpha)}(x) + L_{k-1}^{(\alpha+1)}(x) = (-1)^k \frac{x^k}{k!} + \sum_{j=0}^{k-1} (-1)^j \left(\binom{k+\alpha}{k-j} + \binom{k+\alpha}{k-j-1} \right) \frac{x^j}{j!}$$
$$= \sum_{j=0}^{k-1} (-1)^j \binom{k+\alpha+1}{k-j} \frac{x^j}{j!} = L_k^{(\alpha+1)}(x).$$

The cases $l = k$ and $k > l$ are proved analogously. ■

Given that $|\mathcal{W}(\varphi_k, \varphi_l)|^2$ is a function in $|y|^2$ it is clear that the absolute value of $\mathcal{W}(\varphi_k, \varphi_l)$ is radially symmetric. Figures (3), (4) and (5) exemplary illustrate this behaviour for $\mathcal{W}(\varphi_0)$, $\mathcal{W}(\varphi_3)$ and $\mathcal{W}(\varphi_1, \varphi_3)$.

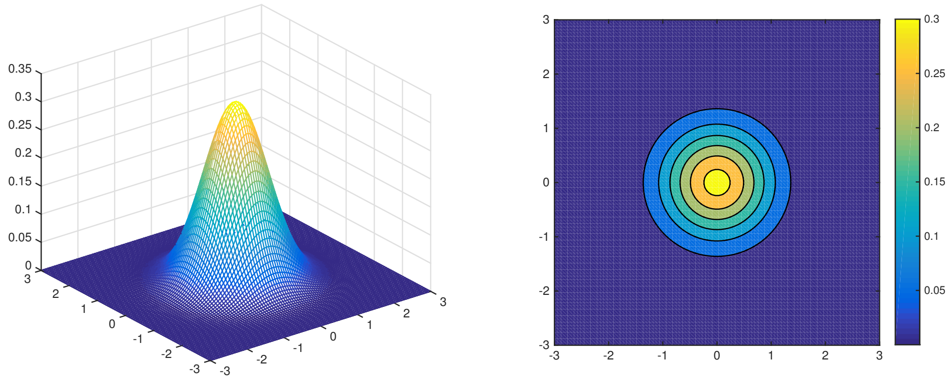

Figure 3.: Absolute value of the symmetric Wigner transform $\mathcal{W}(\varphi_0)$

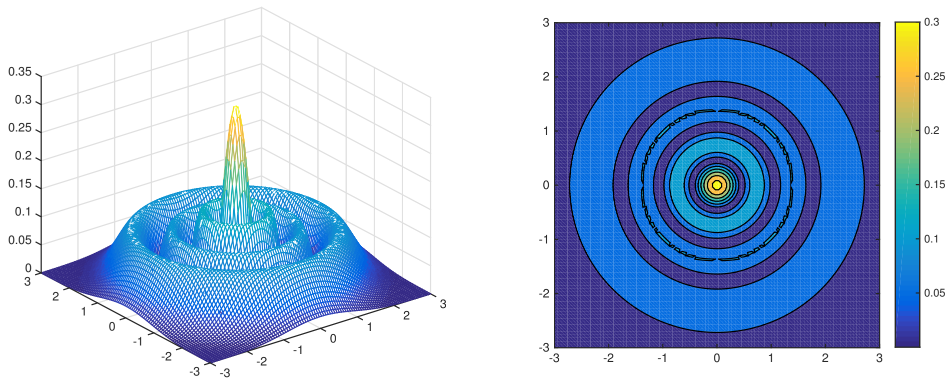

Figure 4.: Absolute value of the symmetric Wigner transform $\mathcal{W}(\varphi_3)$

The only Wigner transform of the form $\mathcal{W}(\varphi_k, \varphi_l)$ that is strictly positive is the Wigner ground state $\mathcal{W}(\varphi_0)$. One can in particular show that the Wigner transform $\mathcal{W}(\varphi)$ of a function $\varphi \in \mathcal{S}(\mathbb{R}^n)$ is non-negative if and only if φ is a Gaussian, see [Gos10, §9.2.1]. This lack of positivity can be cured by the convolution with the Gaussian phase space

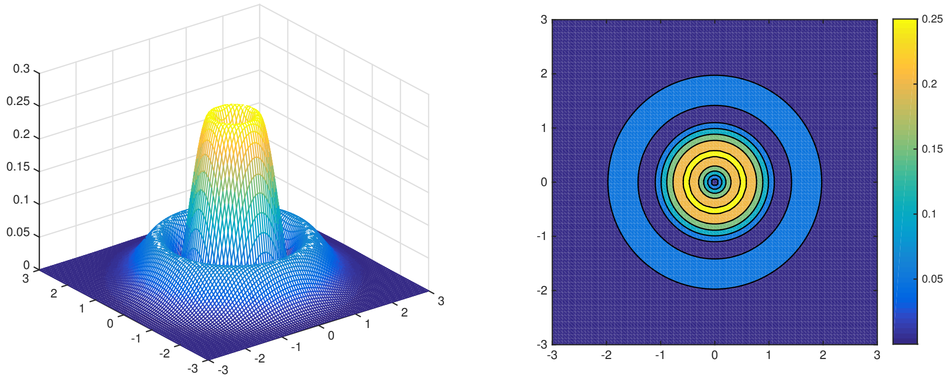

Figure 5.: Absolute value of the mixed Wigner transform $\mathcal{W}(\varphi_1, \varphi_3)$

function $G(z) = \pi^{-n} e^{-|z|^2}$. The resulting positive transform

$$\mathcal{H}(\varphi) = G * \mathcal{W}(\varphi)$$

is called the *Husimi transform* $\mathcal{H} : \mathbb{R}^n \oplus \mathbb{R}^n \mapsto [0;\infty)$. The Husimi transform can also be deduced from the *FBI transform* (Fourier-Bros-Iagolnitzer), which is defined as the inner product with the Gaussian wave packet

$$g(p, q; x) = \pi^{-n/4} e^{-|x-q|^2/2 + \mathrm{i}p^T(x-y)} \tag{3.20}$$

centred in the phase space point $z = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$. That is,

$$(\mathcal{F}_z\varphi)(p, q) = (2\pi)^{-n/2} \langle \varphi, g(p, q) \rangle$$

see for example [Fol09, §3.3]. Then, the Husimi transform appears as the modulus squared of the FBI transform, $\mathcal{H}(\varphi) = |(\mathcal{F}_z\varphi)(p, q)|^2$ for all $z = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$, which immediatly reveals positivity, see [LT14, §1]. The next result can be found as Corollary 2 in [LT14].

Corollary 3.1 — FBI and Husimi transform. Let φ_k be the k-th Hermite function and $z = (\xi, x) \in \mathbb{R}^n \oplus \mathbb{R}^n$. Then, the FBI transform is given by

$$(\mathcal{F}_z\varphi_k)(\xi, x) = \frac{e^{-\mathrm{i}\xi x/2}}{\sqrt{\pi 2^{k+1} k!}} y^k e^{-|y|^2/4}$$

with $y = \mathrm{i}\xi + x$. Consequently, the Husimi transform reads

$$\mathcal{H}(\varphi_k) = \frac{1}{\pi 2^{k+1} k!} |y|^{2k} e^{-|y|^2/2}.$$

Proof. We have

$$(\mathcal{F}_z\varphi_k)(\xi, x) = (2\pi)^{-1/2} \langle \frac{1}{\sqrt{k!}} (\hat{a}^\dagger)^k \varphi_0, g(\xi, x) \rangle = \frac{1}{\sqrt{2\pi k!}} \langle \varphi_0, (\hat{a})^k g(\xi, x) \rangle$$

and since $\hat{a}\, g(\xi, x) = \frac{1}{\sqrt{2}} y\, g(\xi, x)$, it suffices to evaluate the inner product of $g(\xi, x)$ with the coherent ground state φ_0,

$$(\mathcal{F}_z \varphi_k)(\xi, x) = \frac{1}{\sqrt{\pi 2^{k+1} k!}} y^k \langle \varphi_0, g(\xi, x) \rangle.$$

This can be executed by completing the square in the exponent,

$$\begin{aligned}\langle \varphi_0, g(\xi, x) \rangle &= \pi^{-1/2} \int_{\mathbb{R}} e^{-(x'-x)^2 + \mathrm{i}\xi(x'-x)} e^{-x'^2/2} \, dx' \\ &= \pi^{-1/2} e^{-|y|^2/4} e^{-\mathrm{i}\xi x/2} \int_{\mathbb{R}} e^{-(x'-y/2)^2} \, dx' = e^{-|y|^2/4} e^{-\mathrm{i}\xi x/2}.\end{aligned}$$

■

The Husimi transform hence exhibits the same radial symmetry as the Wigner transform, see Figure (6) for an example.

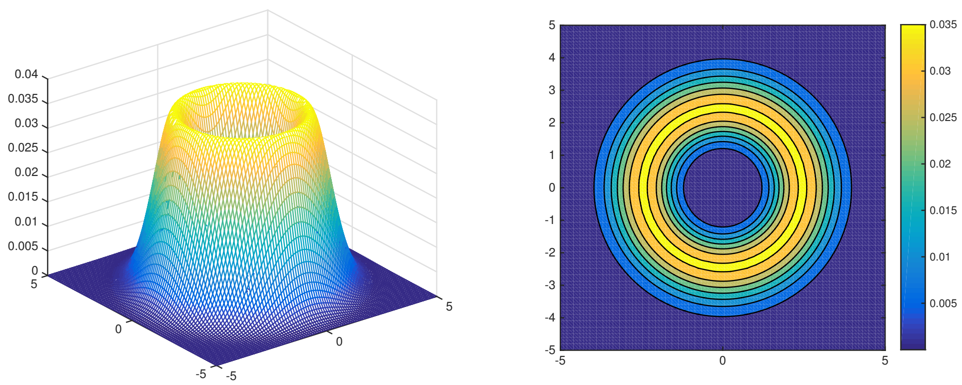

Figure 6.: Absolute value of the Husimi transform $\mathcal{H}(\varphi_3)$

The Gaussian $g(p, q)$ we used to calculate the FBI transform is centred in an arbitrary phase space point $z = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$. Until now we only considered functions centred at the origin, but we can transfer this generalisation also to the Hermite functions:

Let $z = (p, q) \in \mathbb{R} \oplus \mathbb{R}$ and denote by h_k the k-th Hermite polynomial. We set as ground state the shifted Gaussian,

$$\varphi_0(p, q; x) = \pi^{-1/4} e^{-(x-q)^2/2 + \mathrm{i}p(x-q)}$$

and obtain for the Hermite functions centred at z,

$$\varphi_k(p, q; x) = \frac{1}{\sqrt{2^k k!}} h_k(x - q) \varphi_0(p, q; x).$$

Such phase space translations are typically expressed by means of the *Heisenberg- Weyl operator*, see [Gos10, Definition 124],

$$T(z)\psi(x) = e^{\mathrm{i}p^T(x-q/2)} \psi(x - q), \quad \psi \in L^2(\mathbb{R}^n)$$

also for multi-dimensional phase space centres $z = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$. With this notation we find

$$\varphi_k(p, q) = e^{-\mathrm{i}pq/2} T(z)\varphi_k$$

and the shifted Hermite functions $(\varphi_k(p, q))_{k\in\mathbb{N}}$ maintain the orthonormality of the standard Hermite functions $(\varphi_k)_{k\in\mathbb{N}}$.

A nice interpretation of the Fourier transform becomes now visible when we calculate $\mathcal{F}\varphi_k(p, q)$.

Proposition 3.3 Let $z = (p, q) \in \mathbb{R} \oplus \mathbb{R}$. Then, the Fourier transform interchanges the position and momentum centre,

$$(\mathcal{F}\varphi_k(p, q))(\xi) = (-\mathrm{i})^k e^{-\mathrm{i}pq} \varphi_k(-q, p; \xi).$$

Proof. From Lemma 3.4 we know that $\mathcal{F}\varphi_k = (-\mathrm{i})^k \varphi_k$ and thus

$$\mathcal{F}\varphi_(p, q) = e^{-\mathrm{i}pq/2} \mathcal{F}T(z)\mathcal{F}^{-1}\mathcal{F}\varphi_k = (-\mathrm{i})^k e^{-\mathrm{i}pq/2} \mathcal{F}T(z)\mathcal{F}^{-1}\varphi_k$$

and it remains to determine $\mathcal{F}T(z)\mathcal{F}^{-1}$. Let $\varphi \in \mathcal{S}(\mathbb{R})$, then

$$\begin{aligned}(\mathcal{F}T(z)\mathcal{F}^{-1}\varphi)(\xi) &= \tfrac{1}{2\pi} \int_{\mathbb{R}} e^{\mathrm{i}p(x-q/2)} \int_{\mathbb{R}} \varphi(\xi')e^{\mathrm{i}\xi'(x-q)}\, d\xi' e^{-\mathrm{i}x\xi}\, dx \\ &= \tfrac{1}{2\pi} e^{-\mathrm{i}pq/2} \int_{\mathbb{R}^2} \varphi(\xi')e^{\mathrm{i}x(\xi'+p-\xi)}e^{-\mathrm{i}\xi' q}\, dx d\xi'\end{aligned}$$

$$= e^{-\mathrm{i}pq/2} \int_{\mathbb{R}} \varphi(\xi')e^{-\mathrm{i}\xi' q}\delta_{\xi'=\xi-p}\, d\xi' = e^{-\mathrm{i}pq/2}\varphi(\xi - p)e^{-\mathrm{i}q(\xi-p)}.$$

The result follows as $\varphi_k(\xi - p)e^{-\mathrm{i}q(\xi-p)} = \varphi_k(-q, p; \xi)$. ■

In a final step we want to examine the impact of the Heisenberg-Weyl-operator on the Wigner transform. The following general result can for example be found in [Gos10, Proposition 174].

Lemma 3.10 Let $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$ and $z_0, z_1 \in \mathbb{R}^n \oplus \mathbb{R}^n$. Then,

$$\mathcal{W}(T(z_0)\varphi, T(z_1)\psi)(z) = e^{\mathrm{i}(z^T\Omega(z_1-z_0)+\frac{1}{2}z_1^T\Omega z_0)}\mathcal{W}(\varphi, \psi)(z - \tfrac{z_0+z_1}{2}).$$

Proof. Let $z_0 = (p_0, q_0)$ and $z_1 = (p_1, q_1)$. By definition of the Wigner transform, we have

$$\begin{aligned}\mathcal{W}(T(z_0)\varphi, T(z_1)\psi)(\xi, x) =&(2\pi)^{-n}e^{\mathrm{i}x^T(p_1-p_0)}e^{\mathrm{i}(p_0^Tq_0-p_1^Tq_1)/2} \\ &\int_{\mathbb{R}^n} e^{-\mathrm{i}y^T(p_0+p_1)}\overline{\varphi}(x + \tfrac{y}{2} - q_0)\psi(x - \tfrac{y}{2} - q_1)e^{\mathrm{i}y^T\xi}\, dy.\end{aligned}$$

If we substitute $y' = y - (q_0 - q_1)$ we can simplify this further,

$$\begin{aligned}\mathcal{W}(T(z_0)\varphi, T(z_1)\psi)(\xi, x) =&(2\pi)^{-n}e^{\mathrm{i}x^T(p_1-p_0)}e^{\mathrm{i}(p_0^Tq_0-p_1^Tq_1)/2} \\ &\int_{\mathbb{R}^n} e^{\mathrm{i}(y'+(q_0-q_1))^T(\xi-\frac{p_0+p_1}{2})}\overline{\varphi}(x + \tfrac{y'-(q_0+q_1)}{2})\psi(x - \tfrac{y'+(q_0+q_1)}{2})\, dy' \\ =&e^{\mathrm{i}(\xi^T(q_0-q_1)-x^T(p_0-p_1)}e^{\mathrm{i}(p_0^Tq_1-q_0^Tp_1)/2}\mathcal{W}(\varphi, \psi)(z - \tfrac{z_0+z_1}{2}).\end{aligned}$$

■

The Wigner transform of two shifted Hermite functions then follows as an easy application of this lemma.

Corollary 3.2 Let $\varphi_k(p_0, q_0)$ and $\varphi_l(p_1, q_1)$ be the k-th and l-th Hermite function centred at $z_0 = (p_0, q_0) \in \mathbb{R}^2$ resp. $z_1 = (p_1, q_1) \in \mathbb{R}^2$. Then,

$$\mathcal{W}(\varphi_k(p_0, q_0), \varphi_l(p_1, q_1))(z) = e^{\mathrm{i}(z^T \Omega (z_1 - z_0) + \frac{1}{2}(q_1 - q_0)^T (p_1 + p_0))} \mathcal{W}(\varphi_k, \varphi_l)(z - \tfrac{z_0 + z_1}{2}).$$

4. Hagedorn's wave packets

In this chapter we present the construction of a parameter-based orthonormal basis of $L^2(\mathbb{R}^n)$ that was originally developed by George Hagedorn in [Hag85]. These functions appear as product of a multivariate polynomial times a Gaussian, where the polynomials are closely related to the Hermite polynomials we discussed in the previous chapter. However, they form not just simple tensor products of one-dimensional Hermite polynomials. Hagedorn's wave packets generalise Hermite functions to multi-dimensions but also allow for a varying width of the Gaussian and a (small) scaling parameter ε.

In the following work we will always assume that this semiclassical parameter is positive, $\varepsilon > 0$, as it will scale the width of the wave packets to order $\sqrt{\varepsilon}$. We also have to integrate ε in the definition of our operators, the ε- scaled Weyl-quantisation is given by

$$(\mathrm{op}_\varepsilon[a]\varphi)(x) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} a(\xi, \tfrac{1}{2}(x+y)) e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)} \varphi(y)\, d\xi dy \tag{4.1}$$

for all $\varphi \in L^2(\mathbb{R}^n)$, see Appendix A for a detailed study.

For the construction of the wave packets we follow Hagedorn's approach in [Hag98] via ladder operators, but use a different notation introduced in [LST15] based on Lagrangian frames. Then, we proceed similarly to the Hermite functions and deduce coherent states as eigenfunctions of the lowering operator, while excited states are obtained by iteratively applying a raising operator to the coherent state. Both, raising and lowering operator, are linear operators parametrised by a normalised Lagrangian frame. We will show that this approach indeed yields a basis of $L^2(\mathbb{R}^n)$ and specify the structure of the wave packets. Moreover, we discuss several generalisations such as a construction via non-normalised Lagrangian frames or wave packets centered at arbitrary phase space points $z \in \mathbb{C}^n \oplus \mathbb{C}^n$, though we will see that the basic structure of a multivariate polynomial times a Gaussian is preserved in any case.

4.1. Ladder operators

The ladder operators for Hagedorn's wave packets are operators with linear symbols. We use the vector-valued notation

$$\hat{z} = \begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix}$$

introduced in (3.2) where $\hat{q}$ denotes the position and $\hat{p}$ the momentum operator. Moreover, we choose $l \in \mathbb{C}^n \oplus \mathbb{C}^n$ and set

$$\hat{A}(l) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T \Omega \hat{z}, \quad \hat{A}^\dagger(l) = \frac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^* \Omega \hat{z}.$$

Analogously to Dirac's ladder operators we call $\hat{A}(l)$ lowering operator and $\hat{A}^\dagger(l)$ raising operator, see [LST15, §3]. In particular, if we choose $l = (\mathrm{i}, 1)^T$, we find $\hat{A}(l) = \hat{a}$ and $\hat{A}^\dagger(l) = \hat{a}^\dagger$. However, $\hat{A}(l)$ and $\hat{A}^\dagger(l)$ do in general not satisfy the same properties as $\hat{a}$ and $\hat{a}^\dagger$.

Lemma 4.1 — Commutator relations. We have for all $l, l' \in \mathbb{C}^n \oplus \mathbb{C}^n$:

a, $[\hat{A}(l), \hat{A}(l')] = -\frac{\mathrm{i}}{2} l^T \Omega l'$

b, $[\hat{A}(l), \hat{A}^\dagger(l')] = \frac{\mathrm{i}}{2} l^T \Omega \bar{l}' = h(l', l)$

c, $\hat{A}^\dagger(l) = -\hat{A}(\bar{l})$ is (formally) the adjoint operator of $\hat{A}(l)$.

Proof. This result can also be found as [LST15, Lemma 3.2]. The basic Weyl calculus from Appendix A implies

$$[\hat{A}(l), \hat{A}(l')] = \mathrm{i}\varepsilon\, \mathrm{op}_\varepsilon[\nabla A(l)^T \Omega \nabla A(l')] = -\tfrac{\mathrm{i}}{2}\mathrm{op}_\varepsilon[(\Omega^T l)^T \Omega \Omega^T l'] = -\tfrac{\mathrm{i}}{2} l^T \Omega l'$$

and

$$[\hat{A}(l), \hat{A}^\dagger(l')] = \mathrm{i}\varepsilon\, \mathrm{op}_\varepsilon[\nabla A(l)^T \Omega \nabla A^\dagger(l')] = \tfrac{\mathrm{i}}{2}\mathrm{op}_\varepsilon[(\Omega^T l)^T \Omega \Omega^T \bar{l}'] = \tfrac{\mathrm{i}}{2} l^T \Omega \bar{l}'.$$

For the last claim, we find similar to the proof of Lemma 3.2 c,

$$\begin{aligned}
\langle \hat{A}^\dagger(l)\varphi, \psi\rangle &= \frac{\mathrm{i}}{\sqrt{2\varepsilon}} \sum_{j=1}^n \int_{R^n} (\bar{l}_j x_j + \mathrm{i}\varepsilon \bar{l}_{j+n} \partial_{x_j}) \varphi(x) \overline{\psi}(x)\, dx \\
&= \frac{\mathrm{i}}{\sqrt{2\varepsilon}} \sum_{j=1}^n \int_{R^n} \varphi(x) \overline{(l_j x_j + \mathrm{i}\varepsilon l_{j+n} \partial_{x_j}) \psi(x)}\, dx = \langle \varphi, \hat{A}(l)\psi\rangle.
\end{aligned}$$

■

The commutator relations a, and b, give a direct hint to Chapter 3: We see that we can create a set of commuting lowering operators if we choose a set of l's that are skew-orthogonal to each other. Moreover, a set of vectors $\{l_1, \dots, l_n\}$ satisfying both, isotropy (2.8) and normalisation (2.9), parametrises a maximal family of commuting raising and lowering operators,

$$[\hat{A}(l_i), \hat{A}(l_j)] = 0 \quad \text{and} \quad [\hat{A}(l_i), \hat{A}^\dagger(l_j)] = \delta_{ij} \quad \text{for all} \quad 1 \le i, j \le n.$$

Thus, we can associate with every positive Lagrangian subspace $L = \mathrm{span}(l_1, \dots, l_n)$ commuting ladder operators. Following [Hag98, §3] we combine them as an operator vector, see [LST15, Defintiion 3.3].

Definition 4.1 — Ladder operators. For an isotropic matrix $Z \in \mathbb{C}^{2n \times n}$ with columns $l_1, \dots, l_n$ we will denote by $\hat{A}(Z)$ and $\hat{A}^\dagger(Z)$ the vectors of annihilation and creation operators, respectively,

$$\hat{A}(Z) := \left(\hat{A}(l_1), \ldots, \hat{A}(l_n)\right)^T = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} Z^T \Omega \hat{z},$$
$$\hat{A}^\dagger(Z) := \left(\hat{A}^\dagger(l_1), \ldots, \hat{A}^\dagger(l_n)\right)^T = \frac{-\mathrm{i}}{\sqrt{2\varepsilon}} Z^* \Omega \hat{z}.$$

For any multi-index $k \in \mathbb{N}^n$, we set

$$\hat{A}_k(Z) = \hat{A}(l_1)^{k_1} \ldots \hat{A}(l_n)^{k_n}, \quad \hat{A}_k^\dagger(Z) = \hat{A}^\dagger(l_1)^{k_1} \ldots \hat{A}^\dagger(l_n)^{k_n}.$$

Since all columns of an isotropic matrix are mutually skew-orthogonal, all components of the annihilation vector $\hat{A}(Z)$ commute. The same is true for the creation operator $\hat{A}^\dagger(Z)$. Therefore, the operator products $\hat{A}_k(Z)$ and $A_k^\dagger(Z)$ do not depend on the ordering of their individual factors. This is why it suffices to demand isotropy of Z in the definition of the ladder operators. However, to construct a family of orthonormal functions as demonstrated in Section 3.2 for the Hermite functions, we also need the canonical commutator relation to hold, i.e. the normalisation of Z.

In particular, if Z is an isotropic matrix, we can construct a normalised Lagrangian frame Z' with $\mathrm{range}(Z') = \mathrm{range}(Z)$ by taking $Z' = ZN^{-1/2}$ where N is the normalisation of Z, see Definition 2.5. Then,

$$\hat{A}(Z) = \overline{N}^{1/2} \hat{A}(Z') \quad \text{and} \quad \hat{A}^\dagger(Z) = N^{1/2} \hat{A}^\dagger(Z'). \tag{4.2}$$

In general, we can link ladder operators defined by different Lagrangian frames via their mixed isotropy and normalisation.

Corollary 4.1 Let $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ be two Lagrangian frames and $C, D \in \mathbb{C}^{n\times n}$ denote their mixed isotropy (2.17) and their mixed normalisation (2.18). We can expand the ladder operators defined by Z_2 as

$$\hat{A}(Z_2) = D^T \hat{A}(Z_1) + C^T \hat{A}^\dagger(Z_1),$$
$$\hat{A}^\dagger(Z_2) = D^* \hat{A}^\dagger(Z_1) + C^* \hat{A}(Z_1).$$

Proof. The identities follow directly from the definition of the ladder operators. Let $L_1 = \mathrm{range}(Z_1)$, $L_2 = \mathrm{range}(Z_2)$. Then, with the projection from Proposition 2.1,

$$\begin{aligned}\hat{A}(Z_2) &= \hat{A}(\pi_{L_1} Z_2 + \pi_{\overline{L}_1} Z_2) = \hat{A}(\pi_{L_1} Z_2) - \hat{A}^\dagger(\pi_{L_1} \overline{Z}_2)\\ &= \frac{\mathrm{i}}{\sqrt{2\varepsilon}} \left((\tfrac{\mathrm{i}}{2} Z_1 Z_1^* \Omega^T Z_2)^T \Omega \hat{z} + (\tfrac{\mathrm{i}}{2} Z_1 Z_1^* \Omega^T \overline{Z}_2)^* \Omega \hat{z} \right)\\ &= \frac{\mathrm{i}}{\sqrt{2\varepsilon}} \left(D^T Z_1^T \Omega \hat{z} - C^T Z_1^* \Omega \hat{z} \right) = D^T \hat{A}(Z_1) + C^T \hat{A}^\dagger(Z_1)\end{aligned}$$

since $C = \frac{\mathrm{i}}{2} Z_1^T \Omega^T Z_2$ and $D = \frac{\mathrm{i}}{2} Z_1^* \Omega^T Z_2$. The proof for $\hat{A}^\dagger(Z_2)$ works analogously. ■

To conclude the introduction of the ladder operators, we want to add that the definition given here is consistent with the original definition in [Hag98, §3] and the also common notation from [Lub08, §V.2]. We can write

$$\hat{A}_{Hag}(A,B) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}(-\mathrm{i}B\hat{q} + A\hat{p}) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} Z^T \Omega \hat{z} \quad \text{with} \quad Z = \begin{pmatrix} \mathrm{i}B^T \\ A^T \end{pmatrix}$$

or

$$\hat{A}_{Lub}(P,Q) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}(Q^T\hat{p} - P^T\hat{q}) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} Z^T \Omega \hat{z} \quad \text{with} \quad Z = \begin{pmatrix} P \\ Q \end{pmatrix}.$$

We showed in Section 2.3 that both choices of Z define a normalised Lagrangian frame under certain conditions on A, B resp. P, Q.

4.2. Coherent states

As in the previous chapter our coherent states now emerge as eigenfunctions with eigenvalue 0 of a lowering operator, more specifically in the multi-dimensional case as joint eigenfunction of a family of commuting operators that can be parametrised by a Lagrangian subspace $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$. We set

$$I(L) = \{\varphi \in \mathcal{D}'(\mathbb{R}^n)\,;\, \hat{A}(l)\varphi = 0\ \forall l \in L\}, \tag{4.3}$$

see [LST15, §3.1]. In Chapter 3 we initially assumed that $I \subset \mathcal{S}(\mathbb{R}^n)$ and proved this assumption in Lemma 3.3. Here we first go a little bit more into detail.

Let $\mathcal{D}'(\mathbb{R}^n)$ denote the set of all distributions, i.e. the dual space of $C_0^\infty(\mathbb{R}^n) = \mathcal{D}(\mathbb{R}^n)$, see [Hör83, §2] for basic definitions and properties. We define a Gaussian distribution as solution of

$$A(x, \nabla_x)u = 0,$$

where A is a linear function on $\mathbb{C}^{2n}$, see [Hör94, §21.6]. In particular, let $u \in \mathcal{D}'(\mathbb{R}^n)$ with $u \neq 0$ and $A(x,\nabla_x) = \sum_{j=1}^n \alpha_j x_j + \beta_j \partial_{x_j}$ for $\alpha_j, \beta_j \in \mathbb{C}$, $1 \le j \le n$. We then denote

$$I(u) = \{A;\ A(x,\nabla_x)u = 0\}$$

and call u a *Gaussian* if every $v \in \mathcal{D}'(\mathbb{R}^n)$ with $A(x,\nabla_x)v = 0$ for all $A \in I(u)$ is a constant multiple of u, see [Hör95, §5].

From (4.3) we observe that

$$\varphi \in I(L) \quad \text{if and only if} \quad \hat{A}(Z)\varphi = 0$$

for any Lagrangian frame $Z \in F_n(L)$.

Proposition 4.1 Consider a Lagrangian subspace $L = \{(Bx, x)\,;\, x \in \mathbb{C}^n\}$ parametrised by a symmetric matrix $B \in \mathbb{C}^{n\times n}$ as in Lemma 2.3. Then, every element in $I(L)$ is of the form

$$\varphi(x) = c \cdot e^{\frac{\mathrm{i}}{2\varepsilon} x^T B x}$$

for some constant $c \in \mathbb{C}$. Furthermore, L is positive if and only if $I(L) \subset L^2(\mathbb{R}^n)$.

Proof. Motivated by the observation

$$\hat{z}\, e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx} = \begin{pmatrix} Bx \\ x \end{pmatrix} e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx}$$

we denote $l_B(x) = (Bx, x)$ for $x \in \mathbb{C}^n$. Let $l \in L$. Then,

$$\hat{A}(l)e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx} = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T\Omega l_B(x)e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx} = 0$$

using that $l_B(x) \in L$ implies $l^T\Omega l_B(x) = 0$. Hence $e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx} \in I(L)$ and $e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx} \in L^2(\mathbb{R}^n)$ if and only if $\mathrm{Im}(B) > 0$ what is equivalent to the positivity of L by Lemma 2.3. To show uniqueness, we use that

$$\nabla_x \left(e^{-\frac{\mathrm{i}}{2\varepsilon}x^TBx}\varphi(x)\right) = \tfrac{\mathrm{i}}{\varepsilon}\left(-Bx\varphi(x) + \mathrm{i}\varepsilon\nabla_x\varphi(x)\right) e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx}.$$

If $\varphi \in I(L)$, we find

$$\partial_{x_j}\left(e^{-\frac{\mathrm{i}}{2\varepsilon}x^TBx}\varphi(x)\right) = \sqrt{\tfrac{2}{\varepsilon}}A(l_B(e_j))\varphi(x) = 0$$

for $j = 1, \ldots, n$, where e_j denotes the j-th unit vector. Therefore, $\varphi(x) = c \cdot e^{\frac{\mathrm{i}}{2\varepsilon}x^TBx}$ for some $c \in C$ if we utilise that the dimension of L is n. ■

Hagedorn's raising and lowering operators introduced in [Hag98, §3] originate from his earlier parametrisation of coherent states in [Hag85, §1], which can be conveniently expressed in terms of Lagrangian frames as shown in Section 2.3.

Lemma 4.2 — Coherent states. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace and consider a Lagrangian frame $Z \in \mathbb{C}^{2n\times n}$ spanning L. Define $P, Q \in \mathbb{C}^{n\times n}$ by

$$Z = \begin{pmatrix} P \\ Q \end{pmatrix}.$$

Then, P and Q are invertible and

$$\varphi_0(Z; x) = (\pi\varepsilon)^{-n/4}\det(Q)^{-1/2}e^{\frac{\mathrm{i}}{2\varepsilon}x^TPQ^{-1}x} \in I(L). \tag{4.4}$$

Furthermore, $\varphi_0(Z)$ is normalised if and only if the normalisation N of Z satisfies $\det(N) = 1$.

Proof. The proof is based on the properties of P and Q that we stated in Section 2.3. With Lemma 2.2 $L = \mathrm{range}(Z)$ can be written as $L = \{(PQ^{-1}q, q);\, q \in \mathbb{C}^n\}$ and Proposition 4.1 therefore implies that the Gaussian wave packet (4.4) is an element of $I(L)$.

For the normalisation, we find due to Lemma 2.6

$$\begin{aligned}\|\varphi_0(Z)\|^2 &= (\pi\varepsilon)^{-n/2}\det(QQ^*)^{-1/2}\int_{\mathbb{R}^n} e^{-\frac{1}{\varepsilon}x^T\mathrm{Im}(PQ^{-1})x}\,dx \\ &= \det(QQ^*)^{-1/2}\det(\mathrm{Im}(PQ^{-1}))^{-1/2} = \big(\det(QQ^*)\det(Q^{-*}NQ^{-1})\big)^{-1/2} \\ &= \det(N)^{-1/2}.\end{aligned}$$

■

In particular, we can conclude from this lemma that if Z denotes a Lagrangian frame, N its normalisation and $Z' = ZN^{-1/2}$, then

$$\varphi_0(Z') = \det(N)^{1/4}\varphi_0(Z).$$

Taking the root of $\det(N)$ is well-defined as N is Hermitian, for taking the square root of $\det(Q)$ in (4.4), however, we have to specify a branch first. In practice, it will typically be determined by continuity requirements, but to be precise we have to mention here that Equation (4.4) defines $\varphi_0(Z)$ only up to a phase factor.

4.3. Excited states

Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace. We will, as in Section 3.2, apply operators of the form $\hat{A}^\dagger(l)$ to coherent states $\varphi_0 \in I(L)$ with $\|\varphi_0\| = 1$ to create a family of orthonormal functions. The basic idea is to use the commutator relation from Lemma 4.1, $\hat{A}(l)\hat{A}^\dagger(l') = \hat{A}^\dagger(l')\hat{A}(l) + h(l', l)$, for $l, l' \in L$ and obtain

$$\langle \hat{A}^\dagger(l)\varphi_0, \hat{A}^\dagger(l')\varphi_0\rangle = \langle \varphi_0, \hat{A}(l)\hat{A}^\dagger(l')\varphi_0\rangle = h(l', l)$$

since $\|\varphi_0\|^2 = 1$ and $\hat{A}(l)\varphi_0 = 0$ for all $l \in L$. So, if l and l' are columns of a normalised Lagrangian frame, the states $\hat{A}^\dagger(l)\varphi_0$ and $\hat{A}^\dagger(l')\varphi_0$ will be orthogonal to each other if $l \neq l'$ and $\|\hat{A}^\dagger(l)\varphi_0\|^2 = 1$. Moreover, states $\hat{A}^\dagger(l)\varphi_0$ are orthogonal to φ_0 since

$$\langle \hat{A}^\dagger(l)\varphi_0, \varphi_0\rangle = \langle \varphi_0, \hat{A}(l)\varphi_0\rangle = 0.$$

Thus, by iterating this construction we can generate an infinite orthonormal set that turns out to be a basis, see [LST15, Theorem 3.7].

Theorem 4.1 — Orthonormal set. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace and $Z \in F_n(L)$. Then, for any normalised $\varphi_0 \in I(L)$, the set

$$\varphi_k(Z) := \frac{1}{\sqrt{k!}}\hat{A}^\dagger_k(Z)\varphi_0, \quad k \in \mathbb{N}^n, \tag{4.5}$$

is an orthonormal basis of $L^2(\mathbb{R}^n)$. We use here the standard multi-index notation $k! = k_1! \cdot \ldots \cdot k_n!$.

Proof. The result is due to [Hag98, Theorem 3.3]. For the orthogonality let $k, m \in \mathbb{N}^n$

with $k \neq m$. Then,

$$\langle \varphi_k(Z), \varphi_m(Z) \rangle = \tfrac{1}{\sqrt{k!m!}} \langle \varphi_0, \hat{A}_k(Z) \hat{A}^\dagger_m(Z) \varphi_0 \rangle.$$

If $l_1, \dots, l_n$ denote the columns of Z, we can use the commutator relation from Lemma 4.1 and find

$$\hat{A}_k(Z)\hat{A}^\dagger_m(Z) = \hat{A}(l_n)^{k_n} \hat{A}^\dagger(l_n)^{m_n} \dots \hat{A}(l_1)^{k_1} \hat{A}^\dagger(l_1)^{m_1}.$$

If we assume further without loss of generality that $m_1 < k_1$,

$$\begin{aligned}\langle \varphi_0, \hat{A}(l_1)^{k_1} \hat{A}^\dagger(l_1)^{m_1} \varphi_0 \rangle &= \langle \varphi_0, \hat{A}(l_1)^{k_1 - 1} \hat{A}^\dagger(l_1)^{m_1} \hat{A}(l_1) \varphi_0 \rangle + m_1 \langle \varphi_0, \hat{A}(l_1)^{k_1-1} \hat{A}^\dagger(l_1)^{m_1 - 1} \varphi_0 \rangle \\ &= m_1! \langle \varphi_0, \hat{A}(l_1)^{k_1 - m_1} \varphi_0 \rangle = 0.\end{aligned}$$

For the normalisation we use

$$\langle \hat{A}^\dagger_k(Z)\varphi_0, \hat{A}^\dagger_k(Z)\varphi_0 \rangle = \langle \hat{A}^\dagger_{k-e_j}(Z)\varphi_0, \hat{A}(l_j)\hat{A}^\dagger_k(Z)\varphi_0 \rangle = k_j \langle \hat{A}^\dagger_{k-e_j}(Z)\varphi_0, \hat{A}(l_j)\hat{A}^\dagger_{k-e_j}(Z)\varphi_0 \rangle$$

for all $j = 1, \dots, n$ and the claim follows by induction if we start from $\langle \varphi_0, \varphi_0 \rangle = 1$. For the completeness we show that the functions $(\varphi_k(Z))_{k \in \mathbb{N}^n}$ are eigenstates of the self-adjoint elliptic operator

$$\tfrac{1}{2}\left(\hat{A}(Z)^T \hat{A}^\dagger(Z) + \hat{A}^\dagger(Z)^T \hat{A}(Z) \right) = \tfrac{1}{2} \sum_{j=1}^{n} \hat{A}(l_j)\hat{A}^\dagger(l_j) + \hat{A}^\dagger(l_j)\hat{A}(l_j).$$

We can rewrite (4.5) also as

$$\varphi_k(Z) = \tfrac{1}{\sqrt{k_j}} \hat{A}^\dagger(l_j) \varphi_{k-e_j}(Z), \quad 1 \leq j \leq n$$

and with a similar computations as for the Hermite functions

$$\varphi_{k-e_j}(Z) = \tfrac{1}{\sqrt{k_j}} \hat{A}(l_j) \varphi_k(Z), \quad 1 \leq j \leq n.$$

Therefore,

$$\begin{aligned}\tfrac{1}{2}\sum_{j=1}^{n} (\hat{A}(l_j)\hat{A}^\dagger(l_j) + \hat{A}^\dagger(l_j)\hat{A}(l_j))\varphi_k(Z) &= \tfrac{1}{2}\sum_{j=1}^{n} \sqrt{k_j+1}\hat{A}(l_j)\varphi_{k+e_j}(Z) + \sqrt{k_j}\hat{A}^\dagger(l_j)\varphi_{k-e_j}(Z) \\ &= \tfrac{1}{2}\sum_{j=1}^{n} (k_j+1)\varphi_k(Z) + k_j\varphi_k(Z) = (|k| + \tfrac{n}{2})\varphi_k(Z).\end{aligned}$$

Moreover, $\frac{1}{2}\left(\hat{A}(Z)^T \hat{A}^\dagger(Z) + \hat{A}^\dagger(Z)^T \hat{A}(Z) \right)$ is self-adjoint, since $\hat{A}(Z)$ and $\hat{A}^\dagger(Z)$ are formal adjoints. We continue the proof of this result after the next lemma. ■

The number operator $\hat{A}(Z)^T \hat{A}^\dagger(Z)$ we considered in the previous proof has in addition an interesting connection to the symplectic metric of the Lagrangian subspace, see [LST15, Lemma 3.8] that is very useful to prove the completeness of the wave packets.

Lemma 4.3 — Number operator. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace, $Z \in F_n(L)$ and $G \in \mathrm{Sp}(n, \mathbb{R})$ denote the symplectic metric of L. Then, we can write $\hat{A}(Z)^T \hat{A}^\dagger(Z)$ as Weyl-quantised operator $\hat{A}(Z)^T \hat{A}^\dagger(Z) = \mathrm{op}_\varepsilon[\nu]$ with symbol

$$\nu(z) = \tfrac{1}{2\varepsilon}(z^T G z + n\varepsilon), \quad z \in \mathbb{R}^n \oplus \mathbb{R}^n.$$

Proof. With the Moyal product from Corollary A.1, we find

$$\hat{A}(Z)^T \hat{A}^\dagger(Z) = \sum_{j=1}^n \hat{A}(l_j)\hat{A}^\dagger(l_j) = \sum_{j=1}^n \mathrm{op}_\varepsilon[A(l_j)\# A^\dagger(l_j)]$$

where l_j, $j = 1, \dots, n$, denotes the columns of Z and

$$\left(A(l_j)\# A^\dagger(l_j)\right)(z) = \tfrac{1}{2\varepsilon}(z^T \Omega^T l_j l_j^* \Omega z + \tfrac{\mathrm{i}\varepsilon}{2} l_j^T \Omega \bar{l}_j) = \tfrac{1}{2\varepsilon}(z^T \Omega^T l_j l_j^* \Omega z + \varepsilon)$$

for all $z \in \mathbb{R}^{2n}$. Thus,

$$\hat{A}(Z)^T \hat{A}^\dagger(Z) = \mathrm{op}_\varepsilon[\sum_{j=1}^n A(l_j)\# A^\dagger(l_j)] = \mathrm{op}_\varepsilon[z^T G z + n\varepsilon],$$

since $G = \Omega^T Z Z^* \Omega - \mathrm{i}\Omega$. ■

Since we now know the symbol of the number operator, we can use a standard result for hypoelliptic operators to show the existence of a complete eigenbasis.

Proof. To show that ν is a hypoelliptic symbol, we need to verify that there exist constants m, m_0 such that one can find for any compact set $K \subset \mathbb{R}^n$ positive constants $C_1, C_2, R > 0$ with

$$C_1|\xi|^{m_0} \le |\nu(\xi, x)| \le C_2|\xi|^m$$

for all $x \in K$ and $\xi \in \mathbb{R}^n$ with $|\xi| \ge R$. Moreover, there are constants $0 \le \delta < \varrho \le 1$ such that for all compact sets $K \subset \mathbb{R}^n$ there exists a constant $R > 0$ satisfying

$$\left|\frac{\partial_\xi^\alpha \partial_x^\beta \nu(\xi, x)}{\nu(\xi, x)}\right| \le C_{\alpha,\beta,K}|\xi|^{-\varrho|\alpha| + \delta|\beta|}$$

for all multi-indices $\alpha, \beta \in \mathbb{N}^n$, $x \in K$ and $\xi \in \mathbb{R}^n$ with $|\xi| \ge R$ for some constant $C_{\alpha,\beta,K}$, see [Shu87, Definition 5.1]. We write $\nu \in \mathrm{HS}^{m,m_0}_{\rho,\delta}(\mathbb{R}^n \times \mathbb{R}^n)$ resp. $\mathrm{op}_\varepsilon[\nu] \in \mathrm{HL}^{m,m_0}_{\rho,\delta}(\mathbb{R}^n)$.

Clearly, since ν is a quadratic in ξ, we take $m = m_0 = 2$. The existence of a positive lower bound of $|\nu(\xi, x)|$ follows since G is positive definite, i.e. $|\nu(\xi, x)| \ge \frac{n}{2}$. For the upper bound we note that if we choose x in an arbitrary compact set, then due to Corollary 2.3 there exists $C > 0$ such that

$$|\nu(\xi, x)| \le C \cdot |\xi^T Q Q^* \xi| = C \cdot |Q^* \xi|^2 \le C_2|\xi|^2$$

for all $\xi \in \mathbb{R}^n$ and $C_2 > 0$ large enough.

For the estimate of the derivatives we first note that $\partial_\xi^\alpha \partial_x^\beta \nu(\xi, x) = 0$ if $|\alpha| > 2$, if $|\alpha| = 2$ then, $\partial_\xi^\alpha \partial_x^\beta \nu(\xi, x)$ is constant and the fraction bounded by $|\xi|^{-2}$, if $|\alpha| = 1$ it is bounded by $|\xi|^{-1}$. Consequently for all $\alpha, \beta \in \mathbb{N}^n$,

$$\left|\frac{\partial_\xi^\alpha \partial_x^\beta \nu(\xi, x)}{\nu(\xi, x)}\right| \leq C_{\alpha,\beta,K} |\xi|^{-|\alpha|}, \qquad \text{for all } x \in K, |\xi| \geq R.$$

Hence, $\mathrm{op}_\varepsilon[\nu] \in \mathrm{HL}^{2,2}_{1,0}(\mathbb{R}^n)$ and due to [Shu87, Theorem 8.3] there exists a complete orthonormal basis of eigenfunctions of $\mathrm{op}_\varepsilon[\nu]$.

It remains to show that already Hagedorn's wave packets are complete, in other words we can express any eigenfunction of $\mathrm{op}_\varepsilon[\nu]$ as linear combination of Hagedorn's wave packets. In particular, one can show that for any eigenfunction ψ of $\mathrm{op}_\varepsilon[\nu]$ there exists an excitation number $\kappa \in \mathbb{N}$ such that

$$\psi \in \mathrm{span}\{\varphi_k(Z)\,;\, |k| = \kappa\}$$

for a normalised Lagrangian frame $Z \in \mathbb{C}^{2n \times n}$. We first stress that for the raising and lowering operator $\hat{A}(Z)$ and $\hat{A}^\dagger(Z)$ it holds

$$\hat{A}_k(Z)\mathrm{op}_\varepsilon[\nu] = (\mathrm{op}_\varepsilon[\nu] + |k|)\hat{A}_k(Z), \qquad \hat{A}_k^\dagger(Z)\mathrm{op}_\varepsilon[\nu] = (\mathrm{op}_\varepsilon[\nu] - |k|)\hat{A}_k^\dagger(Z),$$

the observation follows from the commutator properties in Lemma 4.1. Assume that ψ is an eigenfunctions of $\mathrm{op}_\varepsilon[\nu]$ with eigenvalue λ, i.e.

$$\mathrm{op}_\varepsilon[\nu]\psi = \lambda\psi.$$

Then, $\lambda > 0$ as $\mathrm{op}_\varepsilon[\nu]$ is a positive operator and if $\hat{A}_k(Z)\psi \neq 0$ then also $\hat{A}_k(Z)\psi$ is an eigenfunction of $\mathrm{op}_\varepsilon[\nu]$ with eigenvalue $\lambda - |k|$. Since all eigenvalues of $\mathrm{op}_\varepsilon[\nu]$ are positive, this implies that there exists a $\kappa \in \mathbb{N}$ such that

$$\hat{A}_l(Z)\psi = 0 \qquad \text{for all } |l| > \kappa.$$

We next proof that this property implies that $\psi \in \mathrm{span}\{\varphi_k(Z)\,;\, |k| = \kappa\}$. Let $k \in \mathbb{N}^n$ with $|k| = \kappa$ and $l_1, \ldots, l_n$ denote the columns of Z. Then it follows for all $j = 1, \ldots, n$ that

$$\hat{A}(l_j)\hat{A}_k(Z)\psi = 0$$

and thus $\hat{A}_k(Z)\psi \in I(L) = \mathrm{span}\{\varphi_0(Z)\}$ by Proposition 4.1. The construction of the wave packets (4.5) then further implies that $\hat{A}_k^\dagger(Z)\hat{A}_k(Z)\psi \in I(L) = \mathrm{span}\{\varphi_k(Z)\}$.

By expanding the number operator

$$\begin{aligned}\mathrm{op}_\varepsilon[\nu]^\kappa &= \left(\hat{A}^\dagger(l_1)\hat{A}(l_1) + \ldots + \hat{A}^\dagger(l_n)\hat{A}(l_n)\right)^\kappa \\ &= \sum_{|m|=\kappa} \binom{\kappa}{m} \left(\hat{A}^\dagger(l_1)\hat{A}(l_1)\right)^{m_1} \ldots \left(\hat{A}^\dagger(l_n)\hat{A}(l_n)\right)^{m_n} = \sum_{|m|=\kappa} \binom{\kappa}{m} \hat{A}_m^\dagger(Z)\hat{A}_m(Z)\end{aligned}$$

where we use the multi-index notation $k! = k_1! \cdot \ldots \cdot k_n!$ we find that

$$\lambda^\kappa \psi = \mathrm{op}_\varepsilon[\nu]^\kappa \psi = \sum_{|m|=\kappa} \binom{\kappa}{m} \hat{A}_m^\dagger(Z)\hat{A}_m(Z)\psi \in \mathrm{span}\{\varphi_k(Z)\,;\, |k| = \kappa\}.$$

The claim follows since $\frac{1}{2}\left(\hat{A}(Z)^T\hat{A}^\dagger(Z) + \hat{A}^\dagger(Z)^T\hat{A}(Z)\right) = \mathrm{op}_\varepsilon[\nu] + \frac{n}{2}$. ■

So far, we showed that we can construct an orthonormal set of functions starting from any normalised element in $I(L)$. But in order to gain more specific statements about the structure of the wave packets we have to fix our ground state.

Hence, we assume in the following that $Z = (P;Q) \in \mathbb{C}^{2n\times n}$ is a normalised Lagrangian frame and choose $\varphi_0(Z)$ from Lemma 4.2 as coherent ground state. Then, it is clear from its definition that applying the raising operator $\hat{A}^\dagger(Z)$ to $\varphi_0(Z)$ will create functions that are of the form polynomial times the Gaussian $\varphi_0(Z)$.

Theorem 4.2 — Polynomial ladder. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace and $Z = (P;Q) \in F_n(L)$. Then, the k-th Hagedorn wave packet $\varphi_k(Z)$, $k \in \mathbb{N}^n$, can be written as

$$\varphi_k(Z;x) = \frac{1}{\sqrt{2^{|k|}k!}} p_k^M\left(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}x\right)\varphi_0(Z;x), \quad x \in \mathbb{R}^n, \tag{4.6}$$

where p_k^M is a multivariate polynomial of degree $|k|$ generated by the recursion

$$p_0^M = 1, \quad (p_{k+e_j}^M)_{j=1}^n = \hat{B}^\dagger p_k^M \quad \text{where} \quad \hat{B}^\dagger = 2x - M\nabla_x \tag{4.7}$$

and $M = M^T = Q^{-1}\overline{Q} \in \mathbb{C}^{n\times n}$. In particular, the polynomial factor p_k^M factorises into Hermite polynomials, i.e.

$$p_k^M(y) = \prod_{j=1}^n h_{k_j}(y_j), \quad y \in \mathbb{R}^n,$$

if and only if $Q \in \mathbb{R}^{n\times n}$.

Proof. This result can also be found as [LT14, Proposition 2] with a different notation. If we write $\hat{A}^\dagger(Z)$ in terms of P and Q, we obtain $\hat{A}^\dagger(Z) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}(P^*\hat{q} - Q^*\hat{p})$. Assuming that the claimed identity (4.6) holds for $k \in \mathbb{N}^n$, we derive with $y = \frac{1}{\sqrt{\varepsilon}}Q^{-1}x$

$$\begin{aligned}
\hat{A}^\dagger(Z)\varphi_k(Z;x) &= \frac{1}{\sqrt{2^{|k|+1}k!}}\frac{\mathrm{i}}{\sqrt{\varepsilon}}\left(P^*x\,p_k^M(y) + \mathrm{i}\varepsilon Q^*\nabla_x p_k^M(y) - Q^*PQ^{-1}x\,p_k^M(y)\right)\varphi_0(Z;x)\\
&= \frac{1}{\sqrt{2^{|k|+1}k!}}\left(\mathrm{i}(P^*Q - Q^*P)y\,p_k^M(y) - Q^*Q^{-T}\nabla_y p_k^M(y)\right)\varphi_0(Z;x)\\
&= \frac{1}{\sqrt{2^{|k|+1}k!}}\left(2y\,p_k^M(y) - M\nabla_y p_k^M(y)\right)\varphi_0(Z;x)\\
&= \frac{1}{\sqrt{2^{|k|+1}k!}}\left(p_{k+e_j}^M\left(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}x\right)\right)_{j=1}^n\varphi_0(Z;x) = \left(\sqrt{k_j+1}\,\varphi_{k+e_j}(Z;x)\right)_{j=1}^n
\end{aligned}$$

where it remains to show that M symmetric. Since $\mathrm{Im}(PQ^{-1}) = (QQ^*)^{-1}$, the matrix QQ^* is real and

$$M - M^T = Q^{-1}\overline{Q} - Q^*Q^{-T} = Q^{-1}\left(\overline{Q}Q^T - QQ^*\right)Q^{-T} = 0.$$

If $Q \in \mathbb{R}^{n\times n}$, we have $M = \mathrm{Id}$ and the polynomial generator $\hat{B}^\dagger$ is the multi-dimensional extension of the generator of the Hermite polynomials $\hat{b}^\dagger$. Vice versa, the operators $\hat{B}_j^\dagger$, $1 \le j \le n$, generate Hermite polynomials if $M = \mathrm{Id}$ what is equivalent to $Q = \overline{Q}$. ■

As initially mentioned in Section 4.1 the construction of the wave packets in Theorem 4.1 only yields an orthonormal basis if Z is normalised. However, the application of $\hat{A}^\dagger(Z)$ to $\varphi_0(Z)$ is well-defined for all Lagrangian frames $Z \in \mathbb{C}^{2n\times n}$. If furthermore the normalisation N of Z is positive definite, we have $\varphi_0(Z) \in L^2(\mathbb{R}^n)$ and we can create a set of L^2-functions that exhibits a similar structure than the standard wave packets.

Corollary 4.2 — Non-normalised Lagrangian frames. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace, $Z = (P;Q) \in \mathbb{C}^{2n\times n}$ a Lagrangian frame that spans L and $N \in \mathbb{C}^{n\times n}$ its normalisation. Then,

$$\varphi_k(Z) := \tfrac{1}{\sqrt{k!}}\hat{A}_k^\dagger(Z)\varphi_0(Z), \quad k \in N^n,$$

where $\varphi_0(Z)$ as in (4.4), can be written as

$$\varphi_k(Z;x) = \tfrac{1}{\sqrt{2^{|k|}k!}}p_k^{M'}(\tfrac{1}{\sqrt{\varepsilon}}NQ^{-1}x)\varphi_0(Z;x), \quad x \in \mathbb{R}^n,$$

with $M' = M'^T = NQ^{-1}\overline{Q}$. The polynomials $p_k^{M'}$ thereby satisfy the same recurrence relation as in Theorem 4.2.

Proof. Let $Z' = \begin{pmatrix} P' \\ Q' \end{pmatrix} := ZN^{-1/2}$. Then, we know from the previous proposition that $\hat{A}^\dagger(Z')\varphi_0(Z';x) = \frac{1}{\sqrt{2}}(\frac{2}{\sqrt{\varepsilon}}Q'^{-1}x)\varphi_0(Z';x)$ and thus,

$$\hat{A}^\dagger(Z)\varphi_0(Z;x) = \det(N)^{-1/4}N^{1/2}\hat{A}^\dagger(Z')\varphi_0(Z';x) = \tfrac{1}{\sqrt{2}}(\tfrac{2}{\sqrt{\varepsilon}}NQ^{-1}x)\varphi_0(Z;x),$$

which legitimates our ansatz. Taking $y := \frac{1}{\sqrt{\varepsilon}}NQ^{-1}x$, we observe

$$\begin{aligned}\hat{A}^\dagger(Z)(p_k^{M'}(y)\varphi_0(Z;x)) &= \hat{A}^\dagger(Z)\varphi_0(Z;x)\cdot p_k^{M'}(y) - \sqrt{\tfrac{\varepsilon}{2}}N^{1/2}Q'^*\nabla_x p_k^{M'}(y)\cdot\varphi_0(Z;x)\\ &= \tfrac{1}{\sqrt{2}}\left(2y\,p_k^{M'}(y) - Q^*Q^{-T}\overline{N}\nabla_y p_k^{M'}(y)\right)\varphi_0(Z;x)\\ &= \tfrac{1}{\sqrt{2}}\left(p_{k+e_j}^{M'}(y)\right)_{j=1}^n\varphi_0(Z;x).\end{aligned}$$

The symmetry of M' we used in the above calculation follows from $N = \frac{1}{2\mathrm{i}}(Q^*P - P^*Q)$ and

$$\begin{aligned}Q^*Q^{-T}\overline{N} &= -\tfrac{1}{2\mathrm{i}}Q^*(\overline{P} - (PQ^{-1})^T\overline{Q}) = -\tfrac{1}{2\mathrm{i}}Q^*(\overline{PQ}^{-1} - PQ^{-1})\overline{Q}\\ &= Q^*\mathrm{Im}(PQ^{-1})\overline{Q} = NQ^{-1}\overline{Q}\end{aligned}$$

by Lemma 2.6. ■

For our illustrations, we choose the Lagrangian frames

$$Z_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i} & \mathrm{i} \\ \mathrm{i} & -\mathrm{i} \\ 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad Z_2 = \frac{1}{2\sqrt{2}} \begin{pmatrix} -1+\mathrm{i} & 1+\mathrm{i} \\ 1+\mathrm{i} & -1+\mathrm{i} \\ 2(1+\mathrm{i}) & 2(1-\mathrm{i}) \\ 2(1-\mathrm{i}) & 2(1+\mathrm{i}) \end{pmatrix} \tag{4.8}$$

and

$$Z_3 = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1-\sqrt{2} & 1 \\ (1+\sqrt{2})\mathrm{i} & \mathrm{i} \\ 2\sqrt{2}\mathrm{i} & -2(2+\sqrt{2})\mathrm{i} \\ 2\sqrt{2} & 2(2-\sqrt{2}) \end{pmatrix}, \quad Z_4 = \begin{pmatrix} 1-2\mathrm{i} & -\mathrm{i} \\ \mathrm{i} & 2+\mathrm{i} \\ -2 & -1+\mathrm{i} \\ 1+\mathrm{i} & 2 \end{pmatrix}. \tag{4.9}$$

The matrices Z_1, Z_2 and Z_3 are normalised Lagrangian frames, while Z_4 is a Lagrangian frame with positive definite normalisation, $N_4 = \begin{pmatrix} 5 & 2-3\mathrm{i} \\ 2+3\mathrm{i} & 3 \end{pmatrix}$. The lower block Q_1

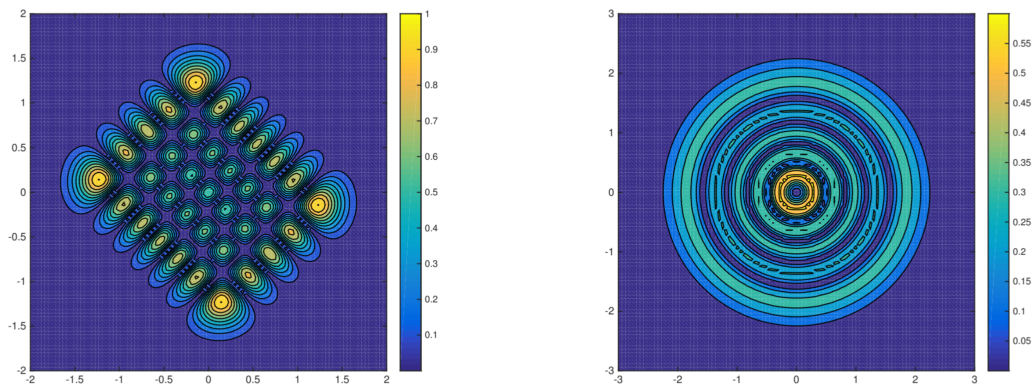

Figure 7.: Contour plots of the absolute values of $\varphi_{(4,6)}(Z_1)$ (left) and $\varphi_{(4,6)}(Z_2)$ (right) for $\varepsilon = 0.1$

of Z_1 is a real matrix and the wave packet $\varphi_{(4,6)}(Z_1)$ can thus be written with a tensor product of Hermite polynomials,

$$\varphi_{(4,6)}(Z_1; x) = \frac{1}{768\sqrt{30}} h_4\left(\frac{1}{\sqrt{2\varepsilon}}(x_1 + x_2)\right) h_6\left(\frac{1}{\sqrt{2\varepsilon}}(x_1 - x_2)\right) \varphi_0(Z_1; x),$$

what explains that the roots of $\varphi_{(4,6)}(Z_1)$ appear as a shifted grid. The wave packet $\varphi_{(4,6)}(Z_2)$ shows a circular structure that will be explained by an analysis of the polynomial prefactor in the next chapter. The wave packets associated with Z_3 and Z_4 demonstrate the various forms Hagedorn's wave packets can in general attain.

4.4. Phase space centres and Fourier transform

The wave packets as introduced in the previous section are centred at the origin. By means of the ε-scaled Heisenberg-Weyl operator

$$T(z)\psi(x) = e^{\frac{\mathrm{i}}{\varepsilon} p^T(x-q/2)} \psi(x-q), \quad z = (p,q) \in \mathbb{C}^n \oplus \mathbb{C}^n \tag{4.10}$$

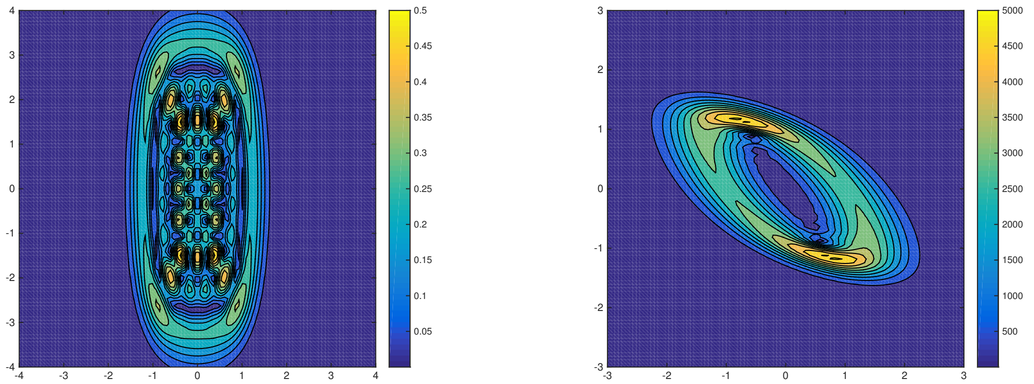

Figure 8.: Contour plots of the absolute values of $\varphi_{(4,6)}(Z_3)$ (left) and $\varphi_{(4,6)}(Z_4)$ (right) for $\varepsilon = 0.1$

that acts on square integrable functions $\psi \in L^2(\mathbb{R}^n)$, see Section 3.4, we can translate Hagedorn's wave packets to any complex center $z \in \mathbb{C}^n \oplus \mathbb{C}^n$. However, to give a physically meaningful interpretation of complex position and momentum values further investigation is needed.

The next lemma follows [LST15, Definition 3.10].

Lemma 4.4 — Centred ladder operators. For $l, z \in \mathbb{C}^n \oplus \mathbb{C}^n$ we define the ladder operators

$$\hat{A}(l, z) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T \Omega(\hat{z} - z), \quad \hat{A}^\dagger(l, z) = \frac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^* \Omega(\hat{z} - \overline{z}),$$

i.e. $\hat{A}^\dagger(l, z) = -\hat{A}(\overline{l}, \overline{z})$ and state that

$$T(w)\hat{A}(l, z)T(w)^{-1} = \hat{A}(l, z + w) \tag{4.11}$$

for all $w \in \mathbb{C}^n \oplus \mathbb{C}^n$.

Proof. It is clear by definition that $T(w)^{-1}\psi(x) = e^{-\frac{\mathrm{i}}{\varepsilon}\eta^T(x-y/2)}\psi(x + y)$ for $w = (\eta, y)$. Thus,

$$\begin{aligned}
T(w)\hat{p}T(w)^{-1}\psi(x) &= T(w)\left(-\mathrm{i}\varepsilon\nabla_x(e^{-\frac{\mathrm{i}}{\varepsilon}\eta^T(x-y/2)}\psi(x + y))\right) = -\eta\psi(x) - \mathrm{i}\varepsilon\nabla_x\psi(x) \\
&= \hat{p}\psi(x) - \eta\psi(x), \\
T(w)\hat{q}T(w)^{-1}\psi(x) &= T(w)\left(xe^{-\frac{\mathrm{i}}{\varepsilon}\eta^T(x-y/2)}\psi(x + y))\right) = (x - y)\psi(x) \\
&= \hat{q}\psi(x) - y\psi(x),
\end{aligned}$$

and the claim follows from $T(w)\hat{z}T(w)^{-1} = \hat{z} - w$. ■

We similarly adjust the vector-valued notation and set

$$\hat{A}(Z, z) = \left(\hat{A}(l_1, z), \ldots, \hat{A}(l_n, z)\right) \quad \text{resp.} \quad \hat{A}^\dagger(Z, z) = \left(\hat{A}^\dagger(l_1, z), \ldots, \hat{A}^\dagger(l_n, z)\right)$$

for any Lagrangian frame $Z \in \mathbb{C}^{2n\times n}$ with columns $l_1, \ldots l_n \in \mathbb{C}^{2n}$. Since adding a constant to an operator does not change its commutation properties, the application of $A_k^\dagger(Z,z)$ to a coherent state is still well-defined. Moreover, with

$$\hat{A}(Z) = \hat{A}(Z,0), \quad \hat{A}^\dagger(Z) = \hat{A}^\dagger(Z,0)$$

and Equation (4.11) we are able to transfer our previous results away from the origin.

Theorem 4.3 — Orthonormal basis. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace and $Z = (P;Q) \in F_n(L)$. Let $z = (p,q) \in \mathbb{C}^n \oplus \mathbb{C}^n$. Then, every element in

$$I(L,z) = \{\varphi \in \mathcal{D}'(\mathbb{R}^n)\,;\, \hat{A}(l,z)\varphi = 0\ \forall l \in L\}$$

is a constant multiple of the normalised coherent state

$$\varphi_0(Z,z;x) = (\pi\varepsilon)^{-n/4}\det(Q)^{-1/2} e^{\frac{\mathrm{i}}{2\varepsilon}(x-q)^T PQ^{-1}(x-q)+\frac{\mathrm{i}}{\varepsilon}p^T(x-q)}$$

and the set $\varphi_k(Z,z) := \frac{1}{\sqrt{k!}}A_k^\dagger(Z,z)\varphi_0(Z,z)$ is an orthonormal basis of $L^2(\mathbb{R}^n)$.

Proof. From Proposition 4.1 we know that every element in $I(L)$ is a constant multiple of $e^{\frac{\mathrm{i}}{2\varepsilon}x^T PQ^{-1}x}$. Let $\varphi \in I(L)$, then

$$0 = \hat{A}(l)\varphi = T(z)^{-1}\hat{A}(l,z)T(z)\varphi$$

and thus $T(z)\varphi \in I(L,z)$. A direct computation yields

$$T(z)e^{\frac{\mathrm{i}}{2\varepsilon}x^T PQ^{-1}x} = e^{\frac{\mathrm{i}}{2\varepsilon}p^T q}e^{\frac{\mathrm{i}}{2\varepsilon}(x-q)^T PQ^{-1}(x-q)+\frac{\mathrm{i}}{\varepsilon}p^T(x-q)} = c\cdot\varphi_0(Z,z;x)$$

for some constant $c \in \mathbb{C}$. Furthermore, by simply substituting $x' = x - q$ one can show that the norm is preserved under translation, $\|T(z)\varphi\|^2 = \|\varphi\|^2$ for all $\varphi \in L^2(\mathbb{R}^n)$. Analogously, one receives

$$\langle T(z)\varphi, T(z)\psi\rangle = \langle\varphi,\psi\rangle, \quad \varphi,\psi \in L^2(R^n)$$

and therefore the wave packets $\varphi_k(Z,z)$ are orthonormal. The completeness follows similarly as in Theorem 4.5 if we consider $\hat{A}(Z,z)^T\hat{A}^\dagger(Z,z)$. ■

Since a translation does not change the overall structure of the wave packets, we can still express the wave packets $\varphi_k(Z,z)$ as a product of a multivariate polynomial and a Gaussian.

Corollary 4.3 — Polynomial ladder. Let $Z = (P;Q) \in \mathbb{C}^{2n\times n}$ be a normalised Lagrangian frame and $z = (p,q) \in \mathbb{C}^n \oplus \mathbb{C}^n$. Then, the k-th Hagedorn wave packet $\varphi_k(Z,z)$, $k \in \mathbb{N}^n$, centred at z can be written as

$$\varphi_k(Z,z;x) = \frac{1}{\sqrt{2^{|k|}k!}}p_k^M\left(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}(x-q)\right)\varphi_0(Z,z;x), \quad x \in \mathbb{R}^n$$

where $M = Q^{-1}\overline{Q}$ and the polynomials p_k^M are recursively defined as in Theorem 4.2.

Proof. We have $\varphi_0(Z,z) = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}T(z)\varphi_0(Z)$ and

$$\hat{A}^\dagger(Z,z)\varphi_0(Z,z) = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}T(z)\hat{A}^\dagger(Z)\varphi_0(Z) = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}\left(T(z)\varphi_{e_j}(Z)\right)_{j=1}^n.$$

Hence, we find by induction that $\varphi_k(Z,z) = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}T(z)\varphi_k(Z)$ and the claim is a direct application of Theorem 4.2. ∎

So, we can create a basis of orthonormal L^2-functions centred at any phase space point $z = (p,q) \in \mathbb{C}^n \oplus \mathbb{C}^n$. However, we want to interpret the coordinates p and q as momentum and position centres of a particle's probability density. Fortunately, it turns out that we can always reduce to the case with real centres $z \in \mathbb{R}^n \oplus \mathbb{R}^n$, see [LST15, §3.3].

To understand why, let us ask which conditions on $z, w \in \mathbb{C}^n \oplus \mathbb{C}^n$ must holds so that $I(L,z) = I(L,w)$. In terms of the annihilation operator this means that for all $l \in L$ and $\varphi \in I(L,z)$,

$$\hat{A}(l,z)\varphi = \hat{A}(l,w)\varphi.$$

Since

$$\hat{A}(l,z) - \hat{A}(l,w) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}l^T\Omega(w-z),$$

this is equivalent to the condition $l^T\Omega(w-z) = 0$ for all $l \in L$ and $w - z$ has to be skew-orthogonal to L. But since L is Lagrangian this means $w - z \in L$. Hence any two complex centres whose difference is in L define the same ladder operators and we just have to find a $v \in \mathbb{C}^n \oplus \mathbb{C}^n$ such that $w = z + \pi_L v$ is real.

Theorem 4.4 — Real centres. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian and $Z \in F_n(L)$. Let $J \in \mathrm{Sp}(n,\mathbb{R})$ denote the complex structure of L and define

$$P_J : \mathbb{C}^n \oplus \mathbb{C}^n \mapsto \mathbb{R}^n \oplus \mathbb{R}^n, \;\; P_J(z) = \mathrm{Re}(z) + J\mathrm{Im}(z).$$

Then, for any $z = (p,q) \in \mathbb{C}^n \oplus \mathbb{C}^n$

$$\hat{A}(Z,z) = \hat{A}(Z,P_J(z)), \quad I(L,z) = I(L,P_J(z))$$

and the coherent states are related by

$$\varphi_0(Z,z) = e^{\frac{\mathrm{i}}{2\varepsilon}(\eta+p)^T(y-q)}\varphi_0(Z,P_J(z)), \quad P_J(z) = (\eta,y).$$

Proof. This result can also be found as [LST15, Theorem 3.12] and it gives a reformulation of [GS12, Theorem 2.1] in terms of Lagrangian frames.

We have

$$z - P_J(z) = (\mathrm{i}\mathrm{Id} - J)\mathrm{Im}(z) = \mathrm{i}(\mathrm{Id} + \mathrm{i}J)\mathrm{Im}(z) = 2\mathrm{i}\pi_L\mathrm{Im}(z)$$

and with the previous considerations $\hat{A}(Z,z) = \hat{A}(Z,P_J(z))$. This directly implies

$$I(L,z) = I(L,P_J(z)).$$

For the coherent states we consider the quadratic function

$$S(x) = \tfrac{1}{2}(x-q)^T B(x-q) + p^T(x-q).$$

Since $z = (p,q)$ is complex, the minimum of S need not to be located at $x = q$, but at $y \in \mathbb{R}^n$ such that $\nabla \mathrm{Im}(S(y)) = 0$. It holds

$$\nabla \mathrm{Im}(S(x)) = \mathrm{Im}\left(B(x-q)+p\right) = \mathrm{Im}(B)x - \mathrm{Im}(B)\mathrm{Re}(q) - \mathrm{Re}(B)\mathrm{Im}(q) + \mathrm{Im}(p)$$

and thus $y = \mathrm{Re}(q) + \mathrm{Im}(B)^{-1}\mathrm{Re}(B)\mathrm{Im}(q) - \mathrm{Im}(B)^{-1}\mathrm{Im}(p)$. Moreover, we set $\eta := \nabla \mathrm{Re}(S(y))$, i.e.

$$\begin{aligned}\eta &= \mathrm{Re}\left(B(-\mathrm{i}\mathrm{Im}(q) + \mathrm{Im}(B)^{-1}\mathrm{Re}(B)\mathrm{Im}(q) - \mathrm{Im}(B)^{-1}\mathrm{Im}(p)) + p\right)\\ &= \mathrm{Re}(p) + (\mathrm{Im}(B) + \mathrm{Re}(B)\mathrm{Im}(B)^{-1}\mathrm{Re}(B))\mathrm{Im}(q) - \mathrm{Re}(B)\mathrm{Im}(B)^{-1}\mathrm{Im}(p).\end{aligned}$$

All together, we have

$$\begin{aligned}\begin{pmatrix}\eta\\ y\end{pmatrix} &= \mathrm{Re}(z) + \begin{pmatrix}-\mathrm{Re}(B)\mathrm{Im}(B)^{-1} & \mathrm{Im}(B) + \mathrm{Re}(B)\mathrm{Im}(B)^{-1}\mathrm{Re}(B)\\ -\mathrm{Im}(B)^{-1} & \mathrm{Im}(B)^{-1}\mathrm{Re}(B)\end{pmatrix}\mathrm{Im}(z)\\ &= \mathrm{Re}(z) + J\mathrm{Im}(z) = P_J(z)\end{aligned}$$

where we used Corollary 2.3. So, S is centered at $P_J(z)$ and we write S as second order expansion around $x = y$,

$$S(x) = S(y) + \nabla S(y)^T(x-y) + \tfrac{1}{2}(x-y)^T B(x-y) = S(y) + \eta^T(x-y) + \tfrac{1}{2}(x-y)^T B(x-y).$$

Thereby the two coherent states are related via

$$\varphi_0(Z,z) = e^{\frac{\mathrm{i}}{\varepsilon}S(y)}\varphi_0(Z,P_J(z))$$

and with $\eta = \nabla S(y) = B(y-q) + p$ we find

$$S(y) = \tfrac{1}{2}(y-q)^T(\eta - p) + p^T(y-q) = \tfrac{1}{2}(y-q)^T(\eta + p).$$

■

In Proposition 3.3 we found that the Fourier transform reverses the position and momentum centres of the Hermite functions. Since we now introduced general phase space centres for Hagedorn's wave packets as well, we can transmit this result to $\varphi_k(Z,z)$. The Fourier transform with the semiclassical parameter $\varepsilon > 0$ reads

$$\mathcal{F}^\varepsilon\varphi(\xi) = (2\pi\varepsilon)^{-n/2}\int_{\mathbb{R}^n}\varphi(x)e^{-\frac{\mathrm{i}}{\varepsilon}x^T\xi}\,dx, \quad \xi \in \mathbb{R}^n,$$

for all $\varphi \in L^2(\mathbb{R}^n)$. We start with the Fourier transform of the coherent ground state.

Lemma 4.5 — Fourier transform. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian and $Z \in F_n(L)$. Then,

$$\mathcal{F}^\varepsilon \varphi_0(Z)(\xi) = \varphi_0(\Omega Z; \xi).$$

Proof. We use the same ansatz as for the Hermite functions in Lemma 3.4. With $\varphi_0(Z) \in I(L)$, we find

$$0 = \mathcal{F}^\varepsilon \hat{A}(Z)\varphi_0(Z) = \mathcal{F}^\varepsilon \hat{A}(Z)(\mathcal{F}^\varepsilon)^{-1}\mathcal{F}^\varepsilon \varphi_0(Z)$$

and thus $\mathcal{F}^\varepsilon \varphi_0(Z)$ is an element of the kernel of $\mathcal{F}^\varepsilon \hat{A}(Z)(\mathcal{F}^\varepsilon)^{-1}$ where we apply the Fourier transform to each component, i,e.

$$\mathcal{F}^\varepsilon \hat{A}(Z)(\mathcal{F}^\varepsilon)^{-1} = \left(\mathcal{F}^\varepsilon \hat{A}(l_1)(\mathcal{F}^\varepsilon)^{-1}, \ldots, \mathcal{F}^\varepsilon \hat{A}(l_n)(\mathcal{F}^\varepsilon)^{-1}\right),$$

where $l_1, \ldots, l_n$ denote the columns of Z. In the proof of Lemma 3.4 we deduced that

$$\mathcal{F}^\varepsilon \hat{z}(\mathcal{F}^\varepsilon)^{-1} = \Omega^T \hat{z}$$

what yields

$$\mathcal{F}^\varepsilon \hat{A}(Z)(\mathcal{F}^\varepsilon)^{-1} = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} Z^T \Omega(\Omega^T \hat{z}) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} (\Omega Z)^T \Omega \hat{z} = \hat{A}(\Omega Z).$$

Since $\mathcal{F}^\varepsilon \varphi_0(Z)$ is normalised it follows that $\mathcal{F}^\varepsilon \varphi_0(Z) = \varphi_0(\Omega Z)$. ∎

With this result we can give explicit formulas for the position density

$$|\varphi_0(Z)|^2 = (\pi\varepsilon)^{-n/2} |\det(Q)|^{-1} e^{-x^T \mathrm{Im}(PQ^{-1})x/\varepsilon}$$

and the momentum density

$$|\mathcal{F}^\varepsilon \varphi_0(Z)|^2 = (\pi\varepsilon)^{-n/2} |\det(P)|^{-1} e^{x^T \mathrm{Im}(QP^{-1})x/\varepsilon}$$

see also Lemma 3.7 b,. Since we know that $\mathrm{Im}(PQ^{-1}) = (QQ^*)^{-1}$ and an analogous computation for the second case yields

$$\mathrm{Im}(QP^{-1}) = \tfrac{1}{2\mathrm{i}}(QP^{-1} - P^{-*}Q^*) = \tfrac{1}{2\mathrm{i}} P^{-*}(P^*Q - Q^*P)P^{-1} = -(PP^*)^{-1}.$$

we find

$$|\varphi_0(Z)|^2 = (\pi\varepsilon)^{-n/2} |\det(Q)|^{-1} e^{-x^T (QQ^*)^{-1} x/\varepsilon},$$
$$|\mathcal{F}^\varepsilon \varphi_0(Z)|^2 = (\pi\varepsilon)^{-n/2} |\det(P)|^{-1} e^{-x^T (PP^*)^{-1} x/\varepsilon},$$

and the matrices $QQ^* \in \mathbb{R}^{n\times n}$ and $PP^* \in \mathbb{R}^{n\times n}$ provide the width of the position and momentum densities, see also [LT14, §3].

Theorem 4.5 — Fourier transform. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian, $Z \in F_n(L)$

and $z = (p, q) \in \mathbb{C}^n \oplus \mathbb{C}^n$. Then,

$$\mathcal{F}^\varepsilon \varphi_k(Z, z)(\xi) = e^{-\frac{\mathrm{i}}{\varepsilon} p^T q} \varphi_k(\Omega Z, \Omega z; \xi)$$

for all $k \in \mathbb{N}^n$.

Proof. This result can also be found in [Lub08, §V.1]. If we apply the Fourier transform to the single components of $\hat{A}^\dagger(Z)$, we have $\left(\mathcal{F}^\varepsilon \hat{A}^\dagger(Z)(\mathcal{F}^\varepsilon)^{-1}\right)^k = \mathcal{F}^\varepsilon \hat{A}^\dagger_k(Z)(\mathcal{F}^\varepsilon)^{-1}$ for all $k \in \mathbb{N}^n$. Thus, with the results from the previous lemma

$$\begin{aligned} \mathcal{F}^\varepsilon \varphi_k(Z) &= \tfrac{1}{\sqrt{k!}} \mathcal{F}^\varepsilon \hat{A}^\dagger_k(Z) \varphi_0(Z) = \tfrac{1}{\sqrt{k!}} \mathcal{F}^\varepsilon \hat{A}^\dagger_k(Z)(\mathcal{F}^\varepsilon)^{-1} \mathcal{F}^\varepsilon \varphi_0(Z) \\ &= \tfrac{1}{\sqrt{k!}} \left(\mathcal{F}^\varepsilon \hat{A}^\dagger(Z)(\mathcal{F}^\varepsilon)^{-1}\right)^k \mathcal{F}^\varepsilon \varphi_0(Z) = \tfrac{1}{\sqrt{k!}} \hat{A}^\dagger(\Omega Z) \varphi_0(\Omega Z) = \varphi_k(\Omega Z). \end{aligned}$$

For the phase space centres we use Proposition 3.3,

$$\mathcal{F}^\varepsilon \varphi_k(Z, z) = \mathcal{F}^\varepsilon e^{-\frac{\mathrm{i}}{2\varepsilon} p^T q} T(z) \varphi_k(Z) = e^{-\frac{\mathrm{i}}{2\varepsilon} p^T q} \mathcal{F}^\varepsilon T(z)(\mathcal{F}^\varepsilon)^{-1} \varphi_k(\Omega Z)$$

and $\mathcal{F}^\varepsilon T(z)(\mathcal{F}^\varepsilon)^{-1} = T(\Omega z)$. The claim follows from $\varphi_k(Z, z) = e^{-\frac{\mathrm{i}}{2\varepsilon} p^T q} T(z) \varphi_k(Z)$. ■

■ **Remark 4.1** In Hagedorn's original work [Hag85] and in [Hag98], where he also used a ladder-based proof, the Fourier transform of the wave packets reads

$$\mathcal{F}^\varepsilon \varphi_k(A, B) = (-\mathrm{i})^{|k|} \varphi_k(B, A).$$

This is indeed consistent with our result: Let $Z = (\mathrm{i}B^T;\ A^T) \in \mathbb{C}^{2n \times n}$. Then,

$$\Omega Z = \begin{pmatrix} -A^T \\ \mathrm{i}B^T \end{pmatrix} = \mathrm{i} \begin{pmatrix} \mathrm{i}A^T \\ B^T \end{pmatrix}$$

and Hagedorn's raising operator $\hat{A}^\dagger_{Hag}(A, B) = \hat{A}_{Hag}(A, B)^*$, see Section 4.1, is equivalent to our raising operator $\hat{A}^\dagger_{Hag}(A, B) = \hat{A}^\dagger(Z)$. Moreover,

$$-\mathrm{i}\hat{A}^\dagger_{Hag}(B, A) = -\mathrm{i}\hat{A}^\dagger\left(\begin{pmatrix} \mathrm{i}A^T \\ B^T \end{pmatrix}\right) = -\mathrm{i}\hat{A}^\dagger(-\mathrm{i}\Omega Z) = \hat{A}^\dagger(\Omega Z)$$

what explains the factor $(-\mathrm{i})^{|k|}$ in the A, B-notation of Hagedorn.

4.5. Generalised wave packets

We conclude the introductory part of Hagedorn's wave packets with a natural generalisation: By Lemma 4.1 the components of $\hat{A}^\dagger(Z)$ commute if the columns of Z are skew-orthogonal to each other. Thus, the iterative application of $\hat{A}^\dagger(Z)$ to any function $\varphi \in L^2(\mathbb{R}^n)$ is well-defined if Z is isotropic. In the further discussion, we focused on coherent states that are elements of $I(L)$ with $L = \mathrm{range}(Z)$. Here we want to continue und also allow for coherent states $\varphi_0 \in I(L)$ where $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ is an arbitrary Lagrangian subspace.

Definition 4.2 — Generalised wave packets. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian, $Z \in F_n(L)$ and $Y \in \mathbb{C}^{2n\times n}$ a normalised Lagrangian frame. We set

$$\varphi_k(Z,Y) = \tfrac{1}{\sqrt{k!}}\hat{A}^\dagger(Y)\varphi_0(Z)$$

for all $k \in \mathbb{N}^n$ and refer to $\varphi_k(Z,Y)$ as *generalised wave packet*.

Due to this definition $\hat{A}^\dagger(Y)$ can still be seen as creator of the generalised wave packets. The annihilator $\hat{A}(Y)$, however, satisfies

$$\hat{A}(Y)\varphi_k(Z,Y) = \left(\sqrt{k_j}\varphi_{k-e_j}(Z,Y)\right)_{j=1}^n$$

if and only if $\hat{A}(Y)\varphi_0(Z) = 0$. Nevertheless, it is obvious that also the generalised wave packets attain the form of a polynomial times the Gaussian $\varphi_0(Z)$.

Proposition 4.2 — Polynomial ladder. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian, $Z = (P;Q) \in F_n(L)$ and $Y \in \mathbb{C}^{2n\times n}$ a normalised Lagrangian frame. We denote by

$$C = \tfrac{1}{2\mathrm{i}}Z^T\Omega Y, \quad D = \tfrac{1}{2\mathrm{i}}Z^*\Omega Y$$

the mixed istropy and the mixed normalisation of Z and Y, see (2.17) and (2.18). Then, we can write the k-th generalised wave packet as

$$\varphi_k(Z,Y;x) = \tfrac{1}{\sqrt{2^{|k|}k!}}p_k^M\left(\tfrac{1}{\sqrt{\varepsilon}}D^*Q^{-1}x\right)\varphi_0(Z;x) \tag{4.12}$$

with $M = -C^*\overline{D} + D^*Q^{-1}\overline{QD}$ and p_k^M as in Theorem 4.2.

Proof. Let $Z = (P;Q)$ and $Y = (V;W)$. We assume that (4.12) holds true and compute

$$\begin{aligned}
\hat{A}^\dagger(Y)\varphi_k(Z,Y;x) &= \tfrac{1}{\sqrt{2^{|k|+1}k!}}\tfrac{\mathrm{i}}{\sqrt{\varepsilon}}\left(V^*xp_k^M(y) - W^*PQ^{-1}xp_k^M(y) + \mathrm{i}\varepsilon W^*\nabla_x p_k^M(y)\right)\varphi_0(Z;x)\\
&= \tfrac{1}{\sqrt{2^{|k|+1}k!}}\left(\mathrm{i}(V^*Q - W^*P)D^{-*}yp_k^M(y) - W^*Q^{-T}\overline{D}\nabla_x p_k^M(y)\right)\varphi_0(Z;x)\\
&= \tfrac{1}{\sqrt{2^{|k|+1}k!}}\left(2yp_k^M(y) - M\nabla_x p_k^M(y)\right)\varphi_0(Z;x)\\
&= \tfrac{1}{\sqrt{2^{|k|+1}k!}}\left(p_{k+e_j}^M(y)\right)_{j=1}^n\varphi_0(Z;x)
\end{aligned}$$

where $y = \frac{1}{\sqrt{\varepsilon}}D^*Q^{-1}x$. It remains to show that $M = W^*Q^{-T}\overline{D}$. We have

$$D^*Q^* = \tfrac{\mathrm{i}}{2}(V^*QQ^* - W^*PQ^*)$$

and since the symplectic metric G of L is symmetric, we can conclude from Corollary 2.3 that $PQ^* = (QP^* + 2\mathrm{i}\mathrm{Id})^T$. Thus,

$$D^*Q^* = \tfrac{\mathrm{i}}{2}(V^*\overline{Q} - W^*\overline{P})Q^T + W^* = C^*Q^T + W^*$$

and $W^*Q^{-T}\overline{D} = D^*Q^{-1}\overline{QD} - C^*\overline{D}$. We further stress that

$$-C^*\overline{D} = \tfrac{1}{4}Y^*\Omega^T\overline{Z}Z^T\Omega\overline{Y} = \tfrac{1}{4}Y^*\Omega^T(\mathrm{Re}(ZZ^*) - \mathrm{i}\Omega)\Omega\overline{Y} = \tfrac{1}{4}Y^*G\overline{Y}$$

what ensures the symmetry of M. ■

With the relation of the ladder operators parametrised by two Lagrangian frames given in Corollary 4.1 we can also give a sharp criterion when the generalised wave packets equal the standard wave packets.

■ **Remark 4.2** Let $Y, Z \in \mathbb{C}^{2n\times n}$ denote two normalised Lagrangian frames, $C = \frac{1}{2\mathrm{i}} Z^T \Omega Y$ their mixed isotropy and $D = \frac{1}{2\mathrm{i}} Z^* \Omega Y$ their mixed normalisation. Then, Y and Z parametrise the same coherent state, $\varphi_0(Y) = \varphi_0(Z)$, if $C = 0$ and the same excited states, $\varphi_k(Z) = \varphi_k(Y)$ for $k \in \mathbb{N}^n$, if in addition $D = \mathrm{Id}$. Thus, $\varphi_k(Z, Y) = \varphi_k(Y)$ if and only if $C = 0$ and $D = \mathrm{Id}$.

Figure 9 displays two generalised wave packets for the Lagrangian frames Z_1, Z_2 and Z_3 given in (4.8) and (4.9). Both wave packets, $\varphi_{(4,6)}(Z_2, Z_1)$ and $\varphi_{(4,6)}(Z_2, Z_3)$, still exhibit a structure similar to Hagedorn's wave packets $\varphi_{(4,6)}(Z_1)$ resp. $\varphi_{(4,6)}(Z_3)$.

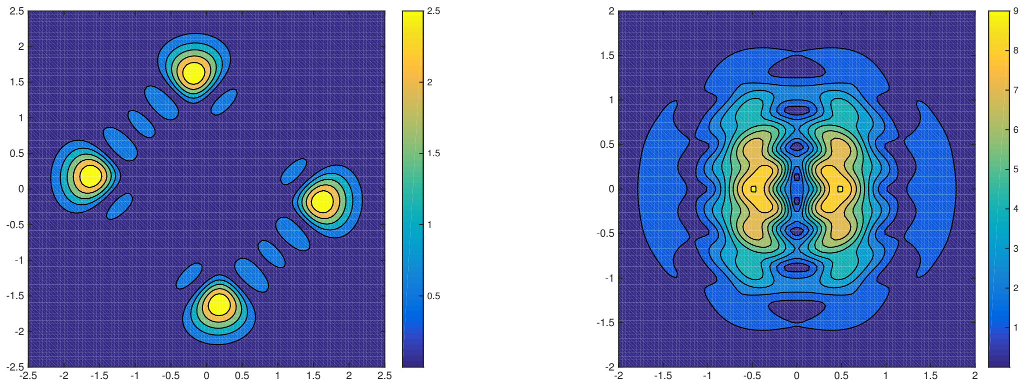

Figure 9.: Contour plots of the absolute values of $\varphi_{(4,6)}(Z_2, Z_1)$ (left) and $\varphi_{(4,6)}(Z_2, Z_3)$ (right) for $\varepsilon = 0.1$

5. Polynomial prefactor

The formulas we found for Hagedorn's wave packets in various cases in the last chapter strongly motivate a closer study of polynomials of the type

$$p_k^M = \hat{B}_k^\dagger 1, \quad \text{where} \quad \hat{B}^\dagger = 2x - M\nabla_x,$$

and M is a symmetric matrix. In the one-dimensional case this definition yields a scaled version of the Hermite polynomials we discussed in Chapter 3. Going over the multi-dimensions, we find that if M is a diagonal matrix, the polynomials are simply tensor products of (scaled) Hermite polynomials. This product structure is usually seen as the generalisation of Hermite polynomials in the multivariate case, see for example [Tha93, §1.1]. However, if M has off-diagonal entries a more complex structure appears and we find in some sense a non-trivial extension of the Hermite polynomials.

One can show that the polynomials $(p_k^M)_{k\in\mathbb{N}^n}$ exhibit similar properties than the standard Hermite polynomials. We can give explicit formulas for the generating function, a type of Rodrigues' formula and a three-term recursion that are closely related to our findings from Section 3.3. Moreover, we are able to generalise the Laguerre connection of the Hermite polynomials also to the polynomials $(p_k^M)_{k\in\mathbb{N}^n}$, this relation will become crucial when we calculate the Wigner transform of Hagedorn's wave packets in the next chapter.

5.1. Polynomials in one dimension

To get an intuition for the polynomials we quickly discuss the univariate case first. The one-dimensional polynomials $(p_k^\gamma)_{k\in\mathbb{N}}$ are generated via

$$p_k^\gamma = \hat{B}_k^\dagger p_0^\gamma(x), \quad \hat{B}^\dagger = 2x - \gamma\nabla_x$$

with $\gamma \in \mathbb{C}$. Starting from $p_0^\gamma(x) = 1$, we produce monomials for $\gamma = 0$, $p_k^0(x) = (2x)^k$ and Hermite polynomials for $\gamma = 1$, $p_k^1(x) = h_k(x)$. For general $\gamma \neq 0$ we create in this manner scaled Hermite polynomials, see [DKT16, §3.1].

We note that the case $\gamma = 0$ is a formal one: all matrices M we deduced in the previous chapter were invertible, so the case $\gamma = 0$ will not appear in the context of Hagedorn's wave packets. We point to monomials to retain a rigorous argument for all polynomials.

Lemma 5.1 — Hermite connection. Let $\gamma \in \mathbb{C}\backslash\{0\}$. Then, the polynomials $(p_k^\gamma)_{k\in\mathbb{N}}$ can be written as

$$p_k^\gamma(x) = \gamma^{k/2} h_k(\tfrac{x}{\sqrt{\gamma}}), \quad x \in \mathbb{R}.$$

Proof. The claim follows by a simple induction over k. We have $p_0^\gamma(x) = h_0(\frac{x}{\sqrt{\gamma}})$ for all $\gamma \neq 0$ and

$$\hat{B}^\dagger \left(\gamma^{k/2} h_k(\tfrac{x}{\sqrt{\gamma}})\right) = \gamma^{(k+1)/2} \left(\tfrac{2x}{\sqrt{\gamma}} h_k(\tfrac{x}{\sqrt{\gamma}}) - \nabla_{(x/\sqrt{\gamma})} h_k(\tfrac{x}{\sqrt{\gamma}})\right) = \gamma^{(k+1)/2} h_{k+1}(\tfrac{x}{\sqrt{\gamma}}).$$

■

Figure 10 displays polynomials of degree $k = 3$ for different values of γ to demonstrate that all polynomials p_3^γ can be obtained by a simple rescaling of h_3.

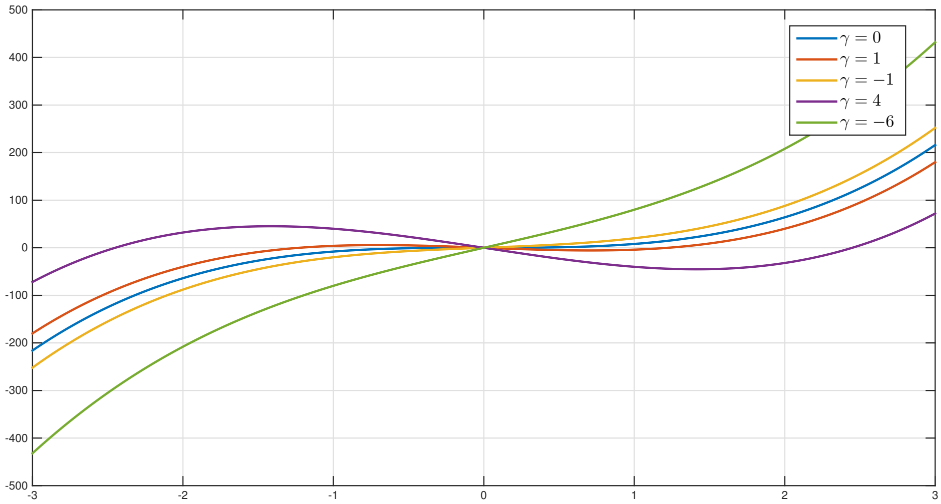

Figure 10.: Polynomials p_3^γ for $\gamma \in \{-6, -1, 0, 1, 4\}$.

We have to stress here that the square root of a complex number γ is not uniquely determined, we have to choose a branch. However, we only use this relation here to adopt the results made in Section 3.3 and will give rigorous proofs for our findings in the multi-dimensional case in the next section.

Corollary 5.1 Let $\gamma \in \mathbb{C}\backslash\{0\}$. The polynomials $(p_k^\gamma)_{k\in\mathbb{N}}$ satisfy the following three relations.

a, Three-term reccurence relation: It holds for all $k \geq 0$

$$p_{k+1}^\gamma(x) = 2x p_k^\gamma(x) - 2\gamma k p_{k-1}^\gamma(x), \quad x \in \mathbb{R},$$

with $p_0^\gamma = 1$ and $p_k^\gamma = 0$ for $k < 0$.

b, Generating function: We have

$$g_\gamma(x,t) = \sum_{k=0}^{\infty} \frac{t^k}{k!} p_k^\gamma(x) = e^{2xt - \gamma t^2}.$$

c, Rodrigues' formula: Let $k \geq 0$. Then,

$$p_k^\gamma(x) = e^{x^2/\gamma}(-\gamma\nabla_x)^k e^{-x^2/\gamma}, \quad x \in \mathbb{R}.$$

Equally, the determinant formula from Proposition 3.1 can be nicely generalised for the polynomials $(p_k^\gamma)_{k\in\mathbb{N}}$.

Corollary 5.2 — Determinant representation. Let $\gamma \in \mathbb{C}\backslash\{0\}$. Then,

$$p_k^\gamma(x) = (-1)^k \det \begin{pmatrix} 1 & x & x^2 & x^3 & x^4 & x^5 & \dots & x^k \\ 2 & 0 & S_1^1\gamma & 0 & \frac{1}{2}S_1^2\gamma^2 & 0 & & \vdots \\ 0 & 2 & 0 & S_2^1\gamma & 0 & \frac{1}{2}S_2^2\gamma^2 & \ddots & \\ \vdots & 0 & 2 & 0 & S_3^1\gamma & 0 & \ddots & 0 \\ & \vdots & 0 & 2 & 0 & S_4^1\gamma & \ddots & \frac{1}{2}S_{k-3}^2\gamma^2 \\ & & & 0 & 2 & 0 & \ddots & 0 \\ & & & \dots & 0 & 2 & \ddots & S_{k-1}^1\gamma \\ 0 & & & & \dots & 0 & 2 & 0 \end{pmatrix}.$$

5.2. Generating function and recurrence relation

In this section we investigate multi-dimensional polynomials $(p_k^M)_{k\in\mathbb{N}^n}$ generated via

$$\left(p_{k+e_j}^M(x)\right)_{j=1}^n = 2x\, p_k^M(x) - M\nabla_x p_k^M(x), \quad x \in \mathbb{R}^n \tag{5.1}$$

starting from $p_0^M(x) = 1$ and $p_k^M(x) = 0$ if $k \notin \mathbb{N}^n$. The recursion matrix M is an invertible, complex symmetric $n \times n$-matrix. In the standard setting of Hagedorn's wave packets M has beyond that another favourable property.

Lemma 5.2 Let $Z = (P; Q) \in \mathbb{C}^{2n\times n}$ be a normalised Lagrangian frame. Then, the matrix $M = Q^{-1}\overline{Q}$ is unitary.

Proof. We have

$$M^*M = Q^T(QQ^*)^{-1}\overline{Q} = \tfrac{1}{2\mathrm{i}}Q^T(PQ^{-1} - Q^{-*}P^*)\overline{Q} = \tfrac{1}{2\mathrm{i}}(P^T\overline{Q} - Q^T\overline{P}) = \mathrm{Id}$$

where we used $(QQ^*)^{-1} = \mathrm{Im}(PQ^{-1})$. ■

The polynomials $(p_k^M)_{k\in\mathbb{N}^n}$ could equivalently to (5.1) also be defined via their generating function or a three-term recurrence relation. We will derive both in this section using the same techniques as for the Hermite polynomials, see Section 3.3. In the polynomial analysis [DKT16], however, we started from the recurrence relation.

Lemma 5.3 — Rodrigues' formula. Let $k \in \mathbb{N}^n$ and $M \in \mathbb{C}^{n\times n}$ be symmetric and invertible. Then, the polynomials $(p_k^M)_{k\in\mathbb{N}^n}$ satisfy

$$p_k^M(x) = e^{x^TM^{-1}x}(-M\nabla_x)^k e^{-x^TM^{-1}x}, \quad x \in \mathbb{R}^n. \tag{5.2}$$

Proof. We calculate with Ansatz (5.2)

$$\begin{aligned}2x\,p_k^M(x) - M\nabla_x p_k^M(x)\\ &= 2x\,p_k^M(x) - M\left(2M^{-1}x\,p_k^M(x) + e^{x^TM^{-1}x}\nabla_x(-M\nabla_x)^k e^{-x^TM^{-1}x}\right)\\ &= e^{x^TM^{-1}x}(-M\nabla_x)^{k+1}e^{-x^TM^{-1}x}\end{aligned}$$

and thus (5.2) fulfils Recursion (5.1). ■

This identity was already shown several times for Hagedorn's wave packets with varying notations, see for example [LT14, Proposition 4], [Hag15, §4] or [DKT16, Eq. (12)]. In [Hag15] there was in addition the generating function of the polynomials determined, again evaluated at $y = \frac{1}{\sqrt{\varepsilon}}Q^{-1}x$ as noted in Theorem 4.2.

Proposition 5.1 — Generating function. Let $M \in \mathbb{C}^{n\times n}$ be symmetric and invertible. Then,

$$g(x,t) = \sum_{k\in\mathbb{N}^n} \frac{t^k}{k!}\, p_k^M(x) = e^{2x^Tt - t^TMt}$$

for all $x, t \in \mathbb{R}^n$.

Proof. We use a similar approach as for the Hermite polynomials in Theorem 3.2 and first expand the exponent,

$$2x^Tt - t^TMt = -(Mt-x)^TM^{-1}(Mt-x) + x^TM^{-1}x.$$

Thus,

$$\begin{aligned}\nabla_t e^{2x^Tt-t^TMt}\,|_{t=0} &= e^{x^TM^{-1}x}\nabla_t e^{-(Mt-x)^TM^{-1}(Mt-x)}\,|_{t=0} = e^{x^TM^{-1}x}(-M\nabla_{t'})e^{-t'^TM^{-1}t'}\,|_{t'=x}\\ &= e^{x^TM^{-1}x}(-M\nabla_x)e^{-x^TM^{-1}x}\end{aligned}$$

where we substituted $t' = -Mt + x$. An iterative argument and the Rodrigues formula (5.2) yield $\nabla_t^k e^{2x^Tt-t^TMt}\,|_{t=0} = p_k^M(x)$ and by expanding $e^{2x^Tt-t^TMt}$ around $t = 0$ we find

$$e^{2x^Tt-t^TMt} = \sum_{k\in\mathbb{N}^n}\frac{t^k}{k!}\left(\nabla_t e^{2x^Tt-t^TMt}\,|_{t=0}\right) = \sum_{k\in\mathbb{N}^n}\frac{t^k}{k!}\,p_k^M(x).$$

■

The generating function enables us to give also a formula for the gradient and the TTRR of the polynomials.

Corollary 5.3 — Appell sequence. We have

$$\nabla_x p_k^M(x) = 2\left(k_j p_{k-e_j}^M(x)\right)_{j=1}^n, \quad x \in \mathbb{R}^n,$$

for all symmetric and invertible $M \in \mathbb{C}^{n\times n}$ and $k \in \mathbb{N}^n$.

Proof. Let $j \in \{1,\dots,n\}$. Then,

$$\begin{aligned}\sum_{k\in\mathbb{N}^n} \frac{t^k}{k!}\partial_{x_j} p_k^M(x) = \partial_{x_j} e^{2x^Tt-t^TMt} &= 2t_j e^{2x^Tt-t^TMt} = 2\sum_{k\in\mathbb{N}^n}\frac{t^{k+e_j}}{k!}\,p_k^M(x)\\ &= 2\sum_{k\in\mathbb{N}^n, k_j\neq 0}\frac{t^k}{(k-e_j)!}\,p_{k-e_j}^M(x)\end{aligned}$$

and comparing the coefficients of t^k shows $\partial_{x_j} p_k^M(x) = 2k_j p_{k-e_j}^M(x)$ if $k_j > 0$. For $k_j = 0$ we find by definition $\partial_{x_j} p_k^M(x) = 0$. ■

So, we can interpret the gradient as a lowering operator of the polynomials, and moreover, find that the polynomials are eigenfunctions of the symmetric operator

$$\tfrac{1}{2}\left((\hat{B}^\dagger)^T\nabla_x + (\nabla_x)^T\hat{B}^\dagger\right).$$

In particular, we have

$$\begin{aligned}\tfrac{1}{2}\left((\hat{B}^\dagger)^T\nabla_x + (\nabla_x)^T\hat{B}^\dagger\right)p_k^M(x) &= (\hat{B}^\dagger)^T\left(k_j p_{k-e_j}^M(x)\right)_{j=1}^n + \tfrac{1}{2}(\nabla_x)^T\left(p_{k+e_j}^M(x)\right)_{j=1}^n\\ &= \sum_{j=1}^n k_j p_k^M(x) + (k_j+1)p_k^M(x) = (2|k|+n)p_k^M(x).\end{aligned}$$

The formula for the gradient also directly implies a recurrence relation for the polynomials.

Corollary 5.4 — Three-term recurrence relation. Let $M \in \mathbb{C}^{n\times n}$ be symmetric and invertible. The polynomials $(p_k^M)_{k\in\mathbb{N}^n}$ satisfy

$$\left(p_{k+e_j}^M(x)\right)_{j=1}^n = 2x\,p_k^M(x) - 2M\left(k_j p_{k-e_j}^M(x)\right)_{j=1}^n, \quad x \in \mathbb{R}^n,$$

with $p_0^M(x) = 1$ and $p_k^M(x) = 0$ for $k \notin \mathbb{N}^n$.

This TTRR of the polynomials furthermore suggests a recursion relation for Hagedorn's wave packets. With $y = \frac{1}{\sqrt{\varepsilon}}Q^{-1}x$ we find

$$\begin{aligned}\left(\sqrt{k_j+1}\varphi_{k+e_j}(Z;x)\right)_{j=1}^n &= \tfrac{1}{\sqrt{2^{|k|+1}k!}}\left(p_{k+e_j}^M(y)\right)_{j=1}^n\varphi_0(Z;x)\\ &= \tfrac{1}{\sqrt{2^{|k|-1}k!}}\left(y\,p_k^M(y) - M(k_j p_{k-e_j}^M(y))_{j=1}^n\right)\varphi_0(Z;x)\\ &= \sqrt{\tfrac{2}{\varepsilon}}Q^{-1}x\,\varphi_k(Z;x) - M(\sqrt{k_j}\varphi_{k-e_j}(Z;x))_{j=1}^n\end{aligned}$$

for any normalised Lagrangian frame $Z = (P;Q) \in \mathbb{C}^{2n\times n}$ and $k \in \mathbb{N}^n$. So, we have restated the three-term recursion

$$Q\left(\sqrt{k_j+1}\varphi_{k+e_j}(Z;x)\right)_{j=1}^{n} = \sqrt{\tfrac{2}{\varepsilon}}x\,\varphi_k(Z;x) - \overline{Q}\left(\sqrt{k_j}\varphi_{k-e_j}(Z;x)\right)_{j=1}^{n}$$

given in [Lub08, §V.2].

5.3. Laguerre connection

When we calculated the Wigner transform of two Hermite functions in Section 3.4, we discovered Laguerre polynomials. This is only one of various connections between Hermite and Laguerre polynomials, see for example [Sze39, §5.6]. We can add a new point here in terms of the polynomials $(p_k^M)_{k\in\mathbb{N}^n}$.

From its form it is clear that the generating function only factorises into m lower-dimensional generating functions if we can rewrite M as a block-diagonal matrix with m blocks, see [DKT16, §3.2]. Therefore, our aim here is to express p_k^M, $k \in \mathbb{N}^n$, as a linear combination of tensor products by deleting off-diagonal entries of M. More precisely, we denote by M' the matrix that remains if we delete the entries $M_{l,m}$ and $M_{m,l}$ of M, i.e.

$$M'_{i,j} = \begin{cases} 0 & \text{if } \{i,j\} = \{l,m\} \\ M_{i,j} & \text{else} \end{cases}.$$

Then, we can express the raising operator $\hat{B}^\dagger$ of the polynomials p_k^M via the raising operator $\hat{B}'^\dagger$ of the polynomials $p_k^{M'}$.

Proposition 5.2 — Laguerre connection. Let $M \in \mathbb{C}^{n\times n}$ be symmetric and invertible. We denote by M' the matrix with deleted entries $M_{l,m} = M_{m,l} = \lambda \in \mathbb{C}$ for $l \neq m$ and by $\hat{B}'^\dagger$ the corresponding polynomial raising operator. Then,

$$\hat{B}_k^\dagger = \hat{B}'^\dagger_{k-k_m(e_l+e_m)}(-2\lambda)^{k_m} k_m! L_{k_m}^{(k_l-k_m)}\left(\tfrac{1}{2\lambda}\hat{b}'^\dagger_l \hat{b}'^\dagger_m\right)$$

if $k_l \geq k_m$ and analogously for $k_m > k_l$. The operator $\hat{b}'^\dagger_l$ thereby denotes the l-th component of $\hat{B}'^\dagger$.

Proof. We can relate the generating functions of p_k^M and $p_k^{M'}$ by

$$e^{2x^Tt-t^TMt} = e^{2x^Tt-t^TM't}e^{-2\lambda t_l t_m} = \left(\sum_{k\in\mathbb{N}^n}\frac{t^k}{k!}\hat{B}'^\dagger_k 1\right)\cdot\left(1 - 2\lambda t_l t_m + \frac{1}{2!}(2\lambda t_l t_m)^2 - \dots\right).$$

Expanding and sorting with respect to the exponent of t then leads to

$$e^{2x^Tt-t^TMt} = \sum_{k\in\mathbb{N}^n}\frac{t^k}{k(l,m)!}\hat{B}'^\dagger_{k(l,m)}\sum_{j=0}^{\min(k_l,k_m)}\frac{(-2\lambda)^j}{j!}\cdot\frac{(\hat{b}'^\dagger_l)^{k_l-j}}{(k_l-j)!}\cdot\frac{(\hat{b}'^\dagger_m)^{k_m-j}}{(k_m-j)!}$$

where $k(l,m) = k - k_l e_l - k_m e_m$. Thus, if we compare the coefficients of t^k we find

$$\hat{B}_k^\dagger = \hat{B}'^\dagger_{k(l,m)} \sum_{j=0}^{\min(k_l,k_m)} \frac{k_l!k_m!(-2\lambda)^j}{j!(k_l-j)!(k_m-j)!} (\hat{b}'^\dagger_l)^{k_l-j} (\hat{b}'^\dagger_m)^{k_m-j}$$

Sums of this type can with a standard procedure be transfered into Laguerre polynomials, see [Fol09, Theorem 1.105]. Let $k_l \geq k_m$. We reorder the sum by means of the index $i = k_m - j$,

$$\begin{aligned}\hat{B}_k^\dagger &= \hat{B}'^\dagger_{k(l,m)}(-2\lambda)^{k_m} k_m!(\hat{b}'^\dagger_l)^{k_l-k_m} \sum_{i=0}^{k_m} \frac{k_l!}{(k_m-i)!(k_l-k_m+i)!i!} \left(-\tfrac{1}{2\lambda}\hat{b}'^\dagger_l \hat{b}'^\dagger_m\right)^i \\ &= \hat{B}'^\dagger_{k-k_m(e_l+e_m)}(-2\lambda)^{k_m} k_m! L_{k_m}^{(k_l-k_m)}(\tfrac{1}{2\lambda}\hat{b}'^\dagger_l \hat{b}'^\dagger_m)\end{aligned}$$

where we utilised that $\hat{b}'^\dagger_l$ and $\hat{b}'^\dagger_m$ commute. ■

The conclusion of the previous proposition can be nicely illustrated in the two-dimensional case. Let

$$M = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{12} & \lambda_{22} \end{pmatrix} \in \mathbb{C}^{2\times 2}$$

be invertible and denote by

$$\hat{b}_j^\dagger = 2x_j - \lambda_{jj}\partial_{x_j}, \quad j = 1,2$$

the raising operator of the Hermite polynomials scaled by λ_{11} resp. λ_{22} that we discussed in the previous section.

Corollary 5.5 — Two-dimensional polynomials. Let $k \in \mathbb{N}^2$ with $k_1 \geq k_2$. Then,

$$\hat{B}_k^\dagger = \begin{cases} (-2\lambda_{12})^{k_2} k_2!(\hat{b}_1^\dagger)^{k_1-k_2} L_{k_2}^{(k_1-k_2)}(\frac{1}{2\lambda_{12}}\hat{b}_1^\dagger \hat{b}_2^\dagger) & \lambda_{12} \neq 0 \\ (\hat{b}_1^\dagger)^{k_1}(\hat{b}_2^\dagger)^{k_2} & \lambda_{12} = 0 \end{cases} \tag{5.3}$$

and the case $k_1 < k_2$ works analogously.

For the case $\lambda_{12} = 0$, this equality directly carries out the factorisation of p_k^M in scaled Hermite functions,

$$p_k^M(x) = p_{k_1}^{\lambda_{11}}(x_1) p_{k_2}^{\lambda_{22}}(x_2) = \sqrt{\lambda_{11}^{k_1}\lambda_{22}^{k_2}} \cdot h_{k_1}(\tfrac{x_1}{\sqrt{\lambda_{11}}}) h_{k_2}(\tfrac{x_2}{\sqrt{\lambda_{22}}}), \quad x \in \mathbb{R}^2.$$

In the case $\lambda_{12} \neq 0$, (5.3) guarantees that p_k^M is a linear combination of at most $\min(k_1,k_2)$ many tensor products of the form

$$(\hat{b}_1^\dagger)^l (\hat{b}_2^\dagger)^m 1 = p_l^{\lambda_{11}}(x_1) p_m^{\lambda_{22}}(x_2)$$

where $l - m = k_1 - k_2$ and $k_1 - k_2 \leq l$, $m \leq k_2$. Moreover, if $\lambda_{11} = \lambda_{22} = 0$, the creation operators $\hat{b}_1^\dagger$ and $\hat{b}_2^\dagger$ produce monomials and we obtain the formula

$$p_k^M(x) = (-2\lambda_3)^{k_2} k_2!(2x_1)^{k_1-k_2} L_{k_2}^{(k_1-k_2)}(\tfrac{2}{\lambda_{12}} x_1 x_2), \quad x \in \mathbb{R}^2,$$

whenever $\lambda_{12} \neq 0$ and $k_1 \geq k_2$. These two special cases can be generalised to arbitrary dimensions.

Corollary 5.6 Let $k \in \mathbb{N}^n$. If $M = \mathrm{Id}$, the polynomials p_k^M are tensor products of one-dimensional Hermite polynomials,

$$p_k^M(x) = \prod_{j=1}^{n} h_{k_j}(x_j), \quad x \in \mathbb{R}^n.$$

Furthermore, if the dimension is even, $n = 2m$, and M of the form

$$M = \begin{pmatrix} 0 & \mathrm{Id}_m \\ \mathrm{Id}_m & 0 \end{pmatrix},$$

the polynomials p_k^M can be written as a tensor product of monomials and Laguerre polynomials, $p_k^M(x) = \prod_{j=1}^{m} \mathcal{L}_{(k_j,k_{j+m})}(x_j, x_{j+m})$ with

$$\mathcal{L}_{(k_j,k_l)}(x_j, x_l) = \begin{cases} (-1)^{k_l} k_l! 2^{k_j} x_j^{k_j-k_l} L_{k_l}^{(k_j-k_l)}(2x_j x_l) & k_j \geq k_l \\ (-1)^{k_j} k_j! 2^{k_l} x_l^{k_l-k_j} L_{k_j}^{(k_l-k_j)}(2x_j x_l) & k_j < k_l \end{cases}.$$

As examples we consider the unitary, symmetric matrices

$$M_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad M_3 = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

as well as the non-unitary matrix

$$M_4 = \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}.$$

The first three matrices are obtained by the Lagrangian frames defined in (4.8) and (4.9), i.e. $M_j = Q_j^{-1}\overline{Q}_j$ where $Z_j = (P_j; Q_j)$ for $j = 1, 2, 3$. The matrix M_4 depicts a more general case that will not arise as part of Hagedorn's wave packets. For a clear illustration, we restrict ourselves here to real matrices.

Figure 11 points out the results of Corollary 5.6: the polynomial $p_{(4,6)}^{M_1}$ factorises in Hermite polynomials, its roots form a grid whose distances equal the roots of the Hermite polynomials. The polynomial $p_{(5,6)}^{M_2}$ is zero evaluated at the x_2-axis since $k_2 > k_1$ and the remaining roots form $\min(k_1, k_2)$-many hyperbolas whose distances are proportional to the roots of the Laguerre polynomials.

Figure 12 illustrates that also in the two-dimensional case the polynomials can attain suprising forms, although $p_{(5,8)}^{M_3}$ and $p_{(8,5)}^{M_4}$ can both be written as a linear combination of only 5 tensor products.

In the setting of Hagedorn's wave packets the polynomials are then evaluated on the rotated grid $Q^{-1}\mathbb{R}^n \subset \mathbb{C}^n$. A real-valued matrix $Q \in \mathbb{R}^{n \times n}$ thereby always corresponds to the matrix $M_1 = \mathrm{Id}_2$ and thus, the only real-valued polynomials one can detect in Hagedorn's wave packets are rescaled or sheared multi-dimensional Hermite polyno-

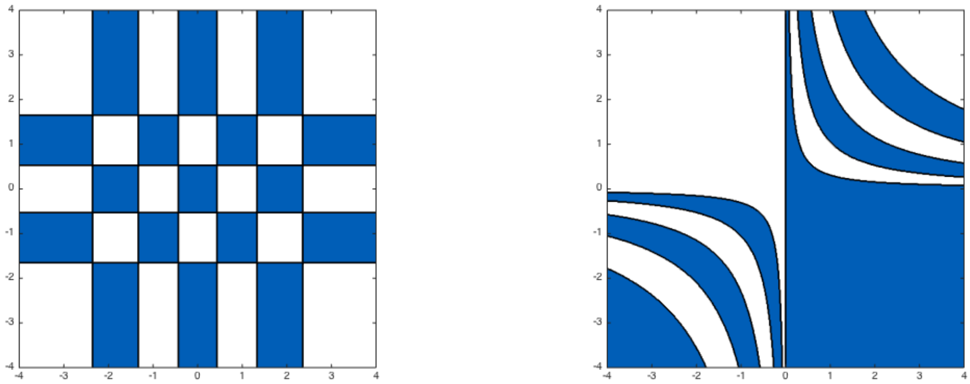

Figure 11.: Plots of the roots of the polynomials $p^{M_1}_{(4,6)}$ (left) and $p^{M_2}_{(5,6)}$ (right), blue regions mark negative values, white regions positive values of the polynomials

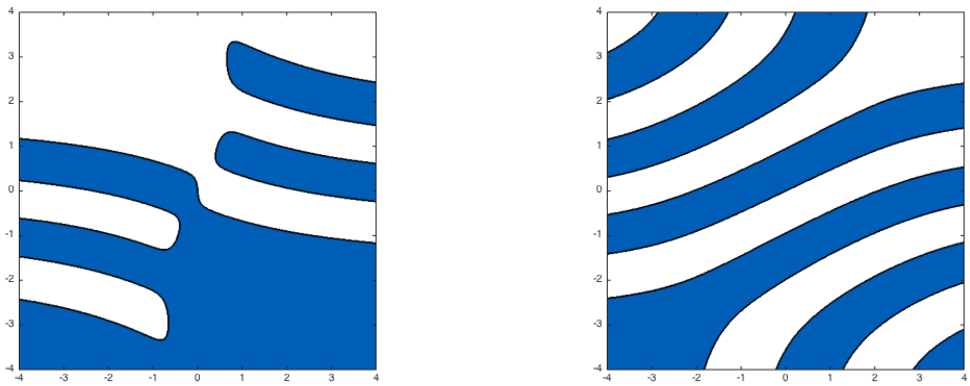

Figure 12.: Plots of the roots of the polynomials $p^{M_3}_{(5,8)}$ (left) and $p^{M_4}_{(8,5)}$ (right), blue regions mark negative values, white regions positive values of the polynomials

mials. All other polynomials will provide complex values. In particular, the complex rotation also explains the circular structure showed in the right picture of Figure 7: Let $Z = (P; Q)$ be a normalised Lagrangian frame and assume that $Q^{-1}\overline{Q} = M_2$. This implies that Q is of the form

$$Q = \begin{pmatrix} a & \overline{a} \\ b & \overline{b} \end{pmatrix}$$

for $a, b \in \mathbb{C}$ with $\mathrm{Im}(a\bar{b}) \neq 0$. From Corollary 5.6 we see that the roots of the rotated polynomial $p^{M_2}_{(4,6)}(Q^{-1}x)$ either form a straight line induced by the monomial factor, or satisfy

$$2(Q^{-1}x)_1(Q^{-1}x)_2 = \frac{1}{2\mathrm{Im}(a\bar{b})^2}(\bar{b}x_1 - \bar{a}x_2)(bx_1 - ax_2) = \eta_j,$$

where η_j, $j = 1, ..., 4$, are the roots of the associated Laguerre polynomial $L^{(2)}_4$. Since the η_j are real, positive and pairwise distinct,

$$\frac{1}{2\mathrm{Im}(a\bar{b})^2}(|b|^2 x_1 + |a|^2 x_2 - 2\mathrm{Re}(a\bar{b})x_1 x_2) = \eta_j$$

produces 4 distinct ellipses. Those are the four dark blue circles in Figure 7 surrounding the origin.

6. Wave packets in phase space

After introducing and studying the properties of Hagedorn's wave packets, our next aim is to deduce the ε-scaled Wigner transform,

$$\mathcal{W}^\varepsilon(\varphi,\psi)(\xi,x) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^n} \overline{\varphi}(x+\tfrac{y}{2})\psi(x-\tfrac{y}{2})e^{\frac{i}{\varepsilon}y^T\xi}\,dy, \quad (\xi,x)\in\mathbb{R}^n\oplus\mathbb{R}^n, \tag{6.1}$$

for $\varphi,\psi\in\mathcal{S}(\mathbb{R}^n)$, of two Hagedorn wave packets. The Wigner function was introduced in 1932 by Wigner, see [Wig32], as a simultaneous probability function for position and momentum. Although $\mathcal{W}^\varepsilon(\varphi,\psi)$ attains negative values if φ and ψ are not simple Gaussian functions, see [Hud74, Theorem 4], the Wigner transform is very valuable as we receive the position and momentum densities of a state as marginal distributions, see Lemma 3.7, and are able to calculate expectation values of operators $\mathrm{op}_\varepsilon[a]$ via

$$\langle\varphi,\hat{a}\psi\rangle = \int_{R^{2n}} \mathcal{W}(\varphi,\psi)(z)a(z)\,d(z), \quad z=(\xi,x)\in\mathbb{R}^n\oplus\mathbb{R}^n.$$

For the Hermite functions we found that the Wigner function can be expressed in terms of Laguerre polynomials and exhibit a circular structure, see Section 3.4. We will show that the same holds true for Hagedorn's wave packets if both wave packets can be parametrised by the same Lagrangian frame. In general, the Wigner transform can be equivalently constructed as Hagedorn's wave packets on position space and we thus obtain wave packets on phase space. This is the main result of this chapter as it allows us to transfer all our previous results directly to phase space, no further investigation is needed. Additionally, we will also determine the FBI transform and, implicitly, the Husimi function of the wave packets, though the findings here are less intuitive than for the Hermite functions.

6.1. Ladders in phase space

We begin with the lift of the ladder operators to phase space. Our goal is to describe the action of the ladder operators of Hagedorn's wave packets as operators that act directly on the Wigner function, i.e.

$$\mathcal{W}^\varepsilon(\hat{A}(Z)\varphi,\psi) = \hat{\mathcal{A}}_1(Z)\mathcal{W}^\varepsilon(\varphi,\psi) \quad \text{resp.} \quad \mathcal{W}^\varepsilon(\varphi,\hat{A}(Z)\psi) = \hat{\mathcal{A}}_2(Z)\mathcal{W}^\varepsilon(\varphi,\psi),$$

for all $\varphi,\psi\in\mathcal{S}(\mathbb{R}^n)$ and analogously for $\hat{A}^\dagger(Z)$. With this, we can describe the Wigner transform of the two Hagedorn wave packets as eigenfunction of the corresponding phase space operator.

Lemma 6.1 Let $l \in \mathbb{C}^n \oplus \mathbb{C}^n$. Then, for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$,

$$\mathcal{W}^\varepsilon(\hat{A}(l)\varphi, \psi)(z) = \tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^*(\Omega z - \tfrac{1}{2}D_z)\mathcal{W}^\varepsilon(\varphi, \psi)(z),$$
$$\mathcal{W}^\varepsilon(\varphi, \hat{A}(l)\psi)(z) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T(\Omega z + \tfrac{1}{2}D_z)\mathcal{W}^\varepsilon(\varphi, \psi)(z),$$

where $z \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $D_z = -\mathrm{i}\varepsilon\nabla_z$ acts on $\mathbb{R}^{2n}$.

Proof. Let $w \in \mathcal{S}(\mathbb{R}^{2n})$. With Lemma 3.7 c, and the Moyal product from Appendix A,

$$\begin{aligned}\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\hat{A}(l)\varphi, \psi)(z)w(z)\,dz &= \langle \hat{A}(l)\varphi, \hat{w}\psi\rangle = \langle \varphi, \hat{A}^\dagger(l)\hat{w}\psi\rangle \\ &= \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi, \psi)(z)(A^\dagger(l)\#w)(z)\,dz\end{aligned}$$

and analogously

$$\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi, \hat{A}(l)\psi)(z)w(z)\,dz = \langle \varphi, \hat{w}\hat{A}(l)\psi\rangle = \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi, \psi)(z)(w\#A(l))(z)\,dz.$$

Since $A(l)$ and $A^\dagger(l)$ are linear functions in z, we can use the expansion formulas $A^\dagger(l)\#w = w \cdot A^\dagger(l) + \frac{\mathrm{i}\varepsilon}{2}\nabla A^\dagger(l)^T\Omega\nabla w$ resp. $w\#A(l) = w \cdot A(l) + \frac{\mathrm{i}\varepsilon}{2}\nabla w^T\Omega\nabla A(l)$ and obtain

$$(A^\dagger(l)\#w)(z) = -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\left(l^*\Omega z \cdot w(z) - \tfrac{\mathrm{i}\varepsilon}{2} l^*\nabla_z w(z)\right) = -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^*\left(\Omega z + \tfrac{1}{2}D_z\right)w(z)$$

and

$$(w\#A(l))(z) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\left(l^T\Omega z \cdot w(z) + \tfrac{\mathrm{i}\varepsilon}{2} l^T\nabla_z w(z)\right) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T\left(\Omega z - \tfrac{1}{2}D_z\right)w(z).$$

By partial integration,

$$\begin{aligned}\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\hat{A}(l)\varphi, \psi)(z)w(z)\,dz &= -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi, \psi)(z)l^*\left(\Omega z + \tfrac{1}{2}D_z\right)w(z)\,dz \\ &= -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\int_{\mathbb{R}^{2n}} l^*\left(\Omega z - \tfrac{1}{2}D_z\right)\mathcal{W}^\varepsilon(\varphi, \psi)(z)w(z)\,dz\end{aligned}$$

and

$$\begin{aligned}\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi, \hat{A}(l)\psi)(z)w(z)\,dz &= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi, \psi)(z)l^T\left(\Omega z - \tfrac{1}{2}D_z\right)w(z)\,dz \\ &= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\int_{\mathbb{R}^{2n}} l^T\left(\Omega z + \tfrac{1}{2}D_z\right)\mathcal{W}^\varepsilon(\varphi, \psi)(z)w(z)\,dz.\end{aligned}$$

Since w was an arbitrary Schwartz function, this proves the claim. ■

If we view the vector-valued operator $\hat{v} = (-\mathrm{i}\varepsilon\nabla_z, z)$ as the phase space analog of $\hat{z} = (\hat{p}, \hat{q})$, i.e. as the Weyl-quantisation of a doubled phase space variable $v = (\zeta, z) \in$

$\mathbb{R}^{2n} \oplus \mathbb{R}^{2n}$, we can rewrite the ladder operators of the previous lemma as

$$\tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^*(\Omega z - \tfrac{1}{2}D_z) = \tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} \begin{pmatrix} -\Omega \bar{l} \\ \frac{1}{2}\bar{l} \end{pmatrix}^T \Omega_{2n} \hat{v}, \qquad \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T(\Omega z + \tfrac{1}{2}D_z) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} \begin{pmatrix} \Omega l \\ \frac{1}{2} l \end{pmatrix}^T \Omega_{2n} \hat{v}, \quad (6.2)$$

where $\Omega_{2n} \in \mathbb{R}^{4n\times 4n}$ denotes the standard skew-symmetric matrix (2.4) of doubled dimension. Since we are interested in Wigner functions of the type $\mathcal{W}^\varepsilon(\varphi_k(Z_1), \varphi_m(Z_2))$, we need to create a phase space operator that acts on the first n components of $\mathcal{W}^\varepsilon$ as $\hat{A}(Z_1)$ and on the second n components as $\hat{A}(Z_2)$.

Definition 6.1 — Phase space frame. For two normalised Lagrangian frames $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ we set

$$\mathcal{Z} = \begin{pmatrix} -\Omega \overline{Z}_1 & \Omega Z_2 \\ \frac{1}{2}\overline{Z}_1 & \frac{1}{2} Z_2 \end{pmatrix} \in \mathbb{C}^{4n\times 2n}$$

and call $\mathcal{Z}$ the *phase space frame* of Z_1 and Z_2.

One can easily verify that $\mathcal{Z}$ is isotropic if and only if Z_1 and Z_2 are isotropic, since

$$\mathcal{Z}^T \Omega_{2n} \mathcal{Z} = \begin{pmatrix} Z_1^* \Omega \overline{Z}_1 & 0 \\ 0 & Z_2^T \Omega Z_2 \end{pmatrix}$$

and with

$$\mathcal{Z}^* \Omega_{2n} \mathcal{Z} = \begin{pmatrix} -Z_1^T \Omega \overline{Z}_1 & 0 \\ 0 & Z_2^* \Omega Z_2 \end{pmatrix}$$

normalised if and only if Z_1 and Z_2 are normalised. So, if $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ are two normalised Lagrangian frames, the phase space frame $\mathcal{Z}$ denotes a normalised Lagrangian frame of doubled dimension and

$$\mathcal{L} := \mathrm{range}(\mathcal{Z}) \subset \mathbb{C}^{4n}$$

is a positive Lagrangian subspace. We can characterise this Lagrangian $\mathcal{L}$ by means of its symplectic metric.

Lemma 6.2 — Phase space metric. Let $L_1, L_2 \subset \mathbb{C}^{2n}$ be two positive Lagrangian subspaces with symplectic metrics G_1 resp. G_2. Let further $Z_1 \in F_n(L_1)$, $Z_2 \in F_n(L_2)$ and $\mathcal{Z}$ denote the corresponding phase space frame. Then, the symplectic metric of $\mathcal{L} = \mathrm{range}(\mathcal{Z})$ is of the form

$$\mathcal{G} = \begin{pmatrix} \frac{1}{4}(G_1^{-1} + G_2^{-1}) & \frac{1}{2}\Omega(G_2 - G_1) \\ \frac{1}{2}(G_1 - G_2)\Omega & G_1 + G_2 \end{pmatrix} \in \mathrm{Sp}(2n, \mathbb{R}).$$

In the special case $L_1 = L_2$ this simplifies to $\mathcal{G} = \begin{pmatrix} \frac{1}{2}G^{-1} & 0 \\ 0 & 2G \end{pmatrix}$, where $G = G_1 = G_2$.

Proof. We have by definition $\mathcal{G} = \Omega_{2n}^T(\mathcal{Z}\mathcal{Z}^* + \mathrm{i}\Omega_{2n})\Omega_{2n}$. The Hermitian square of $\mathcal{Z}$ can be directly computed,

$$\mathcal{Z}\mathcal{Z}^* = \begin{pmatrix} \Omega^T(\overline{Z}_1 Z_1^T + Z_2 Z_2^*)\Omega & \frac{1}{2}\Omega(-\overline{Z}_1 Z_1^T + Z_2 Z_2^*) \\ \frac{1}{2}(\overline{Z}_1 Z_1^T - Z_2 Z_2^*)\Omega & \frac{1}{4}(\overline{Z}_1 Z_1^T + Z_2 Z_2^*) \end{pmatrix}$$

and since $G_1^{-1} = \overline{Z}_1 Z_1^T - \mathrm{i}\Omega$ and $G_2^{-1} = Z_2 Z_2^* + \mathrm{i}\Omega$,

$$\mathcal{Z}\mathcal{Z}^* + \mathrm{i}\Omega_{2n} = \begin{pmatrix} G_1 + G_2 & \frac{1}{2}\Omega(G_2^{-1} - G_1^{-1}) \\ \frac{1}{2}(G_1^{-1} - G_2^{-1})\Omega & \frac{1}{4}(G_1^{-1} + G_2^{-1}) \end{pmatrix}.$$

The claim follows since $G^{-1}\Omega = \Omega G$ holds for any symmetric matrix $G \in \mathrm{Sp}(n, \mathbb{R})$. ■

The definition of the phase space frame $\mathcal{Z}$ was a direct consequence of the form of the phase space ladders. This suffices for the construction of the wave packets in phase space, but we can also verify our phase space lift with a more general argumentation. Let

$$\rho_\pm : \mathbb{C}^{2n} \mapsto \mathbb{C}^{4n}, \quad z \to U_\pm z := \begin{pmatrix} \pm\Omega z \\ \frac{1}{2} z \end{pmatrix},$$

i.e. we can write the ladder operators on phase space in (6.2) as $\hat{A}(\rho_-(\bar{l}))$ and $\hat{A}(\rho_+(l))$. These operators exhibit the same structure as the operators for Hagedorn's wave packets from Section 4.1, but act on $\mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$.

Proposition 6.1 — Double dimension. For all $l, l' \in \mathbb{C}^n \oplus \mathbb{C}^n$ we have

$$\rho_\pm(l)^T \Omega_{2n} \rho_\pm(l') = \pm l^T \Omega l' \quad \text{and} \quad \rho_\pm(l)^T \Omega_{2n} \rho_\mp(l') = 0.$$

This implies that if $L_1, L_2 \subset \mathbb{C}^{2n}$ are positive Lagrangian subspaces, then

$$\mathcal{L} := \rho_-(\overline{L}_1) \oplus \rho_+(L_2) \subset \mathbb{C}^{4n}$$

is a positive Lagrangian subspace. Moreover, if $Z_1 \in F_n(L_1)$ and $Z_2 \in F_n(L_2)$, then $\mathcal{L} = \mathrm{range}(\mathcal{Z})$.

Proof. We compute for all $l, l' \in \mathbb{C}^n \oplus \mathbb{C}^n$,

$$\rho_\pm(l)^T \Omega_{2n} \rho_\pm(l') = \begin{pmatrix} \mp l^T \Omega & \frac{1}{2} l^T \end{pmatrix} \begin{pmatrix} -\frac{1}{2} l' \\ \pm\Omega l' \end{pmatrix} = \pm l^T \Omega l'$$

and

$$\rho_\pm(l)^T \Omega_{2n} \rho_\mp(l') = \begin{pmatrix} \mp l^T \Omega & \frac{1}{2} l^T \end{pmatrix} \begin{pmatrix} -\frac{1}{2} l' \\ \mp\Omega l' \end{pmatrix} = 0.$$

Since $\overline{L}_1$ is a negative Lagrangian while L_2 is positive, we have $\overline{L}_1 \cap L_2 = \{0\}$ and thus $\dim(\mathcal{L}) = 2n$. The isotropy of $\mathcal{L}$ follows from the above equations,

$$\rho_-(\bar{l}_1)^T \Omega_{2n} \rho_-(\bar{l}_1') = 0, \quad \rho_+(l_2)^T \Omega_{2n} \rho_+(l_2') = 0, \quad \rho_-(\bar{l}_1)^T \Omega_{2n} \rho_+(l_2') = 0$$

for all $\bar{l}_1, \bar{l}_1' \in \overline{L}_1$ and $l_2, l_2' \in L_2$ since $\overline{L}_1$ and L_2 are isotropic. Furthermore, if L_1 and

L_2 are positive Lagrangians, then there exist normalised Lagrangian frames Z_1 and Z_2 spanning L_1 and L_2 and by definition

$$\mathrm{range}(\mathcal{Z}) = \{\mathcal{Z}w\,;\, w \in \mathbb{C}^{2n}\} = \{\rho_-(\bar{l}_1) + \rho_+(l_2)\,;\, \bar{l}_1 \in \overline{L}_1, l_2 \in L_2\} = \mathcal{L}.$$

Hence, $\mathcal{L}$ is positive if $\mathcal{Z}$ is normalised, but due to our previous considerations this is equivalent to Z_1 and Z_2 being normalised, i.e. the positivity of L_1 and L_2. ■

Thus, the maps ρ_+ and ρ_- describe a well-defined representation in double phase space. In the literature, see for example [SA16, §2], the standard phase space lift is performed via

$$\tilde{\Omega}_{2n} = \begin{pmatrix} -\Omega & 0 \\ 0 & \Omega \end{pmatrix}.$$

This means for $v = (\zeta, z)$ and $v' = (\zeta', z')$ in $\mathbb{C}^{2n} \oplus \mathbb{C}^{2n}$, we define the symplectic form on double phase space as

$$\tilde{\omega}_2(v, v') = v^T \tilde{\Omega}_{2n} v' = \omega(z, z') - \omega(\zeta, \zeta').$$

This definition is indeed consistent with our lift obtained from the phase space ladders: We first lift the variables via ρ_+ and ρ_- to doubled dimension and then use the standard symplectic form $\omega(v, v') = v^T \Omega_{2n} v'$ for all $v, v' \in \mathbb{C}^{2n} \oplus \mathbb{C}^{2n}$, but

$$\begin{pmatrix} U_- & U_+ \end{pmatrix}^T \Omega_{2n} \begin{pmatrix} U_- & U_+ \end{pmatrix} = \begin{pmatrix} \Omega & \frac{1}{2}\mathrm{Id} \\ -\Omega & \frac{1}{2}\mathrm{Id} \end{pmatrix} \begin{pmatrix} -\frac{1}{2}\mathrm{Id} & -\frac{1}{2}\mathrm{Id} \\ -\Omega & \Omega \end{pmatrix} = \begin{pmatrix} -\Omega & 0 \\ 0 & \Omega \end{pmatrix}.$$

6.2. Coherent and excited states in phase space

With the phase space ladder operators

$$\hat{A}(\mathcal{Z}) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} \mathcal{Z}^T \Omega_{2n} \hat{v} \quad \text{and} \quad \hat{A}^\dagger(\mathcal{Z}) = -\hat{A}(\overline{\mathcal{Z}}) = \tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} \mathcal{Z}^* \Omega_{2n} \hat{v}$$

we are now able to deduce the Wigner transform of two Hagedorn wave packets. Since the ladder operators on phase space possess the same structure than the ladder operators on position space it is already obvious that the Wigner transform will become a wave packet on phase space. To minimise confusion we denote wave packets on position space with small letters, $\varphi : \mathbb{R}^n \mapsto \mathbb{C}$, and wave packets on phase space with capitals, $\Phi : \mathbb{R}^n \oplus \mathbb{R}^n \mapsto \mathbb{C}$, in the following.

Let $L_1, L_2 \subset \mathbb{C}^{2n}$ be two positive Lagrangian subspaces and $Z_1 \in F_n(L_1)$, $Z_2 \in F_n(L_2)$. We start with the coherent state $\mathcal{W}_0(\mathcal{Z}) := \mathcal{W}^\varepsilon(\varphi_0(Z_1), \varphi_0(Z_2))$ and first note that

$$\hat{A}(\mathcal{Z})\mathcal{W}^\varepsilon(\varphi_0(Z_1), \varphi_0(Z_2)) = \mathcal{W}^\varepsilon(\hat{A}(Z_1)\varphi_0(Z_1), \hat{A}(Z_2)\varphi_0(Z_2)) = 0.$$

Thus, $\mathcal{W}_0(\mathcal{Z})$ appears as the eigenfunction of $\hat{A}(\mathcal{Z})$ with eigenvalue 0 and has norm $(2\pi\varepsilon)^{-n/2}$ due to Lemma 3.7.

Proposition 6.2 — Coherent states. Let $I(\mathcal{L}) = \{\Psi \in \mathcal{D}'(\mathbb{R}^n \oplus \mathbb{R}^n)\,;\, \hat{A}(\mathcal{Z})\Psi = 0\}$. Then, every element in $I(\mathcal{L})$ is a constant multiple of

$$\mathcal{W}_0(\mathcal{Z}; z) = (\pi\varepsilon)^{-n} \det(\mathrm{Re}(G))^{1/4} e^{-\frac{1}{\varepsilon} z^T G z}$$

where G denotes the mixed metric of Z_1 and Z_2. If $Z_1 = Z_2$, we have $\det(\mathrm{Re}(G)) = 1$ and $\int_{\mathbb{R}^{2n}} \mathcal{W}_0(\mathcal{Z}; z)\, dz = 1$.

Proof. We denote $\mathcal{Z} = (\mathcal{P}; \mathcal{Q})$ with $\mathcal{P}, \mathcal{Q} \in \mathbb{C}^{2n\times 2n}$. Then, by Lemma 4.2, every element in $I(\mathcal{L})$ is of the form

$$\Psi(z) = c \cdot e^{\frac{\mathrm{i}}{\varepsilon} z^T \mathcal{P}\mathcal{Q}^{-1} z}$$

for $c \in \mathbb{C}$ and it remains to show that $\mathcal{P}\mathcal{Q}^{-1} = 2\mathrm{i}G$. We have

$$\begin{aligned} G\mathcal{Q} &= \tfrac{1}{4}\Omega^T(Z_2 D^{-1} Z_1^* + \overline{Z}_1 D^{-T} Z_2^T)\Omega \begin{pmatrix} \overline{Z}_1 & Z_2 \end{pmatrix} = \tfrac{1}{4}\Omega^T \begin{pmatrix} \overline{Z}_1 D^{-T}(-2\mathrm{i}D^T) & Z_2 D^{-1}(2\mathrm{i}D) \end{pmatrix} \\ &= -\tfrac{\mathrm{i}}{2} \begin{pmatrix} -\Omega\overline{Z}_1 & Z_2 \end{pmatrix} = -\tfrac{\mathrm{i}}{2}\mathcal{P} \end{aligned}$$

since $2\mathrm{i}D = Z_1^* \Omega Z_2$. For the constant factor, we note

$$(2\pi\varepsilon)^{-n} = \|\mathcal{W}_0(\mathcal{Z})\|^2 = |c|^2 \int_{\mathbb{R}^{2n}} e^{-\frac{2}{\varepsilon} z^T \mathrm{Re}(G) z}\, dz = (\tfrac{\pi\varepsilon}{2})^n \det(\mathrm{Re}(G))^{-1/2} |c|^2$$

and thus $c^2 = (\pi\varepsilon)^{-2n} \det(\mathrm{Re}(G))^{1/2}$. If $Z_1 = Z_2$ we have $G = \mathrm{Re}(G)$ and $\det(G) = 1$ since G is real, symplectic and positive definite. Moreover,

$$\int_{\mathbb{R}^{2n}} \mathcal{W}_0(\mathcal{Z}; z)\, dz = \langle \varphi_0(Z_1), \varphi_0(Z_2) \rangle = \|\varphi_0(Z_1)\|^2.$$

■

Starting from the coherent state we can construct now more excited states by applying iteratively the raising operator $\hat{A}^\dagger(\mathcal{Z})$,

$$\mathcal{W}_{(k,l)}(\mathcal{Z}) := \tfrac{1}{\sqrt{k!l!}} \hat{A}^\dagger_{(k,l)}(\mathcal{Z}) \mathcal{W}_0(\mathcal{Z})$$

for all $k, l \in \mathbb{N}^n$. This relation can be read as the phase space analog of the definition of Hagedorn's wave packets in (4.5). With the same approach as for the ground state $\mathcal{W}_0(\mathcal{Z})$ we find

$$\mathcal{W}_{(k,l)}(\mathcal{Z}) = \mathcal{W}^\varepsilon(\tfrac{1}{\sqrt{k!}} \hat{A}^\dagger_k(Z_1)\varphi_0(Z_1), \tfrac{1}{\sqrt{l!}} \hat{A}^\dagger_l(Z_2)\varphi_0(Z_2)) = \mathcal{W}^\varepsilon(\varphi_k(Z_1), \varphi_l(Z_2))$$

and verify that our construction produces the Wigner transform of two arbitrary Hagedorn wave packets. Hence, we can directly conclude that $\mathcal{W}^\varepsilon(\varphi_k(Z_1), \varphi_l(Z_2))$ is a Hagedorn wave packet parametrised by the phase space frame $\mathcal{Z}$ for all normalised Lagrangian frames Z_1 and Z_2,

$$\mathcal{W}_{(k,l)}(\mathcal{Z}) = (2\pi\varepsilon)^{-n/2} \Phi_{(k,l)}(\mathcal{Z}),$$

where $\Phi_{(k,l)}(\mathcal{Z})$ denotes the (k,l)-th Hagedorn wave packet. The statement in the special case of symmetric Wigner functions can be found as [DKT16, Theorem 11].

Theorem 6.1 — Wave packets in phase space. Let $L_1, L_2 \subset \mathbb{C}^{2n}$ be positive Lagrangian subspaces and $Z_1 \in F_n(L_1)$, $Z_2 \in F_n(L_2)$. Then, with $\mathcal{Z} = (\mathcal{P};\mathcal{Q}) \in \mathbb{C}^{4n\times 2n}$

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1),\varphi_l(Z_2))(z) = \tfrac{1}{\sqrt{2^{|k|+|l|}k!l!}}\, p^{\mathcal{M}}_{(k,l)}(\tfrac{1}{\sqrt{\varepsilon}}\mathcal{Q}^{-1}z)\mathcal{W}_0(\mathcal{Z};z), \quad z \in \mathbb{R}^{2n},$$

for all $k,l \in \mathbb{N}^n$. The symmetric and invertible recursion matrix of the polynomials is given by

$$\mathcal{M} = \begin{pmatrix} CD^{-1} & D^{-T} \\ D^{-1} & -D^{-1}\overline{C} \end{pmatrix},$$

where C and D denote the mixed isotropy and normalisation of Z_1 and Z_2.

Proof. The statement is a consequence of Theorem 4.2 and it only remains to confirm the properties of $\mathcal{M} = \mathcal{Q}^{-1}\overline{\mathcal{Q}}$. Let $C = \frac{1}{2\mathrm{i}}Z_1^T\Omega Z_2$ and $D = \frac{1}{2\mathrm{i}}Z_1^*\Omega Z_2$. Then,

$$-\mathrm{i}\mathcal{P}^T\mathcal{Q} = \tfrac{-\mathrm{i}}{2}\begin{pmatrix} Z_1^*\Omega \\ -Z_2^T\Omega \end{pmatrix}\begin{pmatrix} \overline{Z}_1 & Z_2 \end{pmatrix} = \begin{pmatrix} 0 & D \\ D^T & 0 \end{pmatrix}, \quad \text{i.e.} \quad \mathcal{Q}^{-1} = -\mathrm{i}\begin{pmatrix} 0 & D^{-T} \\ D^{-1} & 0 \end{pmatrix}\mathcal{P}^T$$

and

$$\mathcal{M} = \tfrac{-\mathrm{i}}{2}\begin{pmatrix} 0 & D^{-T} \\ D^{-1} & 0 \end{pmatrix}\begin{pmatrix} Z_1^*\Omega \\ -Z_2^T\Omega \end{pmatrix}\begin{pmatrix} Z_1 & \overline{Z}_2 \end{pmatrix} = \begin{pmatrix} 0 & D^{-T} \\ D^{-1} & 0 \end{pmatrix}\begin{pmatrix} \mathrm{Id} & -\overline{C} \\ C^T & \mathrm{Id} \end{pmatrix}.$$

In the proof of Proposition 4.2 where we determined the form of the generalised wave packets we already showed that C^TD is symmetric using the symplectic metric of L_1. The symmetry of CD^{-1} follows since $C^TD = D^TC$ implies $D^{-T}C^T = CD^{-1}$. Similarly,

$$\overline{C}D^T = \tfrac{1}{4}Z_1^*\Omega^T\overline{Z}_2Z_2^T\Omega\overline{Z}_1 = \tfrac{1}{4}Z_1^*\Omega^T\mathrm{Re}(Z_2Z_2^*)\Omega\overline{Z}_1$$

is symmetric and from $\overline{C}D^T = DC^*$ we can conclude $D^{-1}\overline{C} = C^*D^{-T}$. For the invertibility of $\mathcal{M}$ we consider $\mathrm{kern}(\mathcal{M})$: Let $z = (p,q) \in \mathbb{C}^{2n}$ with $\mathcal{M}z = 0$. Then, the second block leads to $p = \overline{C}q$ and the first block to $(CC^* + \mathrm{Id})D^{-T}q = 0$. Since D is invertible and $CC^* + \mathrm{Id}$ positive definite, it follows that $z = 0$. ■

In [LT14, Theorem 1] it was shown that the symmetric Wigner function of Hagedorn's wave packets always factorises into Laguerre polynomials. This behaviour can be explained with the above result and the analysis of the polynomials $(p_k^M)_{k\in\mathbb{N}^n}$ from the previous chapter.

Corollary 6.1 — Symmetric Wigner transform. Let L be a positive Lagrangian subspace and $Z \in F_n(L)$. The Wigner transform of two Hagedorn wave packets parametrised by Z satisfies

$$\mathcal{W}^\varepsilon(\varphi_k(Z),\varphi_l(Z))(z) = \frac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+|l|}k!l!}} e^{-\frac{1}{\varepsilon}z^TGz} \prod_{j=1}^n \mathcal{L}_{(k_j,l_j)}(\tfrac{\mathrm{i}}{\sqrt{\varepsilon}}w_j, \tfrac{-\mathrm{i}}{\sqrt{\varepsilon}}\overline{w}_j), \quad z \in \mathbb{R}^{2n},$$

where $w := Z^T\Omega z$ and the polynomials $\mathcal{L}_{(k_j,l_j)}$ are defined as in Corollary 5.6. In particular

$$\mathcal{W}^\varepsilon(\varphi_k(Z))(z) = (\pi\varepsilon)^{-n}(-1)^{|k|}e^{-\frac{1}{\varepsilon}z^TGz}\prod_{j=1}^n L_{k_j}^{(0)}(\tfrac{2}{\varepsilon}|w_j|^2), \quad z \in \mathbb{R}^{2n}.$$

Proof. If $Z_1 = Z_2$ is a normalised Lagrangian frame, we have $C = 0$, $D = \mathrm{Id}$ and therefore

$$\mathcal{M} = \begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}.$$

Hence, the structure of the polynomials is given by the formula in Corollary 5.6. For the substitution w, we stress that if $Z_1 = Z_2$ then G is real and thus, by Remark 2.2, $\mathcal{P}^*\mathcal{Q} = -\mathrm{i}\mathrm{Id}$, i.e.

$$\mathcal{Q}^{-1}z = \mathrm{i}\mathcal{P}^*z = \mathrm{i}\begin{pmatrix} Z^T\Omega z \\ Z^*\Omega z \end{pmatrix} = \mathrm{i}\begin{pmatrix} w \\ \overline{w} \end{pmatrix}$$

for all $z \in \mathbb{R}^{2n}$. ■

In particular, the representation of $\mathcal{M}$ in terms of C and D shows that the Wigner transform of Hagedorn's wave packets only factorises into Laguerre polynomials if $CD^{-1} = 0$ and $D^{-1} = \mathrm{Id}$. This means it factorises only if Z_1 and Z_2 are two normalised Lagrangian frames satisfying

$$Z_1^T\Omega Z_2 = 0 \quad \text{and} \quad Z_1^*\Omega Z_2 = 2\mathrm{i}\mathrm{Id}.$$

As stated in Remark 2.4 the first condition implies $\mathrm{range}(Z_1) = \mathrm{range}(Z_2)$ while the second conditions ensures $\varphi_k(Z_1) = \varphi_k(Z_2)$ for all $k \in \mathbb{N}^n$. Thus, the Wigner transform will only attain tensor product structure if both wave packets are parametrised by the same Lagrangian frame Z, see also Remark 4.2.

A wave packet with this circular structure is illustrated in the right plot of Figure 7. A tensor product of Hermite polynomials as in the left picture can not occur as Wigner function since in this case $C = \mathrm{Id}$ and $D^{-1} = 0$, what is a contradiction to D being invertible. In general Wigner transforms $\mathcal{W}_{(k,l)}(\mathcal{Z})$ can attain various forms, see for example the left side of Figure 8.

Again, similar as for the Hermite functions, we simplified calculations so far and considered only wave packets centred at the origin. However, by invoking Lemma 3.10, one can easily transfer the result to general wave packets.

Corollary 6.2 — Phase space centers. Let $L_1, L_2 \subset \mathbb{C}^{2n}$ be positive Lagrangian subspaces, $Z_1 \in F_n(L_1)$, $Z_2 \in F_n(L_2)$ and $z_1, z_2 \in \mathbb{R}^{2n} \oplus \mathbb{R}^{2n}$ with $z_1 = (p_1, q_1)$ and

$z_2 = (p_2, q_2)$. It holds for $k, l \in \mathbb{N}^n$

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1, z_1), \varphi_l(Z_2, z_2))(z) = \frac{e^{\frac{\mathrm{i}}{2\varepsilon}(p_1-p_2)^T(q_1+q_2)}}{\sqrt{2^{|k|+|l|}k!l!}} p^{\mathcal{M}}_{(k,l)}\left(\frac{1}{\sqrt{\varepsilon}}\mathcal{Q}^{-1}(z - \tfrac{z_1+z_2}{2})\right) e^{\frac{\mathrm{i}}{\varepsilon}(z_1-z_2)^T\Omega z}\mathcal{W}_0(\mathcal{Z}; z - \tfrac{z_1+z_2}{2})$$

with $z \in \mathbb{R}^{2n}$ and $\mathcal{Z} = (\mathcal{P}; \mathcal{Q})$.

Proof. Using $\varphi_k(Z, z) = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}T(z)\varphi_k(Z)$ for $z = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$, we have

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1, z_1), \varphi_l(Z_2, z_2)) = e^{\frac{\mathrm{i}}{2\varepsilon}(p_1^Tq_1 - p_2^Tq_2)}\mathcal{W}^\varepsilon(T(z_1)\varphi_k(Z_1), T(z_2)\varphi_l(Z_2))$$

and with Lemma 3.10

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1, z_1), \varphi_l(Z_2, z_2))(z) = e^{\frac{\mathrm{i}}{\varepsilon}\left(\frac{1}{2}(p_1^Tq_1 - p_2^Tq_2) + \frac{1}{2}(p_1^Tq_2 - q_1^Tp_2) + z^T\Omega(z_2 - z_1)\right)}\mathcal{W}^\varepsilon(\varphi_k(Z_1), \varphi_l(Z_2))(z - \tfrac{z_1+z_2}{2}).$$

■

To close this section we sum up some references: A formula for the Wigner transform $\mathcal{W}^\varepsilon(\varphi_0(Z, z_1), \varphi_0(Z, z_2))$ of two coherent states can also be found in [CR12, Proposition 16], beyond that [CR12, §2.2] presents a detailed summary of the properties of Wigner functions with a different line of argumentation. In [Gos10, Proposition 242] the author gives a formula for $\mathcal{W}^\varepsilon(\varphi_0(Z))$ based on the representation of G in terms of $\mathrm{Re}(B)$ and $\mathrm{Im}(B)$, see Corollary 2.3, and shows the generalisation $\mathcal{W}^\varepsilon(\varphi_0(Z_1), \varphi_0(Z_2))$ in [Gos10, Proposition 244]. Moreover, the author uses the Wigner transform to define *squeezed coherent states*, see [Gos10, Definition 246], which we will discuss in more detail in the next chapter.

In [LT14, §4.2] phase space ladders and a three-term recurrence relation are determined for Wigner functions of the form $\mathcal{W}^\varepsilon(\varphi_k(Z), \varphi_l(Z))$, $k, l \in \mathbb{N}^n$. One can show that these phase space ladders are equivalent to the ladders we used here: Let $Z = Z_1 = Z_2$ be a normalised Lagrangian frame and write $Z = (P; Q)$. Furthermore, denote by $\mathcal{Z} = (\mathcal{P}; \mathcal{Q})$ the corresponding phase space frame and by $z = (\xi, x)$ our phase space variable. We find

$$\hat{A}(\mathcal{Z}) = -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\left(\mathcal{P}^Tz + \mathrm{i}\varepsilon\mathcal{Q}^*\nabla_z\right) = -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\left(\begin{pmatrix} -P^*x + Q^*\xi \\ P^Tx - Q^T\xi \end{pmatrix} + \tfrac{\mathrm{i}\varepsilon}{2}\begin{pmatrix} P^*\nabla_\xi + Q^*\nabla_x \\ P^T\nabla_\xi + Q^T\nabla_x \end{pmatrix}\right)$$
$$= -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} \cdot \tfrac{1}{2}\begin{pmatrix} -P^*(2x - \mathrm{i}\varepsilon\nabla_\xi) + Q^*(2\xi + \mathrm{i}\varepsilon\nabla_x) \\ P^T(2x + \mathrm{i}\varepsilon\nabla_\xi) - Q^T(2\xi - \mathrm{i}\varepsilon\nabla_\xi) \end{pmatrix}$$

and analogously

$$\hat{A}^\dagger(\mathcal{Z}) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} \cdot \tfrac{1}{2}\begin{pmatrix} -P^T(2x - \mathrm{i}\varepsilon\nabla_\xi) + Q^T(2\xi + \mathrm{i}\varepsilon\nabla_x) \\ P^*(2x + \mathrm{i}\varepsilon\nabla_\xi) - Q^*(2\xi - \mathrm{i}\varepsilon\nabla_\xi) \end{pmatrix}.$$

Thus, the phase space ladders $K, K^\dagger, L, L^\dagger$ from [LT14, Theorem 2] satisfy

$$2\hat{A}(\mathcal{Z}) = \begin{pmatrix} K \\ L \end{pmatrix} \quad \text{and} \quad 2\hat{A}^\dagger(\mathcal{Z}) = \begin{pmatrix} K^\dagger \\ L^\dagger \end{pmatrix}.$$

The recurrence relation for the Wigner transform can be obtained from the TTRR of the polynomials. We have

$$\begin{pmatrix} (\sqrt{k_j+1}\,\mathcal{W}_{k+e_j,l}(z))_{j=1}^n \\ (\sqrt{l_j+1}\,\mathcal{W}_{k,l+e_j}(z))_{j=1}^n \end{pmatrix} = \sqrt{\tfrac{2}{\varepsilon}}\,\mathcal{Q}^{-1} z \mathcal{W}_{k,l}(z) - \mathcal{M} \begin{pmatrix} (\sqrt{k_j}\,\mathcal{W}_{k-e_j,l}(z))_{j=1}^n \\ (\sqrt{l_j}\,\mathcal{W}_{k,l-e_j}(z))_{j=1}^n \end{pmatrix},$$

see Corollary 5.4. In the case $Z = Z_1 = Z_2$, this relation simplifies since

$$\mathcal{M} = \begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{Q}^{-1} z = \mathrm{i}\mathcal{P}^* z = \begin{pmatrix} w \\ -\overline{w} \end{pmatrix}$$

with $w = \mathrm{i} Z^T \Omega z$ as performed in the proof of Corollary 6.1. So,

$$\left(\sqrt{k_j+1}\,\mathcal{W}_{k+e_j,l}(z)\right)_{j=1}^n = \sqrt{\tfrac{2}{\varepsilon}}\,w\,\mathcal{W}_{k,l}(z) - \left(\sqrt{l_j}\,\mathcal{W}_{k,l-e_j}(z)\right)_{j=1}^n,$$

and

$$\left(\sqrt{l_j+1}\,\mathcal{W}_{k,l+e_j}(z)\right)_{j=1}^n = -\sqrt{\tfrac{2}{\varepsilon}}\,\overline{w}\,\mathcal{W}_{k,l}(z) - \left(\sqrt{k_j}\,\mathcal{W}_{k-e_j,l}(z)\right)_{j=1}^n.$$

6.3. FBI and Husimi transform

The findings from the previous section confirm that all Wigner functions except the Wigner transform of coherent states, attain negative values. Hence, the Wigner transforms cannot be viewed as a probability density, but we can gain positivity if we smooth with the ε-scaled Gaussian

$$g^\varepsilon(z;x) = (\pi\varepsilon)^{-n/4} e^{-\frac{1}{2\varepsilon}|x-q|^2 + \frac{\mathrm{i}}{\varepsilon} p^T(x-q)}, \quad x \in \mathbb{R}^n,$$

centred in $z = (p,q) \in \mathbb{R}^n \oplus \mathbb{R}^n$. The generated function $\mathcal{H}^\varepsilon = g^\varepsilon(z) * \mathcal{W}^\varepsilon$ is called Husimi function, see also Section 3.4. We will use the same strategy and first determine the FBI transform of Hagedorn's wave packets

$$(\mathcal{F}_z^\varepsilon \varphi)(z) = (2\pi\varepsilon)^{-n/2} \langle \varphi, g^\varepsilon(z) \rangle, \quad \varphi \in \mathcal{S}(\mathbb{R}^n).$$

The Husimi transform then emerges as the modulus squared, $\mathcal{H}^\varepsilon(\varphi) = |\mathcal{F}_z^\varepsilon \varphi|^2$. Nevertheless, the computations for Hagedorn's wave packets are more involved than the ones for the Hermite functions. This section is a more technical one and as a starter we need two lemmas regarding computations with the polynomials p_k^M.

Lemma 6.3 — Sum formula. Let $M \in \mathbb{C}^{n\times n}$ and $k \in \mathbb{N}^n$. Then, for $x, y \in \mathbb{C}^n$,

$$p_k^M(x+y) = \sum_{l\le k} \binom{k}{l} (2y)^{k-l} p_l^M(x).$$

Proof. A similar result can be found in [LT14, Proposition 3]. For $y \in \mathbb{C}^n$ let τ_y denote the translation operator $(\tau_y f)(x) = f(x+y)$, i.e. $p_k^M(x+y) = \tau_y \hat{B}_k^\dagger 1$. We observe

$$(\tau_y \hat{B}^\dagger f)(x) = 2(x+y)f(x+y) - M\nabla_x f(x+y) = 2yf(x) + (\hat{B}^\dagger \tau_y f)(x)$$

and thus, iteratively,

$$\tau_y \hat{B}_k^\dagger 1 = (2y + \hat{B}^\dagger \tau_y)^k 1 = \sum_{l\le k} \binom{k}{l} (2y)^{k-l} \hat{B}_l^\dagger 1 = \sum_{l\le k} \binom{k}{l} (2y)^{k-l} p_l^M(x).$$

■

The scaled Gaussian $g^\varepsilon(z)$ can also be interpreted as the coherent state $\varphi_0(Z_0, z)$ where

$$Z_0 = \begin{pmatrix} \mathrm{iId} \\ \mathrm{Id} \end{pmatrix}.$$

Therefore, we can already presume that the case where $Z = (P;Q)$ satisfies $B = \mathrm{iId}$ is a simpler special case. Otherwise, the scalar product $\langle \varphi_k(Z), \varphi_0(Z_0)\rangle$, if we neglect translation for a moment, contains a product of the form

$$p_k^M(\tfrac{1}{\sqrt{\varepsilon}} Q^{-1} y)\, e^{\frac{\mathrm{i}}{2\varepsilon} y^T (B + \mathrm{iId}) y}$$

that we need to integrate.

Lemma 6.4 — Integral formula. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian, $Z = (P;Q) \in F_n(L)$ and denote by $M = Q^{-1}\overline{Q}$ and $B = PQ^{-1}$. Then,

$$\int_{\mathbb{R}^n} p_k^M(\tfrac{1}{\sqrt{\varepsilon}} Q^{-1} y)\, e^{\frac{\mathrm{i}}{2\varepsilon} y^T (B + \mathrm{iId}) y}\, dy = c_k$$

where $c_0 = (2\pi\varepsilon)^{n/2} \det(\mathrm{Id} - \mathrm{i}B)^{-1/2}$, $c_k = 0$ if $k \notin \mathbb{N}^n$ and for all $k \in \mathbb{N}^n$ with $|k|$ odd,

$$c_k = 0 \quad \text{and} \quad \left(c_{k+e_j}\right)_{j=1}^n = -2Q^{-1}(B + \mathrm{iId})^{-1}(\overline{B} + \mathrm{iId})\overline{Q}\left(k_j c_{k-e_j}\right)_{j=1}^n.$$

Proof. This statement is a reformulation of [LT14, Proposition 4]. The claim for $|k|$ odd, follows since in this case $p_k^M(x) = -p_k^M(-x)$. Moreover, with the Rodrigues formula from Lemma 5.2 and partial integration

$$\begin{aligned} c_{k+e_j} &= \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{2} y^T Q^T (B+\mathrm{iId}) Q y} e^{y^T M^{-1} y} (-M\nabla_y)^{k+e_j} e^{-y^T M^{-1} y}\, dy \\ &= \int_{\mathbb{R}^n} (M\nabla_y)_j e^{\frac{\mathrm{i}}{2} y^T \left(Q^T (B+\mathrm{iId}) Q - 2\mathrm{i} M^{-1}\right) y} (-M\nabla_y)^k e^{-y^T M^{-1} y}\, dy \end{aligned}$$

for $j = 1, \dots, n$. Since M is symmetric, we further have

$$M\nabla_y e^{\frac{\mathrm{i}}{2}y^T\left(Q^T(B+\mathrm{iId})Q-2\mathrm{i}M^{-1}\right)y} = (\mathrm{i}Q^*(B+\mathrm{iId})Q+2\mathrm{Id})\, ye^{\frac{\mathrm{i}}{2}y^T\left(Q^T(B+\mathrm{iId})Q-2\mathrm{i}M^{-1}\right)y}$$

and with a vector-valued notation where we apply the integral to each component,

$$\left(c_{k+e_j}\right)_{j=1}^n = (\mathrm{i}Q^*(B+\mathrm{iId})Q+2\mathrm{Id})\int_{\mathbb{R}^n} y\, p_k^M(y)e^{\frac{\mathrm{i}}{2}y^TQ^T(B+\mathrm{iId})Qy}\, dy.$$

The three-term recurrence relation of the polynomials finally yields

$$y\, p_k^M = \tfrac{1}{2}\left(p_{k+e_j}^M\right)_{j=1}^n + M\left(k_j p_{k-e_j}^M\right)_{j=1}^n$$

and thus,

$$\begin{aligned}\left(c_{k+e_j}\right)_{j=1}^n &= \left(\tfrac{\mathrm{i}}{2}Q^*(B+\mathrm{iId})Q+\mathrm{Id}\right)\left(c_{k+e_j}\right)_{j=1}^n + (\mathrm{i}Q^*(B+\mathrm{iId})Q+2\mathrm{Id})\, M\left(k_jc_{k-e_j}\right)_{j=1}^n, \\ -\tfrac{1}{2}Q^*(B+\mathrm{iId})Q\left(c_{k+e_j}\right)_{j=1}^n &= (Q^*(B+\mathrm{iId})Q-2\mathrm{iId})\, M\left(k_jc_{k-e_j}\right)_{j=1}^n.\end{aligned}$$

The claim follows since Z is a normalised Lagrangian frame,

$$(Q^*(B+\mathrm{iId})Q-2\mathrm{iId})\, M = (Q^*P+\mathrm{i}Q^*Q-2\mathrm{iId})\, M = (P^*Q+\mathrm{i}Q^*Q)\, M = Q^*\left(B^*+\mathrm{iId}\right)\overline{Q}$$

and B is symmetric. ■

Since we are dealing with wave packets parametrised by two different Lagrangian frames Z_0 and Z, we can also include their mixed isotropy and normalisation,

$$2\mathrm{i}C = Z_0^T\Omega Z = -\mathrm{i}Q+P = (B-\mathrm{iId})Q, \quad 2\mathrm{i}D = Z_0^*\Omega Z = \mathrm{i}Q+P = (B+\mathrm{iId})Q.$$

With this, we can rewrite the recursion for the constants c_k as

$$\left(c_{k+e_j}\right)_{j=1}^n = 2D^{-1}\overline{C}\left(k_jc_{k-e_j}\right)_{j=1}^n.$$

We start with the FBI transform of Hagedorn's wave packets centred at the origin.

Proposition 6.3 — FBI transform. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian and $Z = (P;Q) \in F_n(L)$. Then, the FBI tranform of the k-th Hagedorn wave packet $\varphi_k(Z)$ in $z = (\xi, x) \in \mathbb{R}^n \oplus \mathbb{R}^n$ is given by

$$\begin{aligned}(\mathcal{F}_z^\varepsilon\varphi_k(Z))(\xi,x) = \tfrac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}}\det(Q)^{-1/2}e^{-\frac{1}{2\varepsilon}(|w|^2+|\xi|^2)}e^{\frac{\mathrm{i}}{2\varepsilon}w^T(B+\mathrm{iId})^{-1}w} \\ \sum_{l\le k}\binom{k}{l}\left(\tfrac{1}{\sqrt{\varepsilon}}D^{-1}w\right)^{k-l}c_l.\end{aligned}$$

where $w = x - \mathrm{i}\xi$.

Proof. Let $Z = (P;Q) \in \mathbb{C}^{n\times n}$ and $B = PQ^{-1}$. By definition,

$$(\mathcal{F}_z^\varepsilon \varphi_k(Z))(z) = \tfrac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}} \det(Q)^{-1/2} \int_{\mathbb{R}^n} p_k^M(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}y) e^{\frac{\mathrm{i}}{2\varepsilon}y^T By} e^{-\frac{1}{2\varepsilon}|y-x|^2-\frac{\mathrm{i}}{\varepsilon}\xi^T(y-x)}\, dy$$
$$= \tfrac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}} \det(Q)^{-1/2} e^{-\frac{1}{2\varepsilon}|x|^2+\frac{\mathrm{i}}{\varepsilon}\xi^T x} \int_{\mathbb{R}^n} p_k^M(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}y) e^{\frac{\mathrm{i}}{2\varepsilon}y^T(B+\mathrm{i}\mathrm{Id})y+\frac{1}{\varepsilon}y^T(x-\mathrm{i}\xi)}\, dy.$$

If we complete the square in the exponent we can write the integral in the form of Lemma 6.4. Let $u = \mathrm{i}(B+\mathrm{i}\mathrm{Id})^{-1}(x-\mathrm{i}\xi)$. Then,

$$(\mathcal{F}_z^\varepsilon \varphi_k(Z))(z) =$$
$$= \tfrac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}} \det(Q)^{-1/2} e^{-\frac{1}{2\varepsilon}|x|^2+\frac{\mathrm{i}}{\varepsilon}\xi^T x} e^{-\frac{\mathrm{i}}{2\varepsilon}u^T(B+\mathrm{i}\mathrm{Id})u} \int_{\mathbb{R}^n} p_k^M(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}y) e^{\frac{\mathrm{i}}{2\varepsilon}(y-u)^T(B+\mathrm{i}\mathrm{Id})(y-u)}\, dy$$
$$= \tfrac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}} \det(Q)^{-1/2} e^{-\frac{1}{2\varepsilon}|x|^2+\frac{\mathrm{i}}{\varepsilon}\xi^T x} e^{-\frac{\mathrm{i}}{2\varepsilon}u^T(B+\mathrm{i}\mathrm{Id})u} \int_{\mathbb{R}^n} p_k^M(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}(y'+u)) e^{\frac{\mathrm{i}}{2\varepsilon}y'^T(B+\mathrm{i}\mathrm{Id})y'}\, dy'.$$

The integral can now be simplified by means of the sum and integral formula we introduced at the beginning of this section,

$$\int_{\mathbb{R}^n} p_k^M(\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}(y+u)) e^{\frac{\mathrm{i}}{2\varepsilon}y^T(B+\mathrm{i}\mathrm{Id})y}\, dy = \sum_{l\le k} \binom{k}{l} (\tfrac{2}{\sqrt{\varepsilon}}Q^{-1}u)^{k-l} c_l.$$

Thus,

$$(\mathcal{F}_z^\varepsilon \varphi_k(Z))(z) = \tfrac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}} \det(Q)^{-1/2} e^{-\frac{1}{2\varepsilon}|x|^2+\frac{\mathrm{i}}{\varepsilon}\xi^T x} e^{-\frac{\mathrm{i}}{2\varepsilon}u^T(B+\mathrm{i}\mathrm{Id})u} \sum_{l\le k} \binom{k}{l} (\tfrac{2}{\sqrt{\varepsilon}}Q^{-1}u)^{k-l} c_l$$

and, by inserting u, we find $2\mathrm{i}Q^{-1}(B+\mathrm{i}\mathrm{Id})^{-1}(x-\mathrm{i}\xi) = D^{-1}(x-\mathrm{i}\xi)$ and

$$-\tfrac{\mathrm{i}}{2\varepsilon}u^T(B+\mathrm{i}\mathrm{Id})u = \tfrac{\mathrm{i}}{2\varepsilon}(x-\mathrm{i}\xi)^T(B+\mathrm{i}\mathrm{Id})^{-1}(x-\mathrm{i}\xi).$$

Moreover, $-\frac{1}{2\varepsilon}|x-\mathrm{i}\xi|^2 = -\frac{1}{2\varepsilon}|x|^2 + \frac{\mathrm{i}}{\varepsilon}\xi^T x + \frac{1}{2\varepsilon}|\xi|^2$. ■

We already mentioned that the case $B = \mathrm{i}\mathrm{Id}$ is an interesting special case since then Z_0 and Z are parametrising the same Lagrangian subspace L.

Corollary 6.3 Let $Z = (P;Q) \in \mathbb{C}^{2n\times n}$ be a normalised Lagrangian subspace such that $PQ^{-1} = \mathrm{i}\mathrm{Id}$. The FBI transform of $\varphi_k(Z)$, $k \in \mathbb{N}^n$, simplifies to

$$(\mathcal{F}_z^\varepsilon \varphi_k(Z))(\xi,x) = \tfrac{(\pi\varepsilon)^{-n/2}}{\sqrt{2^{|k|+n}k!}} \det(Q)^{-1/2} e^{-\frac{1}{2\varepsilon}|\xi|^2} e^{-\frac{1}{4\varepsilon}|w|^2} (\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}w)^k$$

where $w = x - \mathrm{i}\xi$ and the Husimi transform is given by

$$(\mathcal{H}^\varepsilon \varphi_k(Z))(\xi,x) = \tfrac{(\pi\varepsilon)^{-n}}{2^{|k|+n}k!} e^{-\frac{1}{\varepsilon}|\xi|^2} e^{-\frac{1}{2\varepsilon}|w|^2} |\tfrac{1}{\sqrt{\varepsilon}}Q^{-1}w|^{2k}.$$

Proof. If $B = \mathrm{i}\mathrm{Id}$ we first note that $c_k = 0$ for all $k \neq 0$. Further, we use $D^{-1} = Q^{-1}$ and summarise in the exponent $-\frac{1}{2\varepsilon}(|w|^2+|\xi|^2) + \frac{1}{4\varepsilon}|w|^2 = -\frac{1}{2\varepsilon}|\xi|^2 - \frac{1}{4\varepsilon}|w|^2$. For the Husimi transform we stress that

$$\det(Q)\det(\overline{Q}) = \det(QQ^*) = \det(\mathrm{Im}(B))^{-1} = 1$$

if $B = \mathrm{iId}$. ■

To translate our results away from the origin, we again make use of the Heisenberg-Weyl operator, see also [LT14, Lemma 2].

Lemma 6.5 — Phase space translation. Let $z, z' \in \mathbb{R}^n \oplus \mathbb{R}^n$ with $z = (\xi, x)$ and $z' = (p, q)$. Then,

$$\mathcal{F}_z^\varepsilon(T(z')\psi)(z) = e^{\frac{\mathrm{i}}{\varepsilon}p^T(x-q/2)}\mathcal{F}_z^\varepsilon(\psi)(z-z')$$

for all Schwartz functions $\psi \in \mathcal{S}(\mathbb{R}^n)$.

Proof. With the definition of $T(z')$ it holds

$$\begin{aligned}\mathcal{F}_z^\varepsilon(T(z')\psi)(z) &= (2\pi\varepsilon)^{-n/2}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}p^T(y-q/2)}\psi(y-q)e^{-\frac{1}{2\varepsilon}|y-x|^2-\frac{\mathrm{i}}{\varepsilon}\xi^T(y-x)}\,dy \\ &= (2\pi\varepsilon)^{-n/2}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}p^T(y'+q/2)}\psi(y')e^{-\frac{1}{2\varepsilon}|y'+q-x|^2-\frac{\mathrm{i}}{\varepsilon}\xi^T(y'+q-x)}\,dy' \\ &= (2\pi\varepsilon)^{-n/2}e^{\frac{\mathrm{i}}{\varepsilon}p^T(x-q/2)}\int_{\mathbb{R}^n}\psi(y')e^{-\frac{1}{2\varepsilon}|y'+q-x|^2-\frac{\mathrm{i}}{\varepsilon}(\xi-p)^T(y'+q-x)}\,dy' \\ &= e^{\frac{\mathrm{i}}{\varepsilon}p^T(x-q/2)}\mathcal{F}_z^\varepsilon(\psi)(z-z').\end{aligned}$$

■

So, we can easily deduce the FBI transform for general Hagedorn wave packets.

Corollary 6.4 — General FBI transform. Let $L \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace, $Z = (P;Q) \in F_n(L)$ and $z' = (p,q) \in \mathbb{R}^n \oplus \mathbb{R}^n$. The FBI transform of the k-th wave packet $\varphi_k(Z,z')$ centred at z' reads

$$\begin{aligned}(\mathcal{F}_z^\varepsilon\varphi_k(Z,z'))(\xi,x) = \frac{(\pi\varepsilon)^{-n}}{\sqrt{2^{|k|+n}k!}}\det(Q)^{-1/2}e^{\frac{\mathrm{i}}{\varepsilon}p^T(x-q)}e^{-\frac{1}{2\varepsilon}(|w|^2+|\xi-p|^2)}e^{\frac{\mathrm{i}}{2\varepsilon}w^T(B+\mathrm{iId})^{-1}w} \\ \sum_{l\le k}\binom{k}{l}(\tfrac{1}{\sqrt{\varepsilon}}D^{-1}w)^{k-l}c_l.\end{aligned}$$

where $z = (\xi, x) \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $w = (x-q) - \mathrm{i}(\xi - p)$.

Proof. We have $\varphi_k(Z,z') = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}T(z')\varphi_k(Z)$ and thus, by the previous corollary,

$$(\mathcal{F}_z^\varepsilon\varphi_k(Z,z'))(\xi,x) = e^{-\frac{\mathrm{i}}{2\varepsilon}p^Tq}e^{\frac{\mathrm{i}}{\varepsilon}p^T(x-q/2)}\mathcal{F}_z^\varepsilon(\varphi_k(Z))(\xi-p,x-q).$$

■

6.4. Generalised wave packets in phase space

The phase space ladder lift in the first section of this chapter did not depend on the normalisation of the Lagrangian frames or on the relation between the ladder operator and the coherent state. This means, for normalised Lagrangian frames $Y_1, Y_2 \in \mathbb{C}^{2n\times n}$ and $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ we have

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1,Y_1),\varphi_l(Z_2,Y_2)) = \tfrac{1}{\sqrt{k!l!}}\hat{A}^\dagger_{(k,l)}(\mathcal{Y})\mathcal{W}^\varepsilon(\varphi_0(Z_1),\varphi_0(Z_2)), \quad k,l \in \mathbb{N}^n,$$

where $\mathcal{Y}$ denotes the phase space frame of Y_1 and Y_2. Thus, it is easy to extend our results for Hagedorn's wave packets also to generalised wave packets and wave packets parametrised by a non-normalised frame. We will simply discover generalised wave packets resp. non-normalised wave packets in phase space.

Proposition 6.4 — Generalised wave packets. Let $Y_1, Y_2 \in \mathbb{C}^{2n\times n}$ and $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ be normalised Lagrangian frames and $k,l \in \mathbb{N}^n$. If we denote

$$\begin{aligned} C_j &= \tfrac{i}{2} Z_j^T \Omega^T Y_j, \quad D_j = \tfrac{i}{2} Z_j^* \Omega^T Y_j, \quad j = 1,2, \\ C &= \tfrac{i}{2} Z_1^T \Omega^T Z_2, \quad D = \tfrac{i}{2} Z_1^* \Omega^T Z_2, \end{aligned}$$

the Wigner transform of two generalised wave packets can be written as

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1,Y_1),\varphi_l(Z_2,Y_2))(z) = \frac{1}{\sqrt{2^{|k|+|l|}k!l!}} p^{\mathcal{M}}_{(k,l)}(\tfrac{1}{\sqrt{\varepsilon}}\mathcal{D}^*\mathcal{Q}^{-1}z)\mathcal{W}_0(\mathcal{Z};z), \quad z \in \mathbb{R}^{2n},$$

where $\mathcal{Z} = (\mathcal{P};\mathcal{Q})$, $\mathcal{M} = -\mathcal{C}^*\overline{\mathcal{D}} + \mathcal{D}^*\mathcal{Q}^{-1}\overline{\mathcal{Q}\mathcal{D}}$ and

$$\mathcal{C} = \begin{pmatrix} \overline{C}_1 & 0 \\ 0 & C_2 \end{pmatrix}, \quad \mathcal{D} = \begin{pmatrix} \overline{D}_1 & 0 \\ 0 & D_2 \end{pmatrix}, \quad \mathcal{Q}^{-1}\overline{\mathcal{Q}} = \begin{pmatrix} CD^{-1} & D^{-T} \\ D^{-1} & -D^{-1}\overline{C} \end{pmatrix}.$$

Proof. The claim is a consequence of Proposition 4.2. We consider the two phase space frames

$$\mathcal{Y} = \begin{pmatrix} -\Omega\overline{Y}_1 & \Omega Y_2 \\ \frac{1}{2}\overline{Y}_1 & \frac{1}{2}Y_2 \end{pmatrix}, \quad \mathcal{Z} = \begin{pmatrix} -\Omega\overline{Z}_1 & \Omega Z_2 \\ \frac{1}{2}\overline{Z}_1 & \frac{1}{2}Z_2 \end{pmatrix}$$

and compute

$$\mathcal{C} = \tfrac{i}{2}\mathcal{Z}^T\Omega^T\mathcal{Y} = \tfrac{i}{2}\begin{pmatrix} Z_1^*\Omega & \frac{1}{2}Z_1^* \\ -Z_2^T\Omega & \frac{1}{2}Z_2^T \end{pmatrix}\begin{pmatrix} \frac{1}{2}\overline{Y}_1 & \frac{1}{2}Y_2 \\ \Omega\overline{Y}_1 & -\Omega Y_2 \end{pmatrix} = \tfrac{i}{2}\begin{pmatrix} Z_1^*\Omega\overline{Y}_1 & 0 \\ 0 & Z_2^T\Omega Y_2 \end{pmatrix} = \begin{pmatrix} \overline{C}_1 & 0 \\ 0 & C_2 \end{pmatrix}$$

and analogously,

$$\mathcal{D} = \tfrac{i}{2}\mathcal{Z}^*\Omega^T\mathcal{Y} = \tfrac{i}{2}\begin{pmatrix} Z_1^T\Omega & \frac{1}{2}Z_1^T \\ -Z_2^*\Omega & \frac{1}{2}Z_2^* \end{pmatrix}\begin{pmatrix} \frac{1}{2}\overline{Y}_1 & \frac{1}{2}Y_2 \\ \Omega\overline{Y}_1 & -\Omega Y_2 \end{pmatrix} = \tfrac{i}{2}\begin{pmatrix} Z_1^T\Omega\overline{Y}_1 & 0 \\ 0 & Z_2^*\Omega Y_2 \end{pmatrix} = \begin{pmatrix} \overline{D}_1 & 0 \\ 0 & D_2 \end{pmatrix}.$$

The same statement for symmetric Wigner functions with a proof that is based in the generating function of the polynomials can be found in [DKT16, Theorem 11]. ■

Proposition 6.5 — Non-normalised phase space frames. Let $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ be two non-normalised Lagrangian frames with positive definite normalisations

$$N_j = \tfrac{1}{2\mathrm{i}} Z_j^* \Omega Z_j, \quad j = 1, 2.$$

Then, $\varphi_k(Z_1), \varphi_l(Z_2)$ are elements of $L^2(\mathbb{R}^n)$ for $k, l \in \mathbb{N}^n$ and their Wigner transform is of the form

$$\mathcal{W}^\varepsilon(\varphi_k(Z_1), \varphi_l(Z_2))(z) = \tfrac{1}{\sqrt{2^{|k|+|l|} k! l!}} p^{\mathcal{M}}_{(k,l)}(\tfrac{1}{\sqrt{\varepsilon}} \mathcal{N} \mathcal{Q}^{-1} z) \mathcal{W}_0(\mathcal{Z}; z), \quad z \in \mathbb{R}^{2n},$$

where $\mathcal{Z} = (\mathcal{P}; \mathcal{Q})$, $\mathcal{M} = \mathcal{N} \mathcal{Q}^{-1} \overline{\mathcal{Q}}$ and

$$\mathcal{N} = \begin{pmatrix} \overline{N}_1 & 0 \\ 0 & N_2 \end{pmatrix}.$$

Proof. Similarly to the previous proof, we refer to Corollary 4.2 and calculate the phase space variables. Let

$$\mathcal{Z} = \begin{pmatrix} -\Omega \overline{Z}_1 & \Omega Z_2 \\ \frac{1}{2} \overline{Z}_1 & \frac{1}{2} Z_2 \end{pmatrix},$$

then,

$$\mathcal{N} = \tfrac{\mathrm{i}}{2} \mathcal{Z}^* \Omega^T \mathcal{Z} = \tfrac{\mathrm{i}}{2} \begin{pmatrix} Z_1^T \Omega & \frac{1}{2} Z_1^T \\ -Z_2^* \Omega & \frac{1}{2} Z_2^* \end{pmatrix} \begin{pmatrix} \frac{1}{2} \overline{Z}_1 & \frac{1}{2} Z_2 \\ \Omega \overline{Z}_1 & -\Omega Z_2 \end{pmatrix} = \tfrac{\mathrm{i}}{2} \begin{pmatrix} Z_1^T \Omega \overline{Z}_1 & 0 \\ 0 & Z_2^* \Omega Z_2 \end{pmatrix} = \begin{pmatrix} \overline{N}_1 & 0 \\ 0 & N_2 \end{pmatrix}.$$

We add that $\mathcal{N}$ is positive definite if N_1 and N_2 are positive definite, since the normalisations are by definition Hermitian. Thus, the coherent state $\mathcal{W}_0(\mathcal{Z})$ is a well-defined L^2-function. ∎

7. Generalised squeezed states

In the literature Hagedorn's wave packets also coexist as (generalised) squeezed states or generalised coherent states. We will name some common approaches in this chapter and show their equivalence to our construction of the wave packets.

In general one obtains squeezed states by translation and transformation of multi-dimensional Hermite functions with a unitary operator. We will again neglect translation here and only focus on the transformation operator. The translation of the squeezed states is, as for Hagedorn's wave packets, obtained by applying the Heisenberg-Weyl operator. The crucial point therefore is the squeezing of the functions.

For the transformation we present three different strategies: The first one is the classical one based on a unitary squeezing operator that is directly applied to the Hermite functions. This approach is probably the most common one, but the originating states are less elementary to handle, see [CR12, §3.4], [AAG14, §2.5] or [Gaz09, §10]. In the second part we show that one can produce equivalent states by adjusting Dirac's ladder operators with a Bogoliubov transformation, see for example [BFG16, §3] or [QWL01]. The squeezed states in this case are easier to handle and the relation to Hagedorn's wave packets gets clearer. To finish the part about the connection between Hermite functions and Hagedorn's wave packets, we also have to mention the ansatz via metapletic operators from [Ohs15]. This result nicely explains why the wave packets adopt many properties of the Hermite functions. In the last section we will use the Wigner function to characterise squeezed states, see [Gos10, §11.3]. This viewpoint gives no structural information about Hermite functions and wave packets, but yields a very short proof for the equivalence of Hagedorn's wave packets and squeezed states.

7.1. Squeezing operators

The classical definition of generalised squeezed states works via a unitary squeezing operator that is applied to multi-dimensional Hermite functions $(\varphi_k)_{k\in\mathbb{N}^n}$ with

$$\varphi_k(x) = (\pi\varepsilon)^{-n/4} e^{-\frac{1}{2\varepsilon}|x|^2} \prod_{j=1}^{n} h_{k_j}(x_j), \quad x \in \mathbb{R}^n.$$

We will reproduce the ansatz in [CR12, §3.4] and start with a complex, symmetric matrix $W \in \mathbb{C}^{n\times n}$ that satisfies $W^*W < \mathrm{Id}$ in the sense that $|Wv|^2 \leq |v|^2$ for all $v \in \mathbb{C}^n$. Then, there exists a unitary matrix $U \in \mathbb{C}^{n\times n}$ such that W can be written as polar decomposition

$$W = U|W|, \quad \text{where} \quad |W| = (W^*W)^{1/2}.$$

and we define a complex symmetric matrix $F \in \mathbb{C}^{n\times n}$ via

$$F = U \arg\tanh(|W|) = W \sum_{j=0}^{\infty} \tfrac{(W^*W)^j}{2j+1}. \tag{7.1}$$

Lemma 7.1 — Squeezing operator. Let $\hat{a}$ and $\hat{a}^\dagger$ denote the ladder operators for the multi-dimensional Hermite functions, i.e. $\hat{a} = \frac{1}{\sqrt{2\varepsilon}}(\hat{q} + \mathrm{i}\hat{p})$ and $\hat{a}^\dagger = \frac{1}{\sqrt{2\varepsilon}}(\hat{q} - \mathrm{i}\hat{p})$. Then, the *squeezing operator*

$$D(F) = e^{\frac{1}{2}((\hat{a}^\dagger)^T F \hat{a}^\dagger - \hat{a}^T F^* \hat{a})}$$

is unitary with inverse $D(F)^{-1} = D(-F)$.

Proof. This result can also be found in [CR12, Lemma 25]. Since $\hat{a}$ and $\hat{a}^\dagger$ are adjoints,

$$D(F)^* = e^{\frac{1}{2}((\hat{a}^\dagger)^T F \hat{a}^\dagger - \hat{a}^T F^* \hat{a})^*} = e^{\frac{1}{2}(\hat{a}^T F^* \hat{a} - (\hat{a}^\dagger)^T F \hat{a}^\dagger)} = D(-F).$$

∎

We now obtain *generalised squeezed states* by applying $D(F)$ to the Hermite functions,

$$\psi_k^F = D(F)\varphi_k, \qquad \forall\, k \in \mathbb{N}^n,$$

see [CR12, §3.4] for coherent states and [CR12, §4.1] for excited states. If we interpret the Hermite functions $(\varphi_k)_{k\in\mathbb{N}^n}$ as Hagedorn wave packets $(\varphi_k(Z_0))_{k\in\mathbb{N}^n}$ with

$$Z_0 = \begin{pmatrix} \mathrm{i}\mathrm{Id} \\ \mathrm{Id} \end{pmatrix}$$

this relation can be rewritten as

$$\psi_k^F = \tfrac{1}{\sqrt{k!}} D(F) \hat{A}_k^\dagger(Z_0)\varphi_0(Z_0) = \tfrac{1}{\sqrt{k!}} D(F)\hat{A}_k^\dagger(Z_0) D(F)^{-1}\, \psi_0^F. \tag{7.2}$$

For the coherent state ψ_0^F we can give a direct formula, see [CR12, Proposition 36].

Proposition 7.1 — Squeezed coherent state. Let $W \in \mathbb{C}^{n\times n}$ be symmetric and $W^*W < \mathrm{Id}$. The squeezed state ψ_0^F, where F is defined in (7.1), is a Gaussian given by

$$\psi_0^F(x) = (\pi\varepsilon)^{-n/4} \det(\mathrm{Id} - |W|^2)^{-1/2} |\det(\mathrm{Id} + W)|^{1/2}\, e^{\frac{\mathrm{i}}{2\varepsilon} x^T \Gamma x}, \quad x \in \mathbb{R}^n,$$

with $\Gamma = \mathrm{i}(\mathrm{Id} - W)(\mathrm{Id} + W)^{-1}$.

The form of Γ in the above proposition already suggests that squeezed coherent states can be expressed as a coherent state $\varphi_0(Z)$ parametrised by

$$Z = \begin{pmatrix} \mathrm{i}(\mathrm{Id} - W) \\ (\mathrm{Id} + W) \end{pmatrix} \in \mathbb{C}^{2n\times n}.$$

One can easily verify that Z satisfies $Z^T \Omega Z = 0$ and $Z^* \Omega Z = 2\mathrm{i}(\mathrm{Id} - W^* W)$ and we thus find a normalised Lagrangian frame by taking

$$Z' = Z(\mathrm{Id} - |W|^2)^{-1/2}.$$

To prove the main result of this section, the relation between Hagedorn's wave packets and generalised squeezed states, we first need the following lemma.

Lemma 7.2 Let $F \in \mathbb{C}^{n\times n}$ with polar decomposition $F = U|F|$, i.e. $U \in \mathbb{C}^{n\times n}$ is unitary and $|F|^2 = F^* F$. Then,

$$\exp\begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix} = \begin{pmatrix} \cosh(|F|) & \sinh(|F|)U^* \\ U\sinh(|F|) & U\cosh(|F|)U^* \end{pmatrix}.$$

Proof. A direct calculations shows that for $k \geq 0$

$$\begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix}^{2k} = \begin{pmatrix} (F^*F)^k & 0 \\ 0 & (FF^*)^k \end{pmatrix}, \quad \begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix}^{2k+1} = \begin{pmatrix} 0 & (F^*F)^k F^* \\ F(FF^*)^k & 0 \end{pmatrix}.$$

Thus, we find for the exponential series

$$\exp\begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix} = \sum_{k=0}^{\infty} \begin{pmatrix} \frac{1}{(2k)!}(F^*F)^k & \frac{1}{(2k+1)!}(F^*F)^k F^* \\ \frac{1}{(2k+1)!}F(FF^*)^k & \frac{1}{(2k)!}(FF^*)^k \end{pmatrix}$$

and with $\sinh(X) = \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} X^{2k+1}$ and $\cosh(X) = \sum_{k=0}^{\infty} \frac{1}{(2k)!} X^{2k}$, for $X \in \mathbb{C}^{n\times n}$,

$$\begin{aligned}
\sum_{k=0}^{\infty} \tfrac{1}{(2k)!}(F^*F)^k &= \sum_{k=0}^{\infty} \tfrac{1}{(2k)!}|F|^{2k} = \cosh(|F|), \\
\sum_{k=0}^{\infty} \tfrac{1}{(2k)!}(FF^*)^k &= \sum_{k=0}^{\infty} \tfrac{1}{(2k)!}U|F|^{2k}U^* = U\cosh(|F|)U^*, \\
\sum_{k=0}^{\infty} \tfrac{1}{(2k+1)!}(FF^*)^k F^* &= \sum_{k=0}^{\infty} \tfrac{1}{(2k+1)!}|F|^{2k+1}U^* = \sinh(|F|)U^*, \\
\sum_{k=0}^{\infty} \tfrac{1}{(2k+1)!}F(FF^*)^k &= \sum_{k=0}^{\infty} \tfrac{1}{(2k+1)!}U|F|^{2k+1} = U\sinh(|F|),
\end{aligned}$$

what finishes the proof. ■

We now summarise our observations in the next proposition, that can also be found as [LT14, Proposition 6].

Proposition 7.2 — Hagedorn's wave packets and generalised squeezed states. Let $W \in \mathbb{C}^{n\times n}$ be symmetric and satisfy $W^*W < \mathrm{Id}$. Then,

$$Z = \begin{pmatrix} \mathrm{i}(\mathrm{Id} - W) \\ (\mathrm{Id} + W) \end{pmatrix} (\mathrm{Id} - |W|^2)^{-1/2} \tag{7.3}$$

is a normalised Lagrangian frame, while the squeezing operator $D(F)$ associated with W satisfies

$$D(F)\hat{a}D(F)^{-1} = \hat{A}(Z) \quad \text{and} \quad D(F)\hat{a}^\dagger D(F)^{-1} = \hat{A}^\dagger(Z).$$

Moreover, there exists a $c \in \mathbb{C}$ with $|c| = 1$ such that $\psi_k^F = c \cdot \varphi_k(Z)$ for all $k \in \mathbb{N}^n$. Conversely, if $Z = (P; Q) \in \mathbb{C}^{2n\times n}$ is a normalised Lagrangian frame, then

$$W = (Q + iP)(Q - iP)^{-1} \in \mathbb{C}^{n\times n}$$

is a complex symmetric matrix with $W^*W < \mathrm{Id}$. The associated squeezing operator satisfies

$$D(F)^{-1}\hat{A}(ZV)D(F) = \hat{a} \quad \text{and} \quad D(F)^{-1}\hat{A}^\dagger(ZV)D(F) = \hat{a}^\dagger$$

where the unitary matrix $V \in \mathbb{C}^{n\times n}$ results from the polar decomposition $Q - iP = |Q - iP|V^*$ and there is a constant $c \in \mathbb{C}$ with $|c| = 1$ such that $\psi_k^F = c \cdot \varphi_k(Z)$.

Proof. We already verified that (7.3) defines a normalised Lagrangian frame if $W = W^T \in \mathbb{C}^{n\times n}$ satisfies $W^*W < \mathrm{Id}$. Vice versa, let $Z = (P; Q)$ be a normalised Lagrangian frame. Then, we first note that

$$W = (Q + iP)(Q - iP)^{-1} = (\mathrm{Id} + \mathrm{i}B)(\mathrm{Id} - \mathrm{i}B)^{-1}$$

where $B = PQ^{-1}$. Since B is symmetric, W fulfils

$$W - W^T = (\mathrm{Id} - \mathrm{i}B)^{-1}\left((\mathrm{Id} - \mathrm{i}B)(\mathrm{Id} + \mathrm{i}B) - (\mathrm{Id} + \mathrm{i}B)(\mathrm{Id} - \mathrm{i}B)\right)(\mathrm{Id} - \mathrm{i}B)^{-1} = 0$$

and

$$\begin{aligned}\mathrm{Id} - W^*W &= (\mathrm{Id} - \mathrm{i}B)^{-*}\left((\mathrm{Id} + \mathrm{i}\overline{B})(\mathrm{Id} - \mathrm{i}B) - (\mathrm{Id} - \mathrm{i}\overline{B})(\mathrm{Id} + \mathrm{i}B)\right)(\mathrm{Id} - \mathrm{i}B)^{-1} \\ &= 4(\mathrm{Id} - \mathrm{i}B)^{-*}\left(\mathrm{Im}(B)\right)(\mathrm{Id} - \mathrm{i}B)^{-1} > 0\end{aligned}$$

since $\mathrm{Im}(B)$ is positive definite. For the ladder operators, we restate [CR12, Lemma 25],

$$D(F)\begin{pmatrix}\hat{a}\\ \hat{a}^\dagger\end{pmatrix}D(F)^{-1} = \begin{pmatrix}(\mathrm{Id} - WW^*)^{-1/2} & -W(\mathrm{Id} - W^*W)^{-1/2}\\ -(\mathrm{Id} - W^*W)^{-1/2}W^* & (\mathrm{Id} - W^*W)^{-1/2}\end{pmatrix}\begin{pmatrix}\hat{a}\\ \hat{a}^\dagger\end{pmatrix}. \tag{7.4}$$

We consider the two operators $\hat{A}_F(t) = D(tF)\hat{a}D(-tF)$ and $\hat{A}_F^\dagger(t) = D(tF)\hat{a}^\dagger D(-tF)$. These operators satisfy

$$\begin{aligned}\frac{d}{dt}\hat{A}_F(t) &= \tfrac{1}{2}\Big(((\hat{a}^\dagger)^T F\hat{a}^\dagger - \hat{a}^T F^*\hat{a})D(tF)\hat{a}D(-tF) - D(tF)\hat{a}((\hat{a}^\dagger)^T F\hat{a}^\dagger - \hat{a}^T F^*\hat{a})D(-tF)\Big) \\ &= \tfrac{1}{2}D(tF)\left[(\hat{a}^\dagger)^T F\hat{a}^\dagger - \hat{a}^T F^*\hat{a}, \hat{a}\right]D(-tF)\end{aligned}$$

since $(\hat{a}^\dagger)^T F\hat{a}^\dagger - \hat{a}^T F^*\hat{a}$ and $D(tF)$ commute and, analogously,

$$\frac{d}{dt}\hat{A}_F^\dagger(t) = \tfrac{1}{2}D(tF)\left[(\hat{a}^\dagger)^T F\hat{a}^\dagger - \hat{a}^T F^*\hat{a}, \hat{a}^\dagger\right]D(-tF).$$

With the commutator relations for $\hat{a}$ and $\hat{a}^\dagger$ from Lemma 3.2, we can simplify the commutators

$$\Big[(\hat{a}^\dagger)^T F \hat{a}^\dagger - \hat{a}^T F^* \hat{a}, \hat{a}\Big] = -F\hat{a}^\dagger, \quad \Big[(\hat{a}^\dagger)^T F \hat{a}^\dagger - \hat{a}^T F^* \hat{a}, \hat{a}^\dagger\Big] = -F^*\hat{a}$$

and obtain the differential equation

$$\frac{d}{dt}\begin{pmatrix} \hat{A}_F(t) \\ \hat{A}_F^\dagger(t) \end{pmatrix} = -\begin{pmatrix} 0 & F \\ F^* & 0 \end{pmatrix}\begin{pmatrix} \hat{A}_F(t) \\ \hat{A}_F^\dagger(t) \end{pmatrix}.$$

Evaluating the solution at $t = 1$ yields

$$D(F)\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} D(F)^{-1} = \exp\left(-\begin{pmatrix} 0 & F \\ F^* & 0 \end{pmatrix}\right)\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix}.$$

and it remains to determine the exponential matrix. With Lemma 7.2

$$\exp\left(-\begin{pmatrix} 0 & F \\ F^* & 0 \end{pmatrix}\right) = \Omega^T \exp\begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix}\Omega = \begin{pmatrix} U\cosh(|F|)U^* & -U\sinh(|F|) \\ -\sinh(|F|)U^* & \cosh(|F|) \end{pmatrix}$$

and since $\cosh(|F|) = (\mathrm{Id} - W^*W)^{-1/2}$, $\sinh(|F|)U^* = \cosh(|F|)W^*$, see [CR12, Eq. (3.55), (3.56)], we have

$$U\sinh(|F|) = (\sinh(|F|)U^*)^* = W\cosh(|F|)$$

and

$$\begin{aligned}(U\cosh(|F|)U^*)^2 &= U(\mathrm{Id} - W^*W)^{-1}U^* = (\mathrm{Id} - U^{-*}|W|^2U^{-1})^{-1} = (\mathrm{Id} - U|W||W|U^*)^{-1} \\ &= (\mathrm{Id} - WW^*)^{-1}.\end{aligned}$$

This proofs Equation (7.4). Let now $Z = (P; Q)$ be defined as in 7.3. Then, it follows,

$$\begin{aligned} D(F)\hat{a}^\dagger D(F)^{-1} &= \tfrac{1}{\sqrt{2\varepsilon}}(\mathrm{Id} - W^*W)^{-1/2}\left(-W^*(\hat{q} + \mathrm{i}\hat{p}) + (\hat{q} - \mathrm{i}\hat{p})\right) \\ &= \tfrac{1}{\sqrt{2\varepsilon}}(\mathrm{Id} - W^*W)^{-1/2}\left((\mathrm{Id} - W^*)\hat{q} - \mathrm{i}(\mathrm{Id} + W^*)\hat{p}\right) \\ &= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}\left(P^*\hat{q} - Q^*\hat{p}\right) = \hat{A}^\dagger(Z) \end{aligned}$$

and the claim for $\hat{A}(Z)$ consequently holds since

$$\begin{aligned} \hat{A}(Z) = \overline{\hat{A}^\dagger(Z)} &= \tfrac{1}{\sqrt{2\varepsilon}}(\mathrm{Id} - WW^*)^{-1/2}\left(-W(\hat{q} - \mathrm{i}\hat{p}) + (\hat{q} + \mathrm{i}\hat{p})\right) \\ &= (\mathrm{Id} - WW^*)^{-1/2}\hat{a} - (\mathrm{Id} - WW^*)^{-1/2}W\hat{a}^\dagger \\ &= (\mathrm{Id} - WW^*)^{-1/2}\hat{a} - W(\mathrm{Id} - W^*W)^{-1/2}\hat{a}^\dagger = D(F)\hat{a}D(F)^{-1}. \end{aligned}$$

For the coherent state $\varphi_0(Z)$ and the squeezed coherent state $\psi_0^F = D(F)\varphi_0$ this implies

$$0 = \hat{a}\varphi_0 = D(F)\hat{a}D(F)^{-1}\psi_0^F = \hat{A}(Z)\psi_0^F,$$

i.e. $\psi_0^F \in I(L)$ and since $D(F)$ is unitary, $\|\psi_0^F\| = 1$. Hence, there exists a $c \in \mathbb{C}$ with

$|c| = 1$ such that $\psi_0^F = c \cdot \varphi_0(Z)$. Moreover, for all $k \geq 0$ by (7.2)

$$\psi_k^F = \frac{1}{\sqrt{k!}} \hat{A}^\dagger(Z)_k \psi_k^F = c \cdot \varphi_k(Z).$$

The inversion can be shown equivalently by inserting $W = (Q + iP)(Q - iP)^{-1}$ into Equation (7.4) und utilise the above construction to related the states. ∎

7.2. Bogoliubov transformation

Another approach to obtain squeezed states is to modify Dirac's ladder operators via a Bogoliubov transformation. We briefly summarise the construction in [BFG16, §3].

A *Bogoliubov transformation* is a mapping from the ladder operators $\hat{a}$ and $\hat{a}^\dagger$ to operators $\hat{a}_S$ and $\hat{a}_S^\dagger$ that preserves the commutator relation, i.e. it holds

$$\left[(\hat{a}_S)_j, (\hat{a}_S^\dagger)_k\right] = \delta_{jk}, \quad \text{for} \quad 1 \leq j, k \leq n. \tag{7.5}$$

Such transforms can be expressed by means of symplectic matrices.

Lemma 7.3 Let $U, V \in \mathbb{C}^{n \times n}$. The matrix

$$S = \begin{pmatrix} U & -\overline{V} \\ -V & \overline{U} \end{pmatrix} \in \mathbb{C}^{2n \times 2n} \tag{7.6}$$

is symplectic if $U^*U - V^*V = \mathrm{Id}$ and $U^TV - V^TU = 0$.

Proof. A direct calculation shows

$$S^T \Omega S = \begin{pmatrix} U^T & -V^T \\ -V^* & U^* \end{pmatrix} \begin{pmatrix} V & -\overline{U} \\ U & -\overline{V} \end{pmatrix} = \begin{pmatrix} U^TV - V^TU & V^T\overline{V} - U^T\overline{U} \\ U^*U - V^*V & V^*\overline{U} - U^*\overline{V} \end{pmatrix}.$$

∎

We will now use symplectic matrices of this form to define a Bogoliubov transform as a linear, symplectic mapping. We assume in the following that S can always be written as (7.6).

Lemma 7.4 — Bogoliubov transform. Let S be symplectic and $\begin{pmatrix} \hat{a}_S \\ \hat{a}_S^\dagger \end{pmatrix} = S^* \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix}$, i.e.

$$\hat{a}_S = U^*\hat{a} - V^*\hat{a}^\dagger \quad \text{and} \quad \hat{a}_S^\dagger = U^T\hat{a}^\dagger - V^T\hat{a}.$$

Then, the components of $\hat{a}_S$ resp. $\hat{a}_S^\dagger$ commute and $\hat{a}_S$ and $\hat{a}_S^\dagger$ satisfy (7.5).

Proof. By definition we find for the components

$$\begin{aligned}[(\hat{a}_S)_j, (\hat{a}_S)_k] &= \left[\sum_{l=1}^n U_{j,l}^*\hat{a}_l - V_{j,l}^*\hat{a}_l^\dagger, \sum_{m=1}^n U_{k,m}^*\hat{a}_m - V_{k,m}^*\hat{a}_m^\dagger\right] = \sum_{l=1}^n \left(V_{j,l}^*\overline{U}_{l,k} - U_{j,l}^*\overline{V}_{l,k}\right) \\ &= \left(V^*\overline{U} - U^*\overline{V}\right)_{j,k},\end{aligned}$$

and

$$\begin{aligned}\left[(\hat{a}_S^\dagger)_j, (\hat{a}_S^\dagger)_k\right] &= \left[\sum_{l=1}^n U_{j,l}^T \hat{a}_l^\dagger - V_{j,l}^T \hat{a}_l, \sum_{m=1}^n U_{k,m}^T \hat{a}_m^\dagger - V_{k,m}^T \hat{a}_m\right] = \sum_{l=1}^n \left(U_{j,l}^T V_{l,k} - V_{j,l}^T U_{l,k}\right) \\ &= \left(U^T V - V^T U\right)_{j,k}.\end{aligned}$$

for all $1 \leq j, k \leq n$. Thus, the components commute if $U^T V - V^T U = 0$ and the commutator relation is equivalent to $U^* U - V^* V = \mathrm{Id}$, since

$$\begin{aligned}\left[(\hat{a}_S)_j, (\hat{a}_S^\dagger)_k\right] &= \left[\sum_{l=1}^n U_{j,l}^* \hat{a}_l - V_{j,l}^* \hat{a}_l^\dagger, \sum_{m=1}^n U_{k,m}^T \hat{a}_m^\dagger - V_{k,m}^T \hat{a}_m\right] = \sum_{l=1}^n \left(U_{j,l}^* U_{l,k} - V_{j,l}^* V_{l,k}\right) \\ &= \left(U^* U - V^* V\right)_{j,k}.\end{aligned}$$

■

This result exhibits the close relation of the Bogoliubov transformation to both, the squeezing operators introduced in the previous section and Hagedorn's wave packets. The form of $\hat{a}_S$ and $\hat{a}_S^\dagger$ in terms of U^*, V^* resp. U^T, V^T strongly reminds us of the form of $\hat{A}(Z)$ and $\hat{A}^\dagger(Z)$ in terms of P and Q. The symplectic map

$$\begin{pmatrix} \hat{a}_S \\ \hat{a}_S^\dagger \end{pmatrix} = \begin{pmatrix} U^* & -V^* \\ -V^T & U^T \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix}$$

on the other hand points to the operators $D(F)\hat{a}D(-F)$, resp. $D(F)\hat{a}^\dagger D(-F)$ we considered in the proof of Proposition 7.2. This connection gets even more obvious with the next statement.

Lemma 7.5 — Matrix factorisation. Let $U, V \in \mathbb{C}^{n\times n}$ satisfy

$$U^* U - V^* V = \mathrm{Id} \quad \text{and} \quad U^T V - V^T U = 0. \tag{7.7}$$

Then, U is invertible and the matrix $W = -VU^{-1} \in \mathbb{C}^{n\times n}$ is symmetric and satisfies

$$W^* W = \mathrm{Id} - (UU^*)^{-1} < \mathrm{Id}. \tag{7.8}$$

Conversely, if $W \in \mathbb{C}^{n\times n}$ is a symmetric matrix that satisfies (7.8), there exist U, V such that $W = -VU^{-1}$ and (7.7) holds true.

Proof. The invertibility of U follows from the first equation in (7.7). Assume that $Ux = 0$ for $x \in \mathbb{C}^n$, then $-|Vx|^2 = |x|^2$ and hence $x = 0$. Moreover, if (7.7) holds true,

$$W^* W = U^{-*} V^* V U^{-1} = U^{-*}(U^* U - \mathrm{Id})U^{-1} = \mathrm{Id} - (UU^*)^{-1}$$

and the inequality follows since UU^* is positive definite. For the symmetry of W we note that

$$W^T - W = -U^{-T} V^T + VU^{-1} = U^{-T}(U^T V - V^T U)U^{-1} = 0.$$

For the conversion we assume that $W = W^T$ fulfils $W^* W < \mathrm{Id}$. Then, we may define

$U = (\mathrm{Id} - W^*W)^{-1/2}$ and $V = -W(\mathrm{Id} - W^*W)^{-1/2}$ and find for this choice $U^TV = V^TU$ since W is symmetric and

$$U^*U - V^*V = (\mathrm{Id} - W^*W)^{-1/2}(\mathrm{Id} - W^*W)(\mathrm{Id} - W^*W)^{-1/2} = \mathrm{Id}.$$

■

Thus, if $W = W^T$ satisfies $W^*W < \mathrm{Id}$, the matrix

$$S^* = \begin{pmatrix} (\mathrm{Id} - W^*W)^{-1/2} & (\mathrm{Id} - W^*W)^{-1/2}W^* \\ W(\mathrm{Id} - W^*W)^{-1/2} & (\mathrm{Id} - WW^*)^{-1/2} \end{pmatrix}$$

is symplectic. Let furthermore F be defined as in (7.1). Then, we can write for the corresponding squeezing operators

$$D(F)\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} D(-F) = \Omega^T S^* \Omega \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} = S^{-*}\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix},$$

what proves the equivalence of the approaches via squeezing operators and the Bogoliubov transform.

With the determined ladder operators, the squeezed states $(\psi_k^S)_{k\in\mathbb{N}^n}$ can then be naturally constructed by the application of $\hat{a}_S^\dagger$ to the coherent squeezed state ψ_0^S that satisfies

$$\hat{a}_S\psi_0^S = 0.$$

We note here that in the indicated literature squeezed states are only defined as coherent states, not as excited states, see [BFG16, §2]. However, the comparison to the squeezing operators of [CR12] justify a more general point of view. With the same arguments as for the Hermite functions and Hagedorn's wave packets one can derive an explicit formula for ψ_0^S.

Proposition 7.3 — Squeezed coherent state. Let S be a symplectic matrix of the form (7.6) and $W = -VU^{-1}$. Then, every squeezed state ψ_0^S can be written as

$$\psi(x) = c \cdot e^{-\frac{1}{2\varepsilon}x^T(\mathrm{Id}-W^*)^{-1}(\mathrm{Id}+W^*)x}$$

for some $c \in \mathbb{C}$. In particular, the matrix $(\mathrm{Id} - W^*)^{-1}(\mathrm{Id} + W^*)$ is symmetric and has a positive definite real part.

Proof. The claim follows from Proposition 7.1 if one takes the inversion and complex conjugation into account. Or, from Lemma 4.2 if one notes that

$$\hat{a}_S\psi = (U^*\hat{a} - V^*\hat{a}^\dagger)\psi = U^*(\hat{a} + W^*\hat{a}^\dagger)\psi = 0$$

is equivalent to $(\hat{a} + W^*\hat{a}^\dagger)\psi = 0$ and

$$\hat{a} + W^*\hat{a}^\dagger = \frac{1}{\sqrt{2\varepsilon}}\left((\mathrm{Id} + W^*)\hat{q} + \mathrm{i}(\mathrm{Id} - W^*)\hat{p}\right).$$

■

If we add normalisation to the coherent squeezed state, $\|\psi_0^S\| = 1$, and define

$$\psi_k^S = \frac{1}{\sqrt{k!}}(\hat{a}_S^\dagger)^k \psi_0^S, \quad k \in \mathbb{N}^n$$

we can also explicitly state the relation to Hagedorn's wave packets. Although the existence of this link is already evident, the formulas are clearer and more convenient as in Proposition 7.1.

Proposition 7.4 — Hagedorn's wave packets and Bogoliubov transforms. Let $Z = (P; Q)$ with $P, Q \in \mathbb{C}^{n\times n}$ be a normalised Lagrangian frame. Then, the matrix S from Equation (7.6) with

$$U = \tfrac{1}{2}(\overline{Q} + \mathrm{i}\overline{P}) \quad \text{and} \quad V = \tfrac{1}{2}(\overline{Q} - \mathrm{i}\overline{P})$$

is symplectic and $\psi_k^S = \varphi_k(Z)$ for all $k \in \mathbb{N}^n$. Vice versa, if S as defined in (7.6) is symplectic, then

$$P = \mathrm{i}(\overline{U} - \overline{V}) \quad \text{and} \quad Q = (\overline{U} + \overline{V})$$

create a normalised Lagrangian frame $Z = (P; Q)$ and $\varphi_k(Z) = \psi_k^S$ for all $k \in \mathbb{N}^n$.

Proof. Let $Z = (P; Q)$ be a normalised Lagrangian frame and

$$S = \frac{1}{2}\begin{pmatrix} \overline{Q} + \mathrm{i}\overline{P} & -Q - \mathrm{i}P \\ -\overline{Q} + \mathrm{i}\overline{P} & Q - \mathrm{i}P \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -\mathrm{iId} & -\mathrm{Id} \\ -\mathrm{iId} & \mathrm{Id} \end{pmatrix}\begin{pmatrix} -\overline{Z} & Z \end{pmatrix}.$$

Then, S is symplectic since

$$S^T\Omega S = -\frac{\mathrm{i}}{2}\begin{pmatrix} -Z^* \\ Z^T \end{pmatrix}\Omega\begin{pmatrix} -\overline{Z} & Z \end{pmatrix} = -\frac{\mathrm{i}}{2}\begin{pmatrix} Z^*\Omega\overline{Z} & -Z^*\Omega Z \\ -Z^T\Omega\overline{Z} & Z^T\Omega Z \end{pmatrix} = \Omega.$$

Conversely, assume that S is symplectic and $Z = \begin{pmatrix} \mathrm{i}(\overline{U} - \overline{V}) \\ \overline{U} + \overline{V} \end{pmatrix}$. Then,

$$Z^*\Omega\overline{Z} = \begin{pmatrix} -\mathrm{i}(U - V)^T & (U + V)^T \end{pmatrix}\begin{pmatrix} -(U + V) \\ -\mathrm{i}(U - V) \end{pmatrix} = 2\mathrm{i}\left(U^TV - V^TU\right) = 0,$$

$$Z^T\Omega\overline{Z} = \begin{pmatrix} \mathrm{i}(U - V)^* & (U + V)^* \end{pmatrix}\begin{pmatrix} -(U + V) \\ -\mathrm{i}(U - V) \end{pmatrix} = -2\mathrm{i}\left(U^*U - V^*V\right) = -2\mathrm{iId}.$$

For the ladder operators, we find for $U = \frac{1}{2}(\overline{Q} + \mathrm{i}\overline{P})$, $V = \frac{1}{2}(\overline{Q} - \mathrm{i}\overline{P})$ with $\hat{a} + \hat{a}^\dagger = \sqrt{\frac{2}{\varepsilon}}\hat{q}$ and $\hat{a} - \hat{a}^\dagger = \sqrt{\frac{2}{\varepsilon}}\mathrm{i}\hat{p}$,

$$\begin{aligned} \hat{A}(Z) &= \frac{\mathrm{i}}{\sqrt{2\varepsilon}}(Q^T\hat{p} - P^T\hat{q}) = \frac{1}{2}(Q^T(\hat{a} - \hat{a}^\dagger) - \mathrm{i}P^T(\hat{a} + \hat{a}^\dagger))) = \frac{1}{2}((Q - \mathrm{i}P)^T\hat{a} - (Q + \mathrm{i}P)^T\hat{a}^\dagger) \\ &= U^*\hat{a} - V^*\hat{a}^\dagger = \hat{a}_S \end{aligned}$$

and analogously $\hat{A}^\dagger(Z) = \hat{a}_S^\dagger$. Moreover, if $P = \mathrm{i}(\overline{U} - \overline{V})$ and $Q = (\overline{U} + \overline{V})$,

$$\begin{aligned}\hat{a}_S &= U^*\hat{a} - V^*\hat{A}^\dagger = \tfrac{1}{\sqrt{2\varepsilon}}(U^*(\hat{q} + \mathrm{i}\hat{p}) - V^*(\hat{q} - \mathrm{i}\hat{p})) = \tfrac{1}{\sqrt{2\varepsilon}}((U-V)^*\hat{q} + \mathrm{i}(U+V)^*\hat{p}) \\ &= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}(Q^T\hat{p} - P^T\hat{q}) = \hat{A}(Z)\end{aligned}$$

and $\hat{a}_S^\dagger = \hat{A}^\dagger(Z)$, what proves the claim for the wave packets. ■

7.3. Metaplectic operators

As a last construction based on Dirac's ladder operators we also want to mention the approach in [Ohs15], where the author applies metaplectic operators to $\hat{a}$ and $\hat{a}^\dagger$.

The definition via squeezing operators presented in the first chapter is well-known, however, the relation between the matrices W and F might seem unintuitive at first sight and calculations can get more involved. The Bogoliubov transformations appeared as a more natural approach and had a clear link to Hagedorn's wave packets. By invoking metaplectic operators now, basic properties of the wave packets follow as a consequence of the properties of the Hermite functions and the metaplectic group, see [Ohs15] for more details.

We will only restate the relation between the operators here and refer to the literature for applications. In [Ohs15, Definition 2.6] the author starts with a more general view on ladder operators.

Definition 7.1 — Ladder operators. Let $X \in \mathbb{C}^{2n\times 2n}$ and set

$$\begin{pmatrix}\hat{a}_X \\ \hat{a}_X^\dagger\end{pmatrix} = X^T\Omega\hat{z}.$$

We call $\hat{a}_X$ and $\hat{a}_X^\dagger$ *ladder operators*, if their components commute, $\hat{a}_X^* = \hat{a}_X^\dagger$ and they satisfy the commutator relation $\left[(\hat{a}_X)_j, (\hat{a}_X^\dagger)_k\right] = \delta_{j,k}$ for all $1 \le j,k \le n$.

The properties required for ladder operators are exactly the ones we needed to define an orthonormal basis set in Section 3.2 and Section 4.3, respectively. By this definition it is clear that we can trace back the properties of $\hat{a}_X$ and $\hat{a}_X^\dagger$ to the properties of X.

Lemma 7.6 The components of $\hat{a}_X$ and $\hat{a}_X^\dagger$ commute and the operators satisfy

$$\left[(\hat{a}_X)_j, (\hat{a}_X^\dagger)_k\right] = \delta_{j,k}, \quad 1 \le j,k \le n$$

if and only if $X^T\Omega X = \frac{\mathrm{i}}{\varepsilon}\Omega$.

Proof. Let $X = \begin{pmatrix} A & B \\ C & D\end{pmatrix} \in \mathbb{C}^{2n\times 2n}$. Then,

$$X^T\Omega X = \begin{pmatrix} C^TA - A^TC & C^TB - A^TD \\ D^TA - B^TC & D^TB - B^TD\end{pmatrix}$$

and we can write the operators $\hat{a}_X$ and $\hat{a}_X^\dagger$ as $\hat{a}_X = C^T\hat{p} - A^T\hat{q}$ and $\hat{a}_X^\dagger = D^T\hat{p} - B^T\hat{q}$. The commutator relation (3.3), $[\hat{q}_j, \hat{p}_k] = \mathrm{i}\varepsilon\delta_{j,k}$, on the other hand yields for $1 \le j,k \le n$,

$$[(\hat{a}_X)_j, (\hat{a}_X)_k] = \mathrm{i}\varepsilon(C^TA - A^TC)_{j,k}, \quad [(\hat{a}_X^\dagger)_j, (\hat{a}_X^\dagger)_k] = \mathrm{i}\varepsilon(D^TB - B^TD)_{j,k}$$
$$[(\hat{a}_X)_j, (\hat{a}_X^\dagger)_k] = \mathrm{i}\varepsilon(C^TB - A^TD)_{j,k}.$$

■

In particular, we can write Dirac's ladder operators as operators of the form $\hat{a}_X$ resp. $\hat{a}_X^\dagger$. We have

$$\begin{pmatrix}\hat{a}\\ \hat{a}^\dagger\end{pmatrix} = \frac{1}{\sqrt{2\varepsilon}}\begin{pmatrix}\hat{q}+\mathrm{i}\hat{p}\\ \hat{q}-\mathrm{i}\hat{p}\end{pmatrix} = \frac{1}{\sqrt{2\varepsilon}}\begin{pmatrix}-\mathrm{Id} & \mathrm{i}\mathrm{Id}\\ -\mathrm{Id} & -\mathrm{i}\mathrm{Id}\end{pmatrix}\begin{pmatrix}0 & -\mathrm{Id}\\ \mathrm{Id} & 0\end{pmatrix}\begin{pmatrix}\hat{p}\\ \hat{q}\end{pmatrix} := X_0^T\Omega\hat{z}$$

and one can easily check that $X_0^T\Omega X_0 = \frac{\mathrm{i}}{\varepsilon}\Omega$. This form turns out to be the canonical form for ladder operators $\hat{a}_X$ and $\hat{a}_X^\dagger$.

Theorem 7.1 The operators $\hat{a}_X$ and $\hat{a}_X^\dagger$ define ladder operators if and only if X can be written as $X = SX_0$ with $S \in \mathrm{Sp}(n,\mathbb{R})$. If $S = \begin{pmatrix}A & B\\ C & D\end{pmatrix} \in \mathbb{R}^{2n\times 2n}$, the operators are given by

$$\begin{aligned}\hat{a}_X &= \frac{\mathrm{i}}{\sqrt{2\varepsilon}}\left((D+\mathrm{i}C)^T\hat{p} - (B+\mathrm{i}A)^T\hat{q}\right)\\ \hat{a}_X^\dagger &= \frac{-\mathrm{i}}{\sqrt{2\varepsilon}}\left((D-\mathrm{i}C)^T\hat{p} - (B-\mathrm{i}A)^T\hat{q}\right).\end{aligned} \tag{7.9}$$

Proof. We will only give a sketch of the proof and refer to [Ohs15, Theorem 2.8] for details. If $S \in \mathrm{Sp}(n,\mathbb{R})$, we have

$$(SX_0)^T\Omega(SX_0) = \frac{\mathrm{i}}{\varepsilon}S^T\Omega S = \frac{\mathrm{i}}{\varepsilon}\Omega$$

and since S is a real-valued matrix, (7.9) directly implies that $\hat{a}_X$ and $\hat{a}_X^\dagger$ are formal adjoints. Thus, if $X = SX_0$, $\hat{a}_X$ and $\hat{a}_X^\dagger$ define ladder operators.

Conversely, assume that $X = \begin{pmatrix}U & V\\ W & Z\end{pmatrix} \in \mathbb{C}^{2n\times 2n}$ parametrises ladder operators $\hat{a}_X$ and $\hat{a}_X^\dagger$. Then, due to the previous lemma, it must hold that $X^T\Omega X = \frac{\mathrm{i}}{\varepsilon}\Omega$ and

$$\hat{a}_X = W^T\hat{p} - U^T\hat{q} \quad \text{and} \quad \hat{a}_X^\dagger = Z^T\hat{p} - V^T\hat{q}$$

are adjoints if and only if $V = \overline{U}$ and $Z = \overline{W}$. Combining these two conditions shows that X can be written in the form SX_0 where S is real and symplectic. ■

With this theorem we can express any ladder operators $\hat{a}_X$ and $\hat{a}_X^\dagger$ via a symplectic matrix and Dirac's ladder operators. Moreover, we can describe the action of S with a metaplectic operator, see [Gos10, §7.1]. Since our notation is varying from the one in the indicated literature we summarise definition and properties of the metaplectic group inAppendix B and here only give a brief overview.

Definition 7.2 — Free symplectic matrix and generating function. We call a matrix

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathrm{Sp}(n, \mathbb{R}) \tag{7.10}$$

a *free* symplectic matrix, if $\det(C) \neq 0$. We moreover associate with every symplectic matrix a quadratic form, the *generating function* of S,

$$\sigma(q, q') = \tfrac{1}{2} q^T C^{-1} D q - q^T C^{-1} q' + \tfrac{1}{2} q'^T A C^{-1} q'.$$

Conversely, if $\sigma(q, q') = \frac{1}{2} q^T K q - q^T L q' + \frac{1}{2} q'^T M q'$ with $K, L, M \in \mathbb{R}^{n \times n}$ and $\det(L) \neq 0$, the matrix

$$S_\sigma = \begin{pmatrix} ML^{-1} & ML^{-1}K - L^T \\ L^{-1} & L^{-1}K \end{pmatrix}$$

is a free symplectic matrix with generating function σ.

Based on its generating function we now assign an operator to any free symplectic matrix S, see [Gos10, Eq. (7.3)].

Definition 7.3 — Quadratic Fourier transform. Let S be a free symplectic matrix of the form (B.1) and σ the corresponding generating function. We define

$$(\hat{S}_\sigma \psi)(x) = (2\pi\varepsilon)^{-n/2} \det(C)^{-1/2} \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\sigma(x,x')} \psi(x')\, dx'$$

for all $\psi \in \mathcal{S}(\mathbb{R}^n)$.

We can also write the standard Fourier transform $\mathcal{F}^\varepsilon$ in this manner: We have

$$\sigma(x, x') = -x^T x',$$

i.e. $K = M = 0$ and $L = \mathrm{Id}$. Hence, the corresponding symplectic matrix is Ω, $\mathcal{F}^\varepsilon = \hat{\Omega}$.

So far, we only considered free symplectic matrices. But the quadratic Fourier forms generate a subgroup of all unitary operators on $L^2(\mathbb{R}^n)$ that is called the *metaplectic group* $\mathrm{Mp}(n, \mathbb{R})$. Elements of $\mathrm{Mp}(n, \mathbb{R})$ are denoted as *metaplectic operators*, see [Gos10, Definition 109]. In particular, one can show that every $\hat{S} \in \mathrm{Mp}(n, \mathbb{R})$ can be written as a product of two quadratic Fourier forms, $\hat{S} = \hat{S}_\sigma \hat{S}_{\sigma'}$, see [Gos10, Proposition 110]. Moreover, the metaplectic group $\mathrm{Mp}(n, \mathbb{R})$ is a twofold covering of the symplectic group and there exists a surjective homomorphism

$$\pi^{\mathrm{Mp}} : \mathrm{Mp}(n, \mathbb{R}) \mapsto \mathrm{Sp}(n, \mathbb{R}), \quad \hat{S} \to S,$$

see Theorem B.3 for a more detailed proof. Thus, for any symplectic matrix S there exists a metaplectic operator $\hat{S}$ such that $\pi^{\mathrm{Mp}}(\hat{S}) = S$, see [Gos10, Theorem 114].

This metaplectic operator now allows us to separate the symplectic matrix and Dirac's ladder operators.

Proposition 7.5 Let $\hat{S} \in \mathrm{Mp}(n,\mathbb{R})$ and $S = \pi^{\mathrm{Mp}}(\hat{S}) \in \mathrm{Sp}(n,\mathbb{R})$. Then, we have

$$\hat{a}_{SX} = \hat{S}\hat{a}_X\hat{S}^{-1} \quad \text{and} \quad \hat{a}^\dagger_{SX} = \hat{S}\hat{a}^\dagger_X\hat{S}^{-1}$$

for all $X \in \mathbb{C}^{2n\times 2n}$.

Proof. This statement is adopted from [Ohs15, Proposition 210]. It is a direct consequence of Theorem B.4 respectively [Gos10, Lemma 120]. One can prove the claim by showing that the relation holds true for the generators of $\mathrm{Sp}(n,\mathbb{R})$ respectively their quadratic Fourier forms that are generators of $\mathrm{Mp}(n,\mathbb{R})$. ∎

The previous proposition implies that all ladder operators can be written as

$$\hat{a}_X = \hat{S}\hat{a}\hat{S}^{-1} \quad \text{and} \quad \hat{a}^\dagger_X = \hat{S}\hat{a}^\dagger\hat{S}^{-1}$$

where $S = \pi^{\mathrm{Mp}}(\hat{S})$ satisfies $X = SX_0$. This means that we can in particular express the ladder operators of Hagedorn's wave packets in this way, we only have to find a suitable symplectic matrix S. But comparing Equation (7.9) and $\hat{A}(Z) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}(Q^T\hat{p} - P^T\hat{q})$ for $Z = (P;Q)$ directly yields

$$S = \begin{pmatrix} \mathrm{Im}(P) & \mathrm{Re}(P) \\ \mathrm{Im}(Q) & \mathrm{Re}(Q) \end{pmatrix}.$$

Proposition 7.6 — Ladder correspondence. Let $Z \in \mathbb{C}^{2n\times n}$ be a normalised Lagrangian frame and $S = \begin{pmatrix} \mathrm{Im}(Z) & \mathrm{Re}(Z) \end{pmatrix} \in \mathbb{R}^{2n\times 2n}$. Then, S is symplectic and

$$\hat{A}(Z) = \hat{S}\hat{a}\hat{S}^{-1}, \qquad \hat{A}^\dagger(Z) = \hat{S}\hat{a}^\dagger\hat{S}^{-1}.$$

Proof. We already stated that if Z is a normalised Lagrangian frame the matrix

$$S' = \begin{pmatrix} \mathrm{Re}(Z) & -\mathrm{Im}(Z) \end{pmatrix}$$

is symplectic, see Remark 2.1. Since $S = S'\Omega^T$ the symplecticity of S is a direct consequence. The statement for the ladders follows from the previous proposition and Equation (7.9). ∎

With the relation of the ladder operators we also found another connection between Hermite functions and Hagedorn's wave packets. Based on this correspondence we could equivalently prove the formulas for the Fourier transform in Theorem 4.5 and the generating functions of the polynomials from Proposition 5.1, see [Ohs15].

Corollary 7.1 — Wave packet correspondence. For a normalised Lagrangian frames $Z \in \mathbb{C}^{2n\times n}$ and $S = \begin{pmatrix} \mathrm{Im}(Z) & \mathrm{Re}(Z) \end{pmatrix}$ it holds

$$\varphi_k(Z) = \hat{S}\varphi_k, \qquad \forall\, k \in \mathbb{N}^n,$$

where φ_k denotes the k-th multi-dimensional Hermite function, $\varphi_k = \varphi_k(Z_0)$.

Proof. For the coherent state $\varphi_0(Z)$ we deduce from

$$0 = \hat{A}(Z)\varphi_0(Z) = \hat{S}\hat{a}\hat{S}^{-1}\varphi_0(Z)$$

that $\hat{S}^{-1}\varphi_0(Z) = \varphi_0$, since all functions satisfying $\hat{a}\psi = 0$ are constant multiples of φ_0 due to Lemma 3.3 and $\hat{S}^{-1}$ as a unitary operator preserves the norm. So $\varphi_0(Z) = \hat{S}\varphi_0$ and we find for the excited states

$$\varphi_k(Z) = \tfrac{1}{\sqrt{k!}}\hat{A}_k^\dagger(Z)\varphi_0(Z) = \tfrac{1}{\sqrt{k!}}(\hat{S}\hat{a}^\dagger\hat{S}^{-1})^k\varphi_0(Z) = \tfrac{1}{\sqrt{k!}}\hat{S}\hat{a}_k^\dagger\varphi_0 = \hat{S}\varphi_k$$

with $k \in \mathbb{N}^n$. ∎

7.4. Wigner functions

The alternative representations of Hagedorn's wave packets we presented so far nicely illustrate the relation of the wave packets to the Hermite functions and give reasons why they adopt many of their properties. A very short proof of the equivalence of Hagedorn's wave packets and generalised squeezed states though can be given if we consider the Wigner function of the wave packets.

We invoke [Gos10, Definition 246] and characterise generalised squeezed states via their phase space representation.

Definition 7.4 — Squeezed states. A function $\psi \in \mathcal{S}(\mathbb{R}^n)$ is called a *squeezed coherent state* if its Wigner transform is

$$\mathcal{W}^\varepsilon(\psi)(z) = (\pi\varepsilon)^{-n}e^{-\frac{1}{\varepsilon}z^TGz}, \quad z \in \mathbb{R}^n \oplus \mathbb{R}^n,$$

where $G \in \mathrm{Sp}(n,\mathbb{R})$ is positive definite: $G = G^T > 0$.

This definition unfortunately only includes coherent states, but we can directly derive from Proposition 6.2 that $\varphi_0(Z)$ is a squeezed coherent state for all normalised Lagrangian frames $Z \in \mathbb{C}^{2n\times n}$. Moreover, we can show that every squeezed state by this characterisation can be written as a Hagedorn wave packet.

Proposition 7.7 — Hagedorn ground states and squeezed coherent states. Let $\psi \in \mathcal{S}(\mathbb{R}^n)$ be a squeezed coherent state. Then, there exists a normalised Lagrangian frame $Z \in \mathbb{C}^{2n\times n}$ such that

$$\psi = c \cdot \varphi_0(Z)$$

for $c \in \mathbb{C}$ with $|c| = 1$.

Proof. Since ψ is a squeezed coherent state, there exists a symmetric, positive definite $G \in \mathrm{Sp}(n,\mathbb{R})$ such that $\mathcal{W}^\varepsilon(\psi)(z) = (\pi\varepsilon)^{-n}e^{-\frac{1}{\varepsilon}z^TGz}$. By Lemma 2.4 we can construct a normalised Lagrangian frame Z with $G = \Omega^T\mathrm{Re}(ZZ^*)\Omega$ and, in particular,

$$\mathcal{W}^\varepsilon\varphi_0(Z) = (\pi\varepsilon)^{-n}e^{-\frac{1}{\varepsilon}z^TGz}.$$

But $\mathcal{W}^\varepsilon(\varphi) = \mathcal{W}^\varepsilon(\psi)$ for $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$ implies

$$\int_{\mathbb{R}^n} \overline{\varphi}(x + \frac{y}{2})\varphi(x - \frac{y}{2})e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)}\, dy = \int_{\mathbb{R}^n} \overline{\psi}(x + \frac{y}{2})\psi(x - \frac{y}{2})e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)}\, dy$$

for all $(\xi, x) \in \mathbb{R}^n \oplus \mathbb{R}^n$. Applying the inverse Fourier transform $(\mathcal{F}^\varepsilon)^{-1}$ on both sides shows

$$\overline{\varphi}(x + \frac{y}{2})\varphi(x - \frac{y}{2}) = \overline{\psi}(x + \frac{y}{2})\psi(x - \frac{y}{2})$$

for almost every $x, y \in \mathbb{R}^n$ and hence $\varphi = c \cdot \psi$ for $c \in \mathbb{C}$ with $|c| = 1$, see [Fol89, Proposition 1.98]. ■

Thus, the coherent states in Hagedorn's parametrisation are equivalent to the squeezed coherent states from [Gos10]. This definition is also consistent with the approach via metaplectic operators from the previous section.

Proposition 7.8 A function $\psi \in \mathcal{S}(\mathbb{R}^n)$ is a squeezed coherent state if and only if there exists a $\hat{S} \in \mathrm{Mp}(n, \mathbb{R})$ such that

$$\psi = e^{\mathrm{i}\gamma}\hat{S}\varphi_0$$

where φ_0 is the standard coherent state and $\gamma \in \mathbb{R}$.

Proof. This result is adopted from [Gos10, Proposition 247]. Since G is symmetric and symplectic, there exists a symplectic matrix $S \in \mathrm{Sp}(n, \mathbb{R})$ such that $G = S^TS$. Thus, if $\psi \in \mathcal{S}(\mathbb{R}^n)$ is a squeezed coherent state,

$$\mathcal{W}^\varepsilon(\psi)(z) = (\pi\varepsilon)^{-n}e^{-\frac{1}{\varepsilon}(Sz)^TSz} = \mathcal{W}^\varepsilon(\varphi_0)(Sz).$$

Moreover, due to the metaplectic covariance formula for the Wigner transform,

$$\mathcal{W}^\varepsilon(\psi)(S^{-1}z) = \mathcal{W}^\varepsilon(\hat{S}\psi)(z),$$

see [Gos10, Corollary 217], we conclude that ψ and $\hat{S}\varphi_0$ possess the same Wigner function. With the same argument as in the previous proof ψ can be written as a phase factor times $\hat{S}\varphi_0$. ■

Part II.

Dynamics

8. Hermitian Schrödinger dynamics

To start with the dynamical part we first examine the well-studied case of a time evolution that is governed by a Hermitian, quadratic Hamiltonian. We also use this preparatory chapter to set some notation and introduce the required essentials of quantum dynamics.

After the first two introductory sections, we restate Hagedorn's findings of the 1980's in [Hag80], [Hag81] and [Hag85] in terms of Lagrangian frames. For quadratic Hamiltonians, it has been shown that the wave packets are exact solutions to Schrödinger's equation, while for general Hamiltonians they provide an approximation of order $\varepsilon^{l/2}$ for arbitrary large l, see Section 8.4. Our aim in this part of the thesis is to transfer this approach to non-Hermitian Hamiltonians.

For this purpose we present an alternative proof of the evolution for quadratic Hamiltonians by means of Lagrangian frames and thereby demonstrate techniques we will build on in the following chapters. We furthermore try to highlight difficulties that will arise under a non-unitary time evolution.

8.1. Time evolution

In classical mechanics the state of a particle is fully described by its position $x \in \mathbb{R}^n$ and its momentum $p \in \mathbb{R}^n$. In quantum mechanics, due to the uncertainty principle, it is not possible to measure both, position and momentum, exactly at the same time. The state of a particle is described by a complex-valued wave function

$$\psi : \mathbb{R}^n \times \mathbb{R} \mapsto \mathbb{C},\ (x,t) \to \psi(x,t).$$

Following the statistical interpretation of Born in [Bor26], we interpret $|\psi(\cdot,t)|^2$ as probability distribution of the position of a particle at time t and therefore demand $\psi(\cdot,t) \in L^2(\mathbb{R}^n)$ and

$$\|\psi(\cdot,t)\|^2 = \int_{\mathbb{R}^n} |\psi(x,t)|^2\, dx = 1.$$

The *state space* of a quantum system can thus be represented by the complex Hilbert space $L^2(\mathbb{R}^n)$ and all possible states correspond to normalised elements of this space.

Characteristics of the particle such as position, momentum or energy then appear due to Bohr's correspondence principle as operators acting on $L^2(\mathbb{R}^n)$, see [CR12, §2.1]. We use the Weyl quantisation briefly introduced in Section 3.1 and studied in more detail in Appendix A to associate with every function $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$ a linear operator $\mathrm{op}_\varepsilon[a]$. The symbol $a = a(p,q)$ is thereby a function of position q and momentum p and called a *classical observable*, the operator $\mathrm{op}_\varepsilon[a] = \hat{a}$ is the corresponding *quantum observable*.

The space $\mathbb{R}^n \oplus \mathbb{R}^n$ is moreover denoted as *phase space*.

As for position and momentum it is in general not possible to measure observables directly, we can only realise their expectation values. If $\psi = \psi(\cdot, t) \in L^2(\mathbb{R}^n)$ is a possible state of a system and $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$ an observable, the expectation value of a in ψ is given by

$$\langle \hat{a} \rangle_\psi = \langle \psi, \hat{a}\psi \rangle = \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\psi)(z) a(z)\, dz, \tag{8.1}$$

see [Gos10, Definition 204].

Our ambition in the following is to deduce the time evolution of Hagedorn's wave packets under quadratic Hamiltonians, i.e. for a given initial state $\psi_0 \in L^2(\mathbb{R}^n)$ we want to determine the state $\psi(x,t)$ at time t. Let us assume that there exist operators $\widehat{\mathcal{U}}(t)$, $t \geq 0$, such that

$$\psi(x,t) = \widehat{\mathcal{U}}(t)\psi_0(x).$$

We call such an operator a *time evolution operator*. To ensure that the so described dynamic is meaningful, the propagation should be unique and satisfy $\psi(x,0) = \psi_0(x)$. This leads to the following definition, see also [Vra03, Definition 2.1.2] or Definition C.1.

Definition 8.1 — One-parameter semigroup. We call a family $\left\{\widehat{\mathcal{U}}(t)\,;\, t \geq 0\right\}$ of operators on $L^2(\mathbb{R}^n)$ a *strongly continuous one-parameter semigroup*, if $\widehat{\mathcal{U}}(0) = \mathrm{id}$,

$$\widehat{\mathcal{U}}(t+s) = \widehat{\mathcal{U}}(t)\widehat{\mathcal{U}}(s) \qquad \text{for all } t, s \geq 0, \tag{8.2}$$

and $\lim\limits_{t \downarrow 0} \widehat{\mathcal{U}}(t)\psi = \psi$ for all $\psi \in L^2(\mathbb{R}^n)$.

Equation (8.2) there contains the addressed uniqueness of the time evolution: we find for an initial state $\psi_0 = \psi(\dot{;}0)$ that

$$\psi(x,t) = \widehat{\mathcal{U}}(t)\psi(x,0) = \widehat{\mathcal{U}}(s)\psi(x,t-s)$$

for $0 \leq s \leq t$, i.e. we end up with the same state $\psi(x,t)$ independently of the starting point of the time evolution. Appendix C provides a closer study of one-parameter semigroups.

Assuming that such a strongly continuous semigroup exists, we can always characterise it by its infinitesimal generator, see Definition C.2 or [EN00, Definition II.1.2].

Definition 8.2 — Hamiltonian. Let $\left\{\widehat{\mathcal{U}}(t)\,;\, t \geq 0\right\}$ be a strongly continuous semigroup that describes the time evolution of our system. Then, the generator

$$\widehat{\mathcal{H}} : D(\widehat{\mathcal{H}}) \mapsto L^2(\mathbb{R}^n),\ \psi \to \widehat{\mathcal{H}}\psi = \lim_{t \downarrow 0} \tfrac{\mathrm{i}\varepsilon}{t}(\widehat{\mathcal{U}}(t)\psi - \psi)$$

is called the *Hamiltonian operator*, or short *Hamiltonian* of the system. The domain $D(\widehat{\mathcal{H}})$ is the subset of $L^2(\mathbb{R}^n)$ where this limit exists.

The Hamiltonian can also be viewed as the quantum observable corresponding to the total energy of the system, see [Tes09, §2.1].

If we consider a closed system, our evolution is conservative and we find for all states $\psi \in L^2(\mathbb{R}^n)$

$$\|\widehat{\mathcal{U}}(t)\psi\| = \|\psi\|.$$

In other words, the operators $\widehat{\mathcal{U}}(t)$, $t \geq 0$, are unitary. The existence of a self-adjoint Hamiltonian then follows by Stone's theorem that was originally found in [Sto30]. For detailed proofs see also [RS80, Theorem VIII.8] or [AF01, Theorem 3.1].

Theorem 8.1 — Stone's theorem. There exists for any strongly continuous one-parameter semigroup $\left\{\widehat{\mathcal{U}}(t)\,;\, t \geq 0\right\}$ of unitary operators on $L^2(\mathbb{R}^n)$ a uniquely self-adjoint operator $\widehat{\mathcal{H}}$ such that

$$\widehat{\mathcal{U}}(t) = e^{-\frac{\mathrm{i}}{\varepsilon} t \widehat{\mathcal{H}}} \quad \text{for all } t \geq 0. \tag{8.3}$$

Vice versa assume that $\widehat{\mathcal{H}}$ is a self-adjoint operator on $L^2(\mathbb{R}^n)$. Then, (8.3) defines a unique family of unitary operators that is strongly continuous and satisfies (8.2).

We stress here that $\widehat{\mathcal{H}}$ is in general an unbounded operator, the exponential in (8.3) can not simply be seen as a power series, but must be interpreted with the spectral theorem for self-adjoint operators, see [RS80, Theorem VIII.7].

If we will allow for an interaction of our system with the environment, i.e. consider a dissipative system, the time evolution operator $\widehat{\mathcal{U}}(t)$ will in general not be unitary, but satisfy

$$\|\widehat{\mathcal{U}}(t)\psi\| \leq \|\psi\| \tag{8.4}$$

for all $\psi \in L^2(\mathbb{R}^n)$. Such a semigroup is called a *contraction semigroup*, see Proposition C.1, or a *quantum dynamical semigroup*, see [CF98, Definition 2.1]. To show the existence of such evolution operators resp. determine the corresponding Hamiltonians we have to expend more effort, see Section 9.1 and Appendix C.

However, we will in the following always assume that $\widehat{\mathcal{U}}(t)$ exists at least for some times $t \in [0;T[$. In any case we can state the following general result for semigroups $\{\widehat{\mathcal{U}}(t)\,;\, t \geq 0\}$ and their generators $\widehat{\mathcal{H}}$, see [HP57, Theorem 10.3.3].

Lemma 8.1 — Time evolution. Let $\{\widehat{\mathcal{U}}(t)\,;\, t \geq 0\}$ be a strongly continuous one-parameter semigroup and $\widehat{\mathcal{H}}$ the corresponding Hamiltonian. Then, we find for all $\psi \in \mathcal{D}(\widehat{\mathcal{H}})$ and $t \geq 0$

$$\mathrm{i}\varepsilon\, \partial_t \widehat{\mathcal{U}}(t)\psi = \widehat{\mathcal{H}}\widehat{\mathcal{U}}(t)\psi. \tag{8.5}$$

This means $\widehat{\mathcal{U}}(t)$ can be seen as the formal solution to

$$\mathrm{i}\varepsilon\, \partial_t \widehat{\mathcal{U}}(t) = \widehat{\mathcal{H}}\widehat{\mathcal{U}}(t), \qquad \widehat{\mathcal{U}}(0) = \mathrm{id}. \tag{8.6}$$

Proof. Let $\psi \in \mathcal{D}(\widehat{\mathcal{H}})$. Then, the main idea is to use (8.2),

$$\mathrm{i}\varepsilon\, \partial_t \widehat{\mathcal{U}}(t)\psi = \lim_{s \to 0} \tfrac{\mathrm{i}\varepsilon}{s}\big(\widehat{\mathcal{U}}(t+s)\psi - \widehat{\mathcal{U}}(t)\psi\big) = \lim_{s \to 0} \tfrac{\mathrm{i}\varepsilon}{s}\big(\widehat{\mathcal{U}}(s) - \mathrm{id}\big)\widehat{\mathcal{U}}(t)\psi = \widehat{\mathcal{H}}\widehat{\mathcal{U}}(t)\psi.$$

A detailed proof considering derivatives from both sides is given in Theorem C.1. ∎

8.2. Quadratic Hamiltonians

Starting from an initial state ψ_0 in the previous lemma leads to the well-known evolution equation

$$\mathrm{i}\varepsilon\,\partial_t\psi(t) = \widehat{\mathcal{H}}\psi(t), \tag{8.7}$$

Schrödinger introduced in [Sch26]. This equality is the fundamental law in physics and chemistry for describing the propagation of non-relativistic particles, see [Lub08, §I.1.2]. For applications one usually chooses ε to be Planck's constant and the Hamiltonian as kinetic and potential energy

$$\widehat{\mathcal{H}} = -\tfrac{\varepsilon^2}{2m}\Delta + V.$$

In this thesis we will pursue a more abstract point of view and consider quadratic Hamiltonians, i.e. Hamiltonians of the above form with a potential V that is quadratic in x or the harmonic oscillator, for example. It is known, that in this case Gaussian functions stay Gaussians over time, see e.g. [Hel75], and also Hagedorn's wave packets keep their structure, see [Hag81].

So far, we only considered the Weyl-quantisation of Schwartz symbols $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$. However, to define quadratic Hamiltonians, we need to invoke a broader class of symbols, see [Fol89, Theorem 2.21].

Definition 8.3 — General symbol classes. Let $\langle x\rangle := (1+|x|^2)^{1/2}$ for $x \in \mathbb{R}^n$. Then, for every function $a \in C^\infty(\mathbb{R}^n \oplus \mathbb{R}^n)$ where constants $K \in \mathbb{R}$ and $\delta < 1$ exist such that

$$\left|\partial_\xi^\alpha \partial_x^\beta a(\xi, x)\right| \le C_{\alpha,\beta}\langle\xi\rangle^{K+\delta(|\alpha|+|\beta|)}$$

for all multiindices $\alpha, \beta \in \mathbb{N}^n$ the corresponding Weyl-quantisation $\mathrm{op}_\varepsilon[a]$ defines a linear operator on $\mathcal{S}(\mathbb{R}^n)$. We call such functions a an *admissible symbol* or an *observable*.

These general symbol classes contain also polynomials in z. A similar formulation can be found in [Zwo11, §4.4] and we also present a more detailed study in Appendix A.

So, taking Weyl-operators of quadratic symbols is well-defined and we can state the following explicit formula in terms of position and momentum operator, see also [Gos10, §15.1.1].

Lemma 8.2 — Quadratic Hamiltonians. Let $\mathcal{H}(z) = \frac{1}{2}z^T H z$ be a quadratic form on $\mathbb{R}^n \oplus \mathbb{R}^n$ with

$$H = H^T = \begin{pmatrix} H_{pp} & H_{pq} \\ H_{qp} & H_{qq} \end{pmatrix} \in \mathbb{C}^{2n\times 2n}. \tag{8.8}$$

Then, the corresponding Weyl-operator can be written as

$$\widehat{\mathcal{H}} = -\tfrac{\varepsilon^2}{2}\nabla_x^T H_{pp}\nabla_x + \tfrac{\varepsilon}{\mathrm{i}}x^T H_{qp}\nabla_x + \tfrac{1}{2}x^T H_{qq}x - \tfrac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(H_{pq})$$

and $\widehat{\mathcal{H}}$ is self-adjoint if and only if $\mathrm{Im}(H) = 0$.

Proof. The form of the Weyl-operator is referenced from Lemma A.4, with $\hat{q} = x$ and

$\hat{p} = -\mathrm{i}\varepsilon\nabla_x$,

$$\begin{aligned}\tfrac{1}{2}\hat{z}^T H \hat{z} &= \tfrac{1}{2}\left(-\varepsilon^2\nabla_x^T H_{pp}\nabla_x - \mathrm{i}\varepsilon\nabla_x^T(H_{pq}x) - \mathrm{i}\varepsilon\, x^T(H_{qp}\nabla_x) + x^T H_{qq}x\right)\\ &= -\tfrac{\varepsilon^2}{2}\nabla_x^T H_{pp}\nabla_x + \tfrac{\varepsilon}{\mathrm{i}}x^T H_{qp}\nabla_x + \tfrac{1}{2}x^T H_{qq}x - \tfrac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(H_{pq}),\end{aligned}$$

the remark about the self-adjointness is a consequence of [Zwo11, Theorem 4.1]. ■

Besides studying the time evolution of the state itself we can also investigate how the expectation of an observable a changes along the solution $\psi(t)$. We have

$$\langle\hat{a}\rangle_{\psi(t)} = \langle\widehat{\mathcal{U}}(t)\psi(0), \hat{a}\,\widehat{\mathcal{U}}(t)\psi(0)\rangle = \langle\psi(0), \widehat{\mathcal{U}}(t)^{-1}\hat{a}\,\widehat{\mathcal{U}}(t)\psi(0)\rangle = \langle\widehat{\mathcal{U}}(t)^{-1}\hat{a}\,\widehat{\mathcal{U}}(t)\rangle_{\psi(0)}$$

and hence define $\hat{a}(t) := \widehat{\mathcal{U}}(t)^{-1}\hat{a}\,\widehat{\mathcal{U}}(t)$. If $\widehat{\mathcal{H}}$ is self-adjoint, we may again use the exponential form and also write

$$\hat{a}_t = e^{\frac{\mathrm{i}}{\varepsilon}t\widehat{\mathcal{H}}}\,\hat{a}\,e^{-\frac{\mathrm{i}}{\varepsilon}t\widehat{\mathcal{H}}},$$

see [Lub08, §I.4.2].

Lemma 8.3 — Heisenberg equation. Let a be an admissible observable and

$$\hat{a}(t) = \widehat{\mathcal{U}}(t)^{-1}\hat{a}\,\widehat{\mathcal{U}}(t).$$

Then, it holds

$$\mathrm{i}\varepsilon\,\partial_t\hat{a}_t = [\hat{a}_t, \widehat{\mathcal{H}}]. \tag{8.9}$$

Proof. A formal calculation using Equation (8.6) yields

$$\mathrm{i}\varepsilon\,\partial_t\hat{a}_t = -\widehat{\mathcal{H}}\widehat{\mathcal{U}}(t)^{-1}\hat{a}\,\widehat{\mathcal{U}}(t) + \widehat{\mathcal{U}}(t)^{-1}\hat{a}\widehat{\mathcal{H}}\,\widehat{\mathcal{U}}(t) = [\hat{a}_t, \widehat{\mathcal{H}}]$$

where we used that $\widehat{\mathcal{U}}(t)$ and $\widehat{\mathcal{H}}$ commute, see [HP57, Theorem 10.3.3] or Theorem C.1. ■

For a quadratic Hamiltonian $\widehat{\mathcal{H}}$ or a symbol $a \in S_\delta(m)$ of at most quadratic growth, we can include the commutator relation (A.2) and obtain for the symbol a_t of $\hat{a}_t$

$$\partial_t a_t = \{a_t, \mathcal{H}\}. \tag{8.10}$$

If $\widehat{\mathcal{H}}$ is not quadratic the above equation provides an approximation of order ε^4 of a_t.

Taking $a_t = p_t$ resp. $a_t = q_t$ in (8.10) directly yields Hamilton's equations,

$$\begin{aligned}\partial_t p_t &= -\partial_q\mathcal{H}(p_t, q_t),\\ \partial_t q_t &= \partial_p\mathcal{H}(p_t, q_t).\end{aligned} \tag{8.11}$$

The relation of the operator $\hat{a}_t$ and the unitary operator $\mathcal{U}(t)$ already points to the metaplectic operators from Section 7.3 respectively Appendix B. The connection becomes more obvious if we regard the flow of the system.

Definition 8.4 — Flow. Let $z_0 = (p_0, q_0) \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $z_t = (p_t, q_t)$ a solution of (8.11) with initial value z_0. We call the map $\Phi_t : \mathbb{R}^n \oplus \mathbb{R}^n \mapsto \mathbb{R}^n \oplus \mathbb{R}^n$ that satisfies

$$z_t = \Phi_t(z_0)$$

the *Hamiltonian flow* of the system.

We note that Equation (8.11) is exact in the sense that the corresponding Weyl-operator $\hat{z}_t$ satisfies (8.9) for every Hamiltonian $\widehat{\mathcal{H}}$ since q_t and p_t are linear. If we now consider a quadratic Hamiltonian, we can simplify (8.11), since

$$\partial_t z_t = \begin{pmatrix} \partial_t p_t \\ \partial_t q_t \end{pmatrix} = \Omega \nabla \mathcal{H}(z_t) = \Omega H z_t$$

for all $z_t \in \mathbb{R}^n \oplus \mathbb{R}^n$. Hence, we can describe the flow of a quadratic Hamiltonian exactly by means of a symplectic matrix.

Lemma 8.4 — Linearised flow. Let $\mathcal{H}$ be a quadratic function with symmetric Hessian matrix $H \in \mathbb{C}^{2n\times 2n}$ and a an admissible observable. We define the matrix $S_t \in \mathbb{C}^{2n\times 2n}$ as a solution of the differential equation

$$\dot{S}_t = \Omega H S_t, \quad S_0 = \mathrm{Id}_{2n}. \tag{8.12}$$

Then, S_t is symplectic and the propagated observable a_t with

$$a_t(z) := a(S_t z) \quad \text{for all } z \in \mathbb{R}^n \oplus \mathbb{R}^n$$

satisfies (8.10).

Proof. The existence of a unique solution of (8.12) follows by the theorem of Picard-Lindelöf and we can write $S_t = e^{t\Omega H}$. Clearly, S_0 is a symplectic matrix and since

$$\partial_t(S_t^T \Omega S_t) = S_t^T H^T \Omega^T \Omega S_t + S_t^T \Omega \Omega H S_t = S_t^T (H^T - H) S_t = 0$$

this property is preserved for all times $t \geq 0$. Moreover, if we denote $z_t = S_t z$, (8.12) implies

$$\partial_t a(z_t) = \nabla a(z_t)^T \dot{S}_t z = \nabla a(z_t)^T \Omega H S_t z = \nabla a(z_t)^T \Omega \nabla \mathcal{H}(z_t) = \{a, \mathcal{H}\}(z_t).$$

■

Thus, we found that in case of a quadratic Hamiltonian it suffices to consider the linearisation of the flow, that is given by a symplectic matrix. Since the operators $\hat{A}(Z)$ resp. $\hat{A}^\dagger(Z)$ are Weyl-quantised phase space functions, the above result applies and we will propagate Lagrangian frames via the linearised flow S_t. This is an essential tool for computations in the remaining thesis.

So far, we considered quadratic Hamiltonians regardless of wether they are self-adjoint or not. The differences between Hermitian and non-Hermitian Hamiltonians will become present in the next section.

8.3. Hermitian dynamics with Hagedorn's wave packets

We now consider the Schrödinger equation (8.7) with a Hermitian, quadratic Hamiltonian $\widehat{\mathcal{H}}$, i.e.

$$\mathcal{H}(z) = \tfrac{1}{2} z^T H z \quad \text{with} \quad H = H^T = \begin{pmatrix} H_{pp} & H_{pq} \\ H_{qp} & H_{qq} \end{pmatrix} \in \mathbb{R}^{2n\times 2n}.$$

As initial value we choose an arbitrary Hagedorn wave packet, $\psi_0 = \varphi_k(Z_0, z_0)$, where $Z_0 \in \mathbb{C}^{2n\times n}$ is a normalised Lagrangian frame, $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $k \in \mathbb{N}^n$. Since H is real, also the linearised flow defined by (8.12) is real. We will see below that this point is crucial for the upcoming calculations.

Our aim in this section is to determine the time evolution $\widehat{\mathcal{U}}(t)\varphi_k(Z_0, z_0)$. As usual we start with a wave packet $\varphi_k(Z_0)$ centred at the origin and regard general phase space centres later on.

The evolution of Hagedorn's wave packets was first investigated in [Hag80] in the univariate case and generalised in [Hag85] to multi-dimensions. We will rewrite the results here in terms of Lagrangian frames and show in the next section their equivalence to the original findings.

Let S_t be the solution to (8.12) and $L_0 = \mathrm{range}(Z_0)$ our initial Lagrangian subspace. Since S_t is symplectic due to Lemma 8.4, $L_t := S_t L_0$ defines a Lagrangian subspaces for all $t \geq 0$. Moreover, we find for $Z_t := S_t Z_0$

$$Z_t^T \Omega Z_t = Z_0^T S_t^T \Omega S_t Z_0 = Z_0^T \Omega Z_0 = 0, \tag{8.13}$$

i.e. Z_t is isotropic and since S_t is real also normalised,

$$Z_t^* \Omega Z_t = Z_0^* S_t^* \Omega S_t Z_0 = Z_0^* \Omega Z_0 = 2\mathrm{i}\mathrm{Id}. \tag{8.14}$$

We stress here that the propagation of a Lagrangian frame becomes costlier when we handle non-unitary time evolutions in the next chapter: If H is a complex-valued matrix, $\mathrm{Im}(S_t) \neq 0$ and we have to normalise Z_t.

However, for the Hermitian dynamics we observe that L_t is a positive Lagrangian subspace spanned by $Z_t \in F_n(L_t)$. Hence we can easily propagate our Lagrangian subspace in time by means of the linearised flow S_t from Lemma 8.4.

For the evolution of the wave packets we first note that

$$\begin{aligned}\widehat{\mathcal{U}}(t)\varphi_k(Z_0) &= \tfrac{1}{\sqrt{k!}} \widehat{\mathcal{U}}(t)\hat{A}_k^\dagger(Z_0)\varphi_0(Z_0) = \tfrac{1}{\sqrt{k!}} \widehat{\mathcal{U}}(t)\hat{A}_k^\dagger(Z_0)\widehat{\mathcal{U}}(t)^{-1}\mathcal{U}(t)\varphi_0(Z_0) \\ &= \tfrac{1}{\sqrt{k!}} (\widehat{\mathcal{U}}(t)\hat{A}^\dagger(Z_0)\widehat{\mathcal{U}}(t)^{-1})^k \widehat{\mathcal{U}}(t)\varphi_0(Z_0),\end{aligned}$$

this means we can adopt our strategy for the Fourier transform and investigate on the one side propagated ladder operators of the form $\widehat{\mathcal{U}}(t)\hat{A}^\dagger(Z_0)\widehat{\mathcal{U}}(t)^{-1}$ and on the other side the time evolution of the coherent state $\widehat{\mathcal{U}}(t)\varphi_0(Z_0)$.

Lemma 8.5 — Ladder evolution. We have for all $l \in \mathbb{C}^n \oplus \mathbb{C}^n$,

$$\widehat{\mathcal{U}}(t)\hat{A}(l)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}(S_t l) \quad \text{and} \quad \widehat{\mathcal{U}}(t)\hat{A}^\dagger(l)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}^\dagger(S_t l).$$

Proof. This result can be seen as a simplification of [LST15, Lemma 4.1]. With the same computation as in the proof of Lemma 8.3, we find for $\hat{A}_t(l) := \widehat{\mathcal{U}}(t)\hat{A}(l)\widehat{\mathcal{U}}(t)^{-1}$

$$\mathrm{i}\varepsilon\, \partial_t \hat{A}_t(l) = [\widehat{\mathcal{H}}, \hat{A}_t(l)] \quad \text{and} \quad \partial_t A_t(l) = \{\mathcal{H}, A_t(l)\}.$$

Similarly to Lemma 8.4 we set $A_t(l;z) = A(l; S_t^{-1}z)$ for all $z \in \mathbb{R}^n \oplus \mathbb{R}^n$ and obtain

$$\partial_t A(l; S_t^{-1}z) = \nabla A(l; S_t^{-1}z)^T \dot{S}_t^{-1} z = -\nabla A(l; S_t^{-1}z)^T \Omega H S_t^{-1} z = \{\mathcal{H}, A(l)\}(S_t^{-1}z)$$

Thus, $A(l; S_t^{-1}z)$ is a solution of the differential equation above and since S_t is symplectic,

$$A(l; S_t^{-1}z) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T \Omega S_t^{-1} z = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T S_t^T \Omega z = A(S_t l; z).$$

The proof for $\hat{A}^\dagger(l)$ works analogously if one takes into account that S_t is real. ∎

This result can directly be adopted for the vector-valued notation. Let $Z \in \mathbb{C}^{2n\times n}$ be an isotropic matrix with columns $l_1, \ldots, l_n$. Then,

$$\widehat{\mathcal{U}}(t)\hat{A}(Z)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}(S_t Z), \quad \text{where} \quad \hat{A}(S_t Z) = \begin{pmatrix} \hat{A}(S_t l_1) & \ldots & \hat{A}(S_t l_n) \end{pmatrix}$$

and analogously, $\widehat{\mathcal{U}}(t)\hat{A}^\dagger(Z)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}^\dagger(S_t Z)$.

We will summarise the propagation of coherent and excited states in the next theorem. An equivalent result for the evolution of Gaussians is given in [Hag80, Theorem 1.1], the evolution of more excited states was treated in [Hag81, Theorem 1.1].

Theorem 8.2 — Coherent and excited state evolution. Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$, $Z_0 \in F_n(L_0)$ and $k \in \mathbb{N}^n$. If S_t is the unique solution of (8.12), $L_t = S_t L_0$ is a Lagrangian subspace spanned by $Z_t = S_t Z_0 \in F_n(L_t)$ for all times $t \geq 0$ and the time evolution of the k-th Hagedorn wave packet $\varphi_k(Z_0)$ is given by

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0) = \varphi_k(Z_t).$$

Proof. We start with the coherent state $\varphi_0(Z_0)$. Since $\varphi_0(Z_0) \in I(L_0)$, we find with Lemma 8.5

$$0 = \widehat{\mathcal{U}}(t)\hat{A}(Z_0)\varphi_0(Z_0) = \widehat{\mathcal{U}}(t)\hat{A}(Z_0)\widehat{\mathcal{U}}(t)^{-1}\widehat{\mathcal{U}}(t)\varphi_0(Z_0) = \hat{A}(S_t Z_0)\widehat{\mathcal{U}}(t)\varphi_0(Z_0)$$

and $\widehat{\mathcal{U}}(t)\varphi_0(Z_0) \in I(L_t)$. Moreover, since $\widehat{\mathcal{U}}(t)$ is unitary, $\|\widehat{\mathcal{U}}(t)\varphi_0(Z_0)\| = 1$ and therefore $\widehat{\mathcal{U}}(t)\varphi_0(Z_0) = \varphi_0(Z_t)$. For the excited states this implies

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0) = \tfrac{1}{\sqrt{k!}}\,(\widehat{\mathcal{U}}(t)\hat{A}^\dagger(Z_0)\widehat{\mathcal{U}}(t)^{-1})^k \widehat{\mathcal{U}}(t)\varphi_0(Z_0) = \tfrac{1}{\sqrt{k!}}\hat{A}_k^\dagger(S_t Z_0)\varphi_0(S_t Z_0) = \varphi_k(S_t Z_0).$$

∎

So, we find that under a Hermitian, quadratic Hamiltonian Hagedorn's wave packets preserve their form and can be parametrised via a Lagrangian frame Z_t that satisfies

$$\dot{Z}_t = \Omega H Z_t.$$

In particular, this equation yields a normalised Lagrangian frame for all times $t \geq 0$.

A very similar conclusion can be made for wave packets with general phase space centres $z \in \mathbb{R}^n \oplus \mathbb{R}^n$.

Proposition 8.1 — Dynamics of the centre. Let $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be parametrised by $Z_0 \in F_n(L_0)$. Then,

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0, z_0) = e^{\frac{i}{\varepsilon}\alpha_t(z_0)}\varphi_k(S_t Z_0, S_t z_0).$$

for all $k \in \mathbb{N}^n$, where S_t denotes the unique solution of (8.12) and

$$\alpha_t(z_0) := \int_0^t \left(p_\tau^T \dot{q}_\tau - \mathcal{H}(z_\tau)\right) d\tau \quad \text{with} \quad z_\tau = \begin{pmatrix} p_\tau \\ q_\tau \end{pmatrix} = S_\tau z_0.$$

Proof. This result is a special case of [LST15, Propositon 4.8]. The claim is obtained with the same line of argumentation as in Theorem 8.2 if one notices that

$$A(l, z_0; S_t^{-1}z) = \tfrac{i}{\sqrt{2\varepsilon}} l^T \Omega (S_t^{-1}z - z_0) = \tfrac{i}{\sqrt{2\varepsilon}} l^T \Omega S_t^{-1}(z - S_t z_0) = A(S_t l, S_t z_0; S_t^{-1}z).$$

Thus, $\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0) \in I(L_t, S_t z_0)$ and

$$\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0) = c_t \cdot \varphi_0(Z_t, S_t z_0)$$

for $c_t \in \mathbb{C}$. We determine c_t be inserting $\varphi_0(t) := c_t \cdot \varphi_0(S_t Z_0, S_t z_0)$ into Schrödinger's equation (8.7) and therefore denote

$$Z_t = S_t Z_0 = \begin{pmatrix} P_t \\ Q_t \end{pmatrix}, \qquad z_t = S_t z_0 = \begin{pmatrix} p_t \\ q_t \end{pmatrix}, \tag{8.15}$$

and $B_t = P_t Q_t^{-1}$. On the one side, we have for the time derivative

$$\partial_t \varphi_0(t) = \left(\tfrac{\dot{c}_t}{c_t} - \tfrac{1}{2}\mathrm{tr}(\dot{Q}_t Q_t^{-1}) + \tfrac{i}{\varepsilon}\left(\tfrac{1}{2}(x - q_t)^T \dot{B}_t (x - q_t) + (\dot{p}_t - B_t \dot{q}_t)^T (x - q_t) - p_t^T \dot{q}_t\right)\right)\varphi_0(t)$$

where we used Jacobi's determinant formula, $\partial_t \det(Q_t) = \det(Q_t)\mathrm{tr}(\dot{Q}_t Q_t^{-1})$.

On the other hand, we find for a quadratic Hamiltonian as in Lemma 8.2

$$\begin{aligned} &-\tfrac{\varepsilon^2}{2}\nabla_x^T H_{pp} \nabla_x \varphi_0(t) \\ &\quad = \left(-\tfrac{i\varepsilon}{2}\mathrm{tr}(H_{pp}B_t) + \tfrac{1}{2}(x - q_t)^T B_t H_{pp} B_t (x - q_t) + p_t^T H_{pp} B_t (x - q_t) + p_t^T H_{pp} p_t\right)\varphi_0(t) \end{aligned}$$

and

$$\tfrac{\varepsilon}{\mathrm{i}} x^T H_{qp} \nabla_x \varphi_0(t)$$
$$= \left((x-q_t)^T H_{qp} B_t (x-q_t) + (H_{pq} p_t + B_t H_{pq} q_t)^T (x-q_t) + q_t^T H_{qp} p_t\right) \varphi_0(t).$$

To be able to sort by powers of $(x-q_t)$, we moreover expand

$$\tfrac{1}{2} x^T H_{qq} x\, \varphi_0(t) = \left(\tfrac{1}{2}(x-q_t)^T H_{qq}(x-q_t) + q_t^T H_{qq}(x-q_t) + \tfrac{1}{2} q_t^T H_{qq} q_t\right) \varphi_0(t).$$

Hence, $\varphi_0(t)$ is a solution of (8.7), if

$$\begin{aligned} \mathrm{i}\varepsilon \tfrac{\dot c_t}{c_t} - \tfrac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\dot Q_t Q_t^{-1}) + p_t^T \dot q_t &= -\tfrac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(H_{pp}B_t + H_{pq}) + \mathcal{H}(z_t), \\ B_t \dot q_t - \dot p_t &= B_t \partial_{q_t}\mathcal{H}(z_t) + \partial_{p_t}\mathcal{H}(z_t), \\ -\dot B_t &= B_t H_{pp} B_t + B_t H_{qp} + H_{pq} B_t + H_{qq}. \end{aligned}$$

For the first equation, we note that (8.12) implies $\dot Q_t Q_t^{-1} = H_{pp}B_t + H_{pq}$ and c_t is the solution to

$$\tfrac{\dot c_t}{c_t} = \tfrac{\mathrm{i}}{\varepsilon}(p_t^T \dot q_t - \mathcal{H}(z_t)).$$

The second equation is equivalent to Hamilton's equation of motion (8.11). The last identity equals [GS12, Eq. (39)] and the authors show in [GS12, Theorem 3.3] the equivalence to the propagation via S_t in (8.15).

For the more excited states we further stress that

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0,z_0) = \tfrac{1}{\sqrt{k!}} \hat A_k^\dagger(Z_t,z_t)\widehat{\mathcal{U}}(t)\varphi_0(Z_0,z_0) = c_t \cdot \varphi_k(Z_t,z_t).$$

■

So, the dynamics of a phase space centre z_0 is described by the differential equation

$$\dot z_t = \Omega H z_t,$$

what is consistent with Hamilton's equations (8.11) for a quadratic Hamiltonian. For the non-Hermitian case we will find a different picture: the dynamics of the centre will not only be driven by the real and imaginary part of the Hamiltonian, but also by the symplectic metric of L_t, see also [GS11].

8.4. Large order asymptotics

In this section we want to show that our previous findings for the Hermitian dynamics are consistent with the results for the semiclassical dynamics in [Hag81], [Hag85] and [HJ00]. In these works the authors considered the time-dependent Schrödinger equation

$$i\varepsilon\, \partial_t \psi(x,t) = -\tfrac{\varepsilon^2}{2}\Delta\psi(x,t) + V(x)\psi(x,t), \tag{8.16}$$

where Δ denotes the Laplace operator, $\Delta = \sum_{j=1}^{n} \partial_{x_j}^2$ and $V(x)$ a potential depending on the position $x \in \mathbb{R}^n$. Hagedorn's wave packets are then used to approximate solutions via

$$\psi_l(x,t) = e^{\frac{i}{\varepsilon}\alpha_t(z_0)} \sum_{|j|\le J} \varphi_j(Z_t, z_t; x)$$

up to an exponentially small error. Our main purpose is now to prove that the propagation

$$Z_t = S_t Z_0 \quad \text{resp.} \quad z_t = S_t z_0$$

is indeed equivalent to the classical equations of motion given in [Hag85, Eq. (1.6)-(1.10)] and [HJ00, Eq.(2.3)].

Let $Z_t = (P_t; Q_t) \in \mathbb{C}^{2n\times n}$ and $z_t = (p_t, q_t) \in \mathbb{R}^n \oplus \mathbb{R}^n$. If the potential V is a real quadratic form, then the Hamiltonian

$$\mathcal{H}(p,q) = \tfrac{1}{2}|p|^2 + V(q) \quad \text{with} \quad D^2\mathcal{H}(p,q) = \begin{pmatrix} \mathrm{Id} & 0 \\ 0 & D^2V(q) \end{pmatrix}$$

is Hermitian and quadratic. Our results from the previous section imply that

$$\psi(x,t) = e^{\frac{i}{\varepsilon}\alpha_t(z_0)} \varphi_k(Z_t, z_t; x)$$

is an exact solution of (8.16) if

$$\dot{Z}_t = \Omega D^2\mathcal{H}(z_t) Z_t, \quad \dot{z}_t = \Omega D^2\mathcal{H}(z_t) z_t \quad \text{and} \quad \dot{\alpha}_t(z_0) = p_t^T \dot{q}_t - \mathcal{H}(p_t, q_t).$$

Thereby, $D^2\mathcal{H}$ and D^2V denote the Hessian matrix of $\mathcal{H}$ resp. V. The first two equations are equivalent to

$$\begin{pmatrix} \dot{P}_t \\ \dot{Q}_t \end{pmatrix} = \begin{pmatrix} -D^2V(q_t)Q_t \\ P_t \end{pmatrix}, \qquad \begin{pmatrix} \dot{p}_t \\ \dot{q}_t \end{pmatrix} = \begin{pmatrix} -D^2V(q_t)q_t \\ p_t \end{pmatrix} = \begin{pmatrix} -\nabla V(q_t) \\ p_t \end{pmatrix},$$

while the third equation yields

$$\dot{\alpha}_t(z_0) = |p_t|^2 - \tfrac{1}{2}|p_t|^2 - V(q_t) = \tfrac{1}{2}|p_t|^2 - V(q_t).$$

Denoting $A(t) = Q_t$, $B(t) = -iP_t$, $a(t) = q_t$, $\eta(t) = p_t$ and $S(t) = \alpha_t(z_0)$, we can rewrite these equations as

$$\begin{aligned} \dot{A}(t) &= iB(t), & \dot{B}(t) &= iD^2V(a(t))A(t), \\ \dot{a}(t) &= \eta(t), & \dot{\eta}(t) &= -\nabla V(a(t)), \\ \dot{S}(t) &= \tfrac{1}{2}|\eta(t)|^2 - V(a(t)), \end{aligned}$$

what exactly matches with [Hag85, Eq. (1.6)-(1.10)] resp. [HJ00, Eq.(2.3)].

For general potentials V, one can show that the wave packets $e^{\frac{i}{\varepsilon}\alpha_t(z_0)}\varphi_k(Z_t, z_t; x)$ approximate solutions of (8.16) by considering the Taylor expansion of V up to second order, see [HJ00, Theorem 3.1].

Theorem 8.3 — Asymptotics. Let $V \in \mathbb{C}^\infty(\mathbb{R}^n)$ be a real, positive function and $\psi(x,t)$ a solution of (8.16) satisfying

$$\psi(x,0) = \sum_{|j|\leq J} c_j \varphi_j(Z_0, z_0; x) \quad \text{with} \quad \sum_{|j|\leq J} |c_j|^2 = 1,$$

where $Z_0 \in \mathbb{C}^{2n\times n}$ is a normalised Lagrangian frame, $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n \backslash \{0\}$ and $c_j \in \mathbb{C}$ for all $j \in \mathbb{N}^n$ with $|j| \leq J$. Then,

$$\psi_l(x,t) = e^{\frac{\mathrm{i}}{\varepsilon}\alpha_t(z_0)} \sum_{|j|\leq \tilde{J}(l)} c_j(l,t)\varphi_j(Z_t, z_t; x)$$

with $\tilde{J}(l) = J + 3(l-1)$ is an approximation of $\psi(x,t)$ up to order $\varepsilon^{l/2}$, i.e. for all $T > 0$

$$\sup_{t\in[-T;T]} \|\psi_l(x,t) - \psi(x,t)\| \leq C(l)\varepsilon^{l/2}$$

for some constant $C(l) > 0$.

By tightening the constraints on the potential V, in particular demanding that V is analytic on $D = \{x + \mathrm{i}y \in \mathbb{C}^n\,;\, |y_j| < \delta,\, j = 1,\dots,n\}$ for $\delta > 0$ and satisfies for all $x + \mathrm{i}y \in D$

$$|V(x + \mathrm{i}y)| \leq c \cdot e^{\tau|x+\mathrm{i}y|^2}$$

for constants $c, \tau > 0$, one can optimise the upper bound further and find an exponentially small error, see [HJ00, Theorem 4.1]. We stress here that this approximation result is only valid for Hermitian Hamiltonians. To obtain a similar statement for the non-Hermitian Hamiltonians investigated in the following an additionally study would be needed and might make a good enhancement of this thesis.

8.5. Example: Harmonic Oscillator

As a quick first example we review the dynamics under the harmonic oscillator

$$\widehat{\mathcal{H}} = \tfrac{\omega_0}{2}(\hat{p}^2 + \hat{q}^2), \qquad H = \omega_0 \cdot \mathrm{Id}_2,$$

for $\omega_0 \in \mathbb{R}$ in the one-dimensional setting. In particular, we can compare our findings here to the results for the non-Hermitian Swanson oscillator in Section 9.6 where we add the complex mixed term $-\frac{\mathrm{i}}{2}(\hat{p}\hat{q} + \hat{q}\hat{p})$ to the harmonic oscillator.

In the univariate setting we can write our initial Lagrangian subspace as

$$L_0 = \mathrm{span}\{l_0\}, \qquad l_0 = \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \in \mathbb{C}^2,$$

and note that l_0 is normalised if $\mathrm{Im}(p_0\overline{q}_0) = 1$. The time evolved subspace is then given by $L_t = \mathrm{span}\{l_t\}$ with

$$l_t = \begin{pmatrix} p_t \\ q_t \end{pmatrix} = S_t l_0.$$

From our discussion in Section 3.2 we know that the Hermite functions generated from $l_0 = (\mathrm{i}, 1)^T$ are eigenfunctions of the harmonic oscillator.

Linearised flow

For the linearised flow the evolution equation (8.12) implies

$$\begin{aligned} S_t = e^{t\Omega H} &= \sum_{k=0}^{\infty} \tfrac{(\omega_0 t)^k}{k!}\Omega^k = \sum_{k=0}^{\infty} \tfrac{(-1)^k}{(2k)!}(\omega_0 t)^{2k}\mathrm{Id}_2 + \sum_{k=0}^{\infty} \tfrac{(-1)^k}{(2k+1)!}(\omega_0 t)^{2k+1}\Omega \\ &= \cos(t\omega_0)\mathrm{Id}_2 + \sin(t\omega_0)\Omega \end{aligned}$$

and S_t is a real, symplectic matrix.

Evolved coherent state

The time evolution of the Lagrangian subspace is accordingly described by

$$l_t = S_t l_0 = \begin{pmatrix} \cos(t\omega_0)p_0 - \sin(t\omega_0)q_0 \\ \sin(t\omega_0)p_0 + \cos(t\omega_0)q_0 \end{pmatrix}$$

and the width of the propagated coherent state is given by $b_t = \frac{p_t}{q_t}$. If $l_0 = (\mathrm{i}, 1)^T$ then one can easily verify that $b_t = \mathrm{i}$ for all times t.

Evolved excited states

To determine the excited states completely we need in addition the recursion matrix M_t that is in the one-dimensional case only a scaling factor, see Section 5.1. We have

$$M_t = \frac{\overline{q}_t}{q_t} = \frac{\sin(t\omega_0)\overline{p}_0 + \cos(t\omega_0)\overline{q}_0}{\sin(t\omega_0)p_0 + \cos(t\omega_0)q_0}$$

and if we consider again the standard Hermite functions, $l_0 = (\mathrm{i}, 1)^T$, this simplifies to $M_t = (-\mathrm{i}\sin(t\omega_0) + \cos(t\omega_0))^2 = e^{-2\mathrm{i}t\omega_0}$. Thus, also the coherent state $\varphi_0(l_t)$ may stay unaltered, the excited states oscillate in time, see Figure 13.

Dynamics of the centre

Finally, we can state for the dynamics of an initial centre $z_0 = (\xi_0, x_0) \in \mathbb{R}^2$,

$$z_t = S_t z_0 = \begin{pmatrix} \cos(t\omega_0)\xi_0 - \sin(t\omega_0)x_0 \\ \sin(t\omega_0)\xi_0 + \cos(t\omega_0)x_0 \end{pmatrix}$$

and we find the characteristic circular behaviour, see Figure 14. We want to particularly stress that the centres here are real-valued for all times t. Moreover, we can also

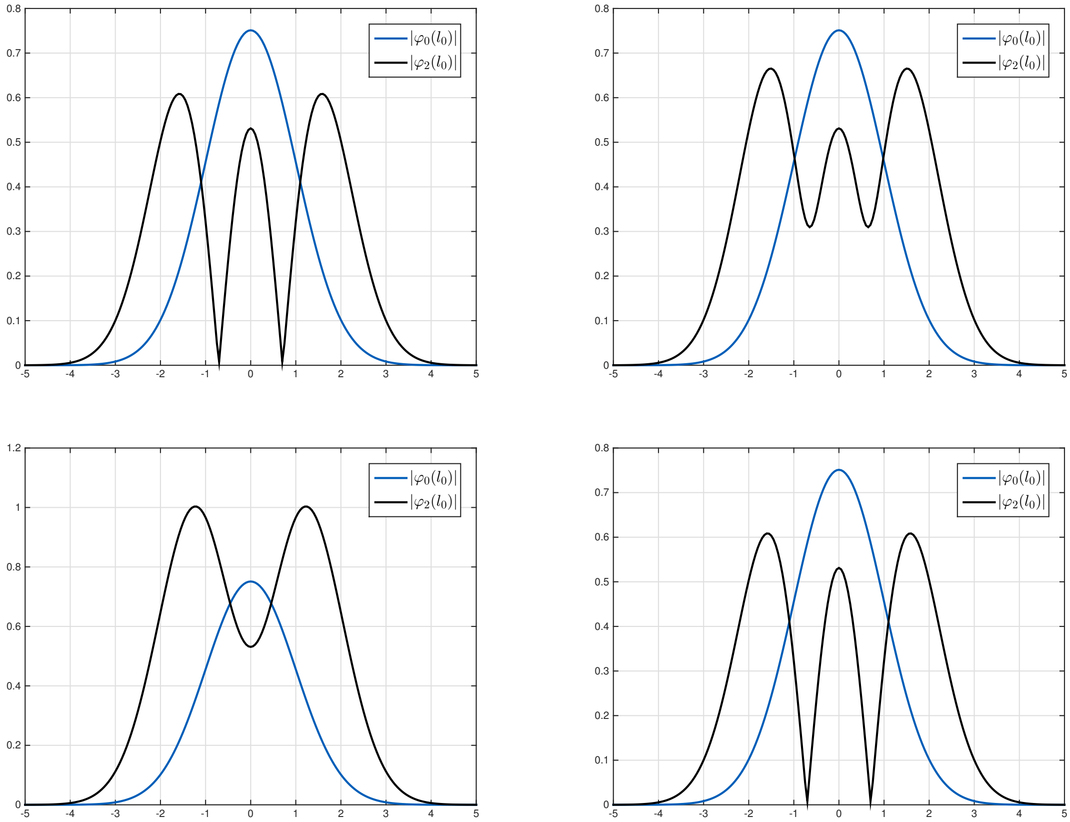

Figure 13.: Absolute values of the wave packets $\varphi_0(l_t)$ and $\varphi_2(l_t)$ starting from $l_0 = (\mathrm{i}, 1)^T$ at time $t = 0$ (upper left), $t = 0.3925 \approx \frac{\pi}{8}$ (upper right), $t = 1.57 \approx \frac{\pi}{8}$ (lower left) and $t = 3.14 \approx \pi$ (lower right) for $\varepsilon = 1$ and $\omega_0 = 1$.

compute the symplectic metric G_t of L_t,

$$G_t = \Omega^T \mathrm{Re}(l_t l_t^*)\Omega =$$

$$|p_0|^2 \cdot \mathrm{Id}_2 + (|q_0|^2 - |p_0|^2) \begin{pmatrix} \cos^2(t\omega_0) + \sin(2t\omega_0)\frac{\mathrm{Re}(p_0\bar{q}_0)}{|q_0|^2 - |p_0|^2} & \sin(t\omega_0)\cos(t\omega_0) \\ \sin(t\omega_0)\cos(t\omega_0) & \sin^2(t\omega_0) - \sin(2t\omega_0)\frac{\mathrm{Re}(p_0\bar{q}_0)}{|q_0|^2 - |p_0|^2} \end{pmatrix}$$

and for the standard Hermite functions we obtain $G_t = \mathrm{Id}_2$ for all $t \geq 0$.

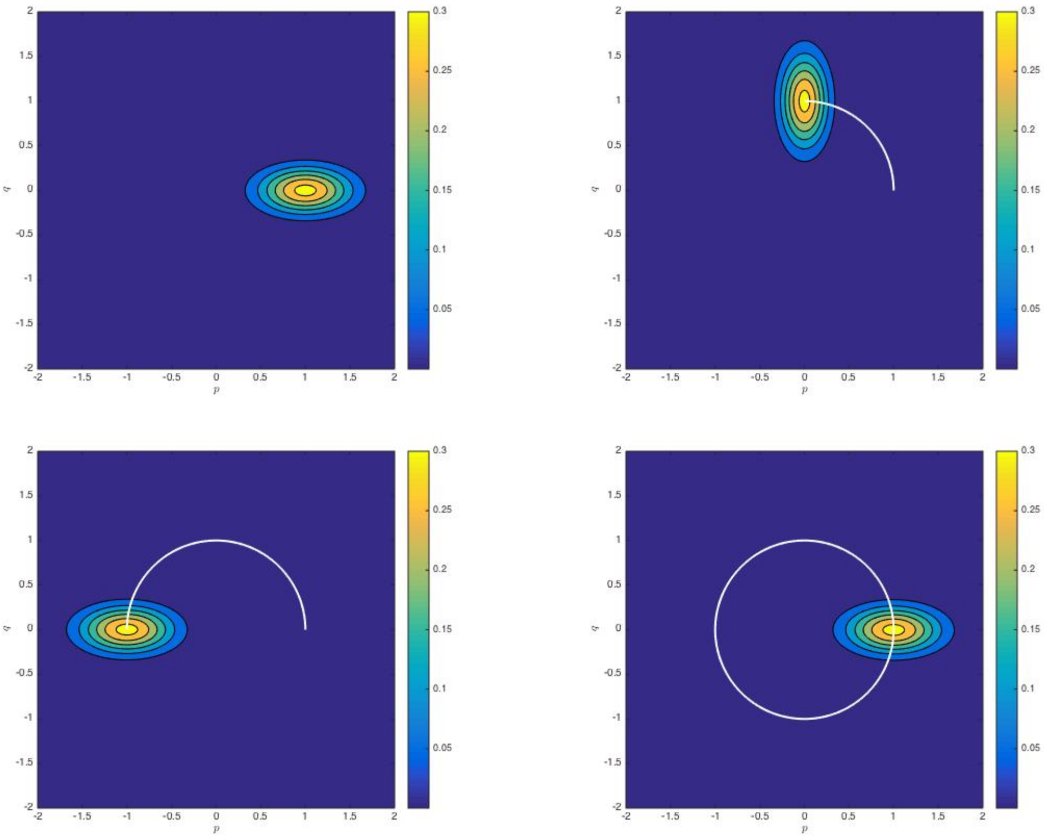

Figure 14.: Trajectory of the centre z_t with initial value $z_0 = (1, 0)$ and contour plot of the absolute value of the Wigner transform $\mathcal{W}^\varepsilon(\varphi_0(l_t))$ for $l_0 = (4, 2 - 0.25\mathrm{i})$ at time $t = 0$ (upper left), $t = 1.57 \approx \frac{\pi}{2}$ (upper right), $t = 3.14 \approx \pi$ (lower left) and $t = 6.28 \approx 2\pi$ (lower right) for $\varepsilon = 1$ and $\omega_0 = 1$.

9. Non-Hermitian Schrödinger dynamics

In this chapter we generalise our results and investigate the Schrödinger equation (8.7) with a quadratic but non-Hermitian Hamiltonian $\widehat{\mathcal{H}}$. This means $\mathcal{H}$ can be written as $\mathcal{H}(z) = \frac{1}{2}z^T H z$ with $H \in \mathbb{C}^{2n\times 2n}$ symmetric and $\mathrm{Im}(H) \neq 0$.

A similar problem with coherent states as ansatz functions was treated in [GS12]. We now combine their findings with Hagedorn's approach from [Hag85] and in this way extend [GS12, Theorem 3.4] to excited states. We will show explicitly in Section 9.4 that in contrast to the Hermitian setting, here we have to take for the propagation of excited wave packets also lower excited wave packets into account, see Theorem 9.2.

We start our analysis again with the time evolution operator. In this case $\widehat{\mathcal{U}}(t)$ will not be unitary, in other words the norm of the initial state will not be preserved. This can be favourable if one wants to model physical effects such as diffusion, decoherence, see [BH02, §5], or absorption, see [Mug+04]. However, it is not clear that $\widehat{\mathcal{U}}(t)$ exists, since $\widehat{\mathcal{H}}$ is not self-adjoint and thus Stone's theorem can not be applied. Hence, we have to provide a closer study of $\widehat{\mathcal{U}}(t)$ in Section 9.1 resp. Appendix C.

Yet for the evolution of the wave packets we can still define the linearised flow S_t as solution of

$$\dot{S}_t = \Omega H S_t, \qquad S_0 = \mathrm{Id}.$$

We recall that the linearisation is exact for all quadratic Hamiltonians, see Lemma 8.12. But, as indicated in the previous chapter for a symmetric, complex matrix H, we find a symplectic, but complex flow S_t. This notably complicates our computations, we need to include the theories for non-normalised Lagrangian frames and comparable ladder operators we established in Section 2.5 and 4.1, respectively.

Our proceeding nevertheless is similar to the one for Hermitian Hamiltonians:
Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace and $Z_0 \in F_n(L_0)$. We determine the time evolution

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0) = \frac{1}{\sqrt{k!}}\widehat{\mathcal{U}}(t)A_k^\dagger(Z_0)\widehat{\mathcal{U}}(t)^{-1}\widehat{\mathcal{U}}(t)\varphi_0(Z_0)$$

of the k-th Hagedorn wave packet by first investigating the evolution of the ladder operators and the coherent states and then apply these results to the construction of excited states. After that we continue and include also general phase space centres $z \in \mathbb{R}^n \oplus \mathbb{R}^n$.

To finish this chapter we demonstrate our findings by means of the Davies-Swanson Oscillator, see [Dav99b] and [Swa04], a harmonic oscillator with a complex potential.

9.1. Time evolution

First of all, we have to ensure that our approach via the time evolution operator $\widehat{\mathcal{U}}(t)$ is still valid also in the non-Hermitian case. It is known that some non-selfadjoint Hamiltonians define a unitary time evolution, see for example [BBJ03], where the authors studied a class of *PT*-symmetric operators. Or, one can replace non-Hermitian Hamiltonians with an equivalent pseudo-Hermitian operator, see for example [MFF06], where the Davies-Swanson oscillator is also studied as an example.

Since we restrict ourselves to quadratic Hamiltonians in this thesis, we can give a more general result for the existence of the time evolution operator.

Proposition 9.1 Let $\mathcal{H}(z) = \frac{1}{2} z^T H z$ be a complex quadratic form with $H = H^T \in \mathbb{C}^{2n\times 2n}$ invertible and

$$\mathrm{Im}(H) \le 0.$$

Then, the operator $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ generates a continuous contraction semigroup $\{\widehat{\mathcal{U}}(t)\,;\, t \ge 0\}$ such that

$$\mathrm{i}\varepsilon\, \partial_t \widehat{\mathcal{U}}(t) = \widehat{\mathcal{H}}\widehat{\mathcal{U}}(t), \tag{9.1}$$

for all $t \ge 0$ and $\widehat{\mathcal{U}}(0) = \mathrm{id}$.

Proof. This statement is adopted from [PS08, Theorem 2.1], where semigroups of elliptic quadratic operators are treated in detail. The proof is based on the fact that $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ and its adjoint are both closed, dissipative operators if $\mathrm{Im}(H) \le 0$ and thus a consequence of the Lumer-Phillips theorem, see [EN00, Theorem II.3.15] respectively [EN00, Corollary II.3.17] . We present a more detailed study of this result in Appendix C. ■

Equation (9.1) herein is the same formal identity as in Lemma 8.1, the equality should hold true in the strong sense.

The above result verifies our findings for Hamiltonians with non-positive definite imaginary part and especially for the Lindblad equation. For a general Hamiltonian it is not clear wether Equation (9.1) possesses a solution or not. This point was also addressed in [GS12, §3]. There are some approaches that give hope that there exists a time evolution operator at least for times $t \in [0; T[$ with $T > 0$, for example [AV14] identifying the evolution operators with operators on Fock spaces or a direct calculation of $\mathcal{U}(t)$ as in [CR06, §5]. With the second strategy we are able to show that the evolution operator exists for times $t \ge 0$ such that the linearised flow $S_t = e^{t\Omega H}$ satisfies

$$\mathrm{i}(\Omega - S_t^* \Omega S_t) \ge 0.$$

However, we were not able yet to trace this condition back to a valid argument for the Hamiltonian $\mathcal{H}$. For the examples studied in this thesis with indefinite or positive definite imaginary part, namely the Davies-Swanson oscillator and the Fokker-Planck equation we refer to the literature for existence results, see [Ris84, §4.2.1] and [Gra+14, §2].

9.2. Ladder evolution

Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ denote our initial positive Lagrangian subspace and $Z_0 \in F_n(L_0)$. Analogue to our considerations in the previous chapter we evolve the Lagrangian subspace along S_t,

$$L_t := S_t Z_0.$$

Since S_t is symplectic this still yields a Lagrangian subspace spanned by the isotropic matrix $S_t Z_0 \in \mathbb{C}^{2n\times n}$, see (8.13). Unfortunately, since S_t is complex, $S_t Z_0$ will not be normalised, see (8.14). We have to resume our idea from Section 2.5 and utilise the normalisation matrix

$$N_t = \tfrac{1}{2\mathrm{i}} Z_0^* S_t^* \Omega S_t Z_0 \in \mathbb{C}^{n\times n}$$

to define a normalised Lagrangian frame with the same range by

$$Z_t := S_t Z_0 N_t^{-1/2}.$$

This approach is well-defined as long as $N_t > 0$, see Lemma 2.5. If $\mathrm{Im}(H) \leq 0$, we have

$$N_t = N_0 + \int_0^t \dot{N}_\tau \, d\tau = \mathrm{Id} - \int_0^t Z_0^* S_\tau^* \mathrm{Im}(H) S_\tau Z_0 \, d\tau > 0 \tag{9.2}$$

for all times $t \geq 0$. For a general Hamiltonian a continuity argument yields that there exits a $T > 0$ such that L_t is positive for all $t \in [0; T[$ since $N_0 = \mathrm{Id}$. We assume that this time interval lies within the range where our time evolution operator $\widehat{\mathcal{U}}(t)$ exists. However, we lack a rigorous proof for this presumption and admit that further investigation here would be required.

Lemma 9.1 — Ladder evolution. For all $l \in \mathbb{C}^n \oplus \mathbb{C}^n$, we find

$$\widehat{\mathcal{U}}(t)\hat{A}(l)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}(S_t l) \quad \text{and} \quad \widehat{\mathcal{U}}(t)\hat{A}^\dagger(l)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}^\dagger(\overline{S}_t l).$$

Proof. This statement is also given in [LST15, Lemma 4.1]. The proof works completely analogue to the proof of Lemma 8.5, we only note for the raising operator,

$$\hat{A}^\dagger(l; S_t^{-1} z) = -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^* \Omega S_t^{-1} z = -\tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^* S_t^T \Omega z = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} (\overline{S}_t l)^* \Omega z = \hat{A}^\dagger(\overline{S}_t l; z)$$

for all $z \in \mathbb{R}^n \oplus \mathbb{R}^n$ since $\mathrm{Im}(S_t) \neq 0$. ■

For any isotropic matrix $Z \in \mathbb{C}^{2n\times n}$ this result motivates the notation

$$\widehat{\mathcal{U}}(t)\hat{A}(Z_0)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}(S_t Z_0) \quad \text{and} \quad \widehat{\mathcal{U}}(t)\hat{A}^\dagger(Z_0)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}^\dagger(\overline{S}_t Z_0).$$

Since S_t is symplectic, both matrices $S_t Z_0$ and $\overline{S}_t Z_0$ are isotropic, but as initially pointed out none of them is normalised. Moreover, the raising operator $\hat{A}^\dagger(\overline{S}_t Z_0)$ does not correspond to the evolved Lagrangian L_t and is in particular not adjoint to $\hat{A}(S_t Z_0)$,

$$\hat{A}(S_t Z_0)^* \neq \hat{A}^\dagger(\overline{S}_t Z_0).$$

Thus, we found ladder operators parametrised by two different Lagrangian frames. We investigated this setting already in Corollary 4.1 and noted that ladder operators can always be related by means of the mixed isotropy and the mixed normalisation of the frames.

Corollary 9.1 — Ladder decomposition. We denote the mixed isotropy and mixed normalisation of Z_t and $\overline{S}_t Z_0$ by

$$C_t = \tfrac{1}{2\mathrm{i}} Z_t^T \Omega \overline{S}_t Z_0 \quad \text{and} \quad D_t = \tfrac{1}{2\mathrm{i}} Z_t^* \Omega \overline{S}_t Z_0,$$

see (2.17) and (2.18). Then, the corresponding ladder operators are related via

$$\hat{A}(\overline{S}_t Z_0) = D^T \hat{A}(Z_t) + C^T \hat{A}^\dagger(Z_t) \quad \text{and} \quad \hat{A}^\dagger(\overline{S}_t Z_0) = D_t^* \hat{A}^\dagger(Z_t) + C_t^* \hat{A}(Z_t).$$

Proof. This result is a consequence of Corollary 4.1. For a direct proof, see [LST15, Lemma 4.4]. ■

Since the raising operator $\hat{A}^\dagger(\overline{S}_t Z_0)$ not only involves the creator $\hat{A}^\dagger(Z_t)$, but also the annihilator $\hat{A}(Z_t)$, this corollary already predicts that evolved excited states will not simply preserve their structure, but also activate lower excited states. For the coherent state then again, we only have to correct its definition via the non-normalised Lagrangian frame $S_t Z_0$.

9.3. Coherent state evolution

In the following we will always consider the evolution of states on time intervals $[0;T[$ so that

$$L_t = S_t L_0$$

is a positive Lagrangian subspace. If we propagate $\varphi_0(Z_0)$ with Lemma 9.1 and Equation (4.2)

$$0 = \widehat{\mathcal{U}}(t)\hat{A}(Z_0)\varphi_0(Z_0) = \hat{A}(S_t Z_0)\widehat{\mathcal{U}}(t)\varphi_0(Z_0).$$

We obtain $\widehat{\mathcal{U}}(t)\varphi_0(Z_0) \in I(L_t)$ for all $t \in [0;T[$, but $\|\widehat{\mathcal{U}}(t)\varphi_0(Z_0)\| \neq 1$. This means, unlike the unitary evolution of coherent states in Theorem 8.2 we find an additional damping factor $\beta_t \in \mathbb{R}$.

Proposition 9.2 — Coherent state evolution. Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ and $L_t = S_t L_0$ be positive Lagrangian subspaces for $t \in [0;T[$. Let $G_t \in \mathrm{Sp}(n,\mathbb{R})$ be the symplectic metric of L_t and consider $Z_t = S_t Z_0 N_t^{-1/2}$. Then,

$$\widehat{\mathcal{U}}(t)\varphi_0(Z_0) = \varphi_0(S_t Z_0) = e^{\beta_t}\varphi_0(Z_t)\,, \qquad t \in [0;T[\,,$$

with

$$\beta_t = \tfrac{1}{4}\int_0^t \mathrm{tr}(G_\tau^{-1}\mathrm{Im}(H))\,d\tau.$$

Proof. This result can also be found as [LST15, Proposition 4.2]. We know that

$$\widehat{\mathcal{U}}(t)\varphi_0(Z_0) = c_t \cdot \varphi_0(S_t Z_0)$$

for $c_t \in \mathbb{C}$. A similar computation as for Proposition 8.1 shows that inserting this ansatz into the Schrödinger equation (8.7) yields $c_t = 1$, i.e. $\widehat{\mathcal{U}}(t)\varphi_0(Z_0) = \varphi_0(S_t Z_0)$. Moreover, it is clear by definition that

$$\varphi_0(S_t Z_0) = \det(N_t)^{-1/4}\varphi_0(Z_t).$$

With Jacobi's determinant formula, $\partial_t \det(N_t) = \det(N_t)\mathrm{tr}(\partial_t N_t N_t^{-1})$, we have

$$\partial_t \det(N_t)^{-1/4} = -\tfrac{1}{4}\det(N_t)^{-1/4}\mathrm{tr}(\partial_t N_t N_t^{-1}).$$

We now use the Hamiltonian system (8.12) to differentiate the normalisation

$$\partial_t N_t = \tfrac{1}{2\mathrm{i}}\partial_t\left(Z_0^* S_t^* \Omega S_t Z_0\right) = \tfrac{1}{2\mathrm{i}}\left(Z_0^* S_t^* \overline{H} S_t Z_0 - Z_0^* S_t^* H S_t Z_0\right) = -Z_0^* S_t^* \mathrm{Im}(H) S_t Z_0$$

and by Proposition 2.2,

$$\begin{aligned}\mathrm{tr}\left(\partial_t N_t N_t^{-1}\right) &= \mathrm{tr}\left(N_t^{-1/2}\partial_t N_t N_t^{-1/2}\right) = \mathrm{tr}\left(-Z_t^*\mathrm{Im}(H)Z_t\right) = -\mathrm{tr}\left(\mathrm{Im}(H)(G_t^{-1} - \mathrm{i}\Omega)\right)\\ &= -\mathrm{tr}\left(G_t^{-1}\mathrm{Im}(H)\right).\end{aligned}$$

Thus, $\det(N_t)^{-1/4}$ is a solution of $\partial_t \det(N_t)^{-1/4} = \frac{1}{4}\mathrm{tr}\left(G_t^{-1}\mathrm{Im}(H)\right)\det(N_t)^{-1/4}$ and we can write $\det(N_t)^{-1/4} = e^{\beta_t}$ with

$$\partial_t \beta_t = \tfrac{1}{4}\mathrm{tr}(G_t^{-1}\mathrm{Im} H)\,, \qquad \beta_0 = 0.$$

■

Since β_t is a real factor, we find

$$\|\widehat{\mathcal{U}}(t)\varphi_0(Z_0)\| = e^{\beta_t},$$

that is β_t models the gain or loss of the non-conservative system. One can directly see the factor β_t is fully governed by the dynamics of the symplectic metric G_t and this dynamic can be described by the following Riccati equation.

Theorem 9.1 — Riccati equation. Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ and $L_t = S_t L_0$ be positive Lagrangian subspaces for $t \in [0; T[$. Denote by $G_t, J_t \in \mathrm{Sp}(n, \mathbb{R})$ the symplectic metric and the complex structure of L_t, respectively. Then,

$$\begin{aligned}\dot{G}_t &= \mathrm{Re}(H)\Omega G_t - G_t\Omega\mathrm{Re}(H) - \mathrm{Im}(H) - G_t\Omega\mathrm{Im}(H)\Omega G_t,\\ \dot{J}_t &= \Omega\mathrm{Re}(H)J_t - J_t\Omega\mathrm{Re}(H) - \Omega\mathrm{Im}(H) + J_t\Omega\mathrm{Im}(H)J_t.\end{aligned}$$

Proof. The equations of motion for G_t and J_t have been derived in [GS12, Theorem 3.3] using the Siegel half space and rational relations. [LST15, Appendix B] provides an alternative proof based on Lagrangian frames that we will restate here.

We have $G_t = \Omega^T \mathrm{Re}(Z_t Z_t^*)\Omega$ with $Z_t Z_t^* = S_t Z_0 N_t^{-1} Z_0^* S_t^*$ and due to the time derivative of the normalisation from the previous proof,

$$\begin{aligned}\partial_t(Z_t Z_t^*) &= \dot{S}_t Z_0 N_t^{-1} Z_0^* S_t^* - S_t Z_0 N_t^{-1} \dot{N}_t N_t^{-1} Z_0^* S_t^* + S_t Z_0 N_t^{-1} Z_0^* \dot{S}_t^* \\ &= \Omega H Z_t Z_t^* + Z_t Z_t^* \mathrm{Im}(H) Z_t Z_t^* - Z_t Z_t^* \overline{H}\Omega.\end{aligned}$$

With $\partial_t \mathrm{Re}(Z_t Z_t^*) = \mathrm{Re}(\partial_t(Z_t Z_t^*))$ and $\mathrm{Im}(Z_t Z_t^*) = -\Omega$ this yields

$$\begin{aligned}\partial_t \mathrm{Re}(Z_t Z_t^*) &= \Omega \mathrm{Re}(H)\mathrm{Re}(Z_t Z_t^*) + \Omega \mathrm{Im}(H)\Omega + \mathrm{Re}(Z_t Z_t^*)\mathrm{Im}(H)\mathrm{Re}(Z_t Z_t^*) \\ &\quad - \Omega \mathrm{Im}(H)\Omega - \mathrm{Re}(Z_t Z_t^*)\mathrm{Re}(H)\Omega + \Omega \mathrm{Im}(H)\Omega \\ &= \Omega \mathrm{Re}(H)\mathrm{Re}(Z_t Z_t^*) - \mathrm{Re}(Z_t Z_t^*)\mathrm{Re}(H)\Omega + \Omega \mathrm{Im}(H)\Omega \\ &\quad + \mathrm{Re}(Z_t Z_t^*)\mathrm{Im}(H)\mathrm{Re}(Z_t Z_t^*).\end{aligned}$$

Thus, we find for G_t,

$$\partial_t G_t = \mathrm{Re}(H)\Omega G_t - G_t \Omega \mathrm{Im}(H)\Omega G_t - \mathrm{Im}(H) - G_t \Omega \mathrm{Re}(H)$$

and since $J_t = -\Omega G_t$,

$$\partial_t J_t = -\Omega \partial_t G_t = \Omega \mathrm{Re}(H) J_t + J_t \Omega \mathrm{Im}(H) J_t + \Omega \mathrm{Im}(H) - J_t \Omega \mathrm{Re}(H).$$

■

9.4. Excited state evolution

We now apply the raising operator $\hat{A}^\dagger(\overline{S}_t Z_0)$ to the propagated coherent state. With Corollary 9.1, we have

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0) = \tfrac{1}{\sqrt{k!}} \hat{A}_k^\dagger(\overline{S}_t Z_0)\widehat{\mathcal{U}}(t)\varphi_0(Z_0) = \tfrac{e^{\beta_t}}{\sqrt{k!}}(D_t^* \hat{A}^\dagger(Z_t) + C_t^* \hat{A}(Z_t))^k \varphi_0(Z_t).$$

Here the annihilation part of the decomposition becomes visible. All terms of the form $\hat{A}_m(Z_t)\varphi_0(Z_t)$, $m \le k$, vanish and we reformulate the remaining terms with the commutator relation for $\hat{A}^\dagger(Z_t)$ and $\hat{A}(Z_t)$, see Lemma 4.1. In this manner we encounter lower excited wave packets $\varphi_m(Z_t)$, $m \le k$, see [LST15, Theorem 4.5].

Theorem 9.2 — Excited state evolution. Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ and $L_t = S_t L_0$ be positive Lagrangian subspaces for $t \in [0; T[$. Consider $Z_t = S_t Z_0 N_t^{-1/2} \in F_n(L_t)$ and denote by $G_t \in \mathrm{Sp}(n, \mathbb{R})$ the symplectic metric of L_t. Define

$$M_t = \tfrac{1}{4}(S_t \overline{Z}_0)^T G_t (S_t \overline{Z}_0) = \tfrac{1}{2\mathrm{i}} N_t^{-1} (S_t Z_0)^* \Omega (S_t \overline{Z}_0)$$

and the polynomials q_k, $k \in \mathbb{N}^n$, via the recursion relation

$$q_0(x) = 1\,, \qquad \big(q_{k+e_j}(x)\big)_{j=1}^n = x q_k(x) - M_t \nabla q_k(x). \tag{9.3}$$

Then, we have for any $k \in \mathbb{N}^n$

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0) = \frac{e^{\beta_t}}{\sqrt{k!}}\, q_k(N_t^{-1/2}A^\dagger(Z_t))\varphi_0(Z_t), \quad t \in [0;T[. \tag{9.4}$$

Proof. We find with Corollary 9.1 for the components of the raising operator $\hat{A}^\dagger(\overline{S}_t Z_0)$

$$e_j^T \hat{A}^\dagger(\overline{S}_t Z_0) = e_j^T D_t^* \hat{A}^\dagger(Z_t) + e_j^T C^* \hat{A}(Z_t) = \hat{A}^\dagger(Z_t D_t e_j) + \hat{A}(Z_t \overline{C}_t e_j) := \hat{u}_j + \hat{v}_j.$$

In this way we can rewrite $\hat{A}_k^\dagger(\overline{S}_t Z_0)\varphi_0(Z_t) = \prod_{j=1}^n (\hat{u}_j + \hat{v}_j)^{k_j}\varphi_0(Z_t)$ for all $k \in \mathbb{N}^n$. Since $\hat{v}_j\varphi_0(Z_t) = 0$, it is clear that

$$\hat{A}_k^\dagger(\overline{S}_t Z_0)\varphi_0(Z_t) = q_k(\hat{u})\varphi_0(Z_t)$$

where $q_k(\hat{u}) = q_k(\hat{u}_1, \ldots, \hat{u}_n)$ is a polynomial of degree $|k|$ in n variables. We obtain this polynomial q_k be successively swapping $\hat{v}_j$ to the right, i.e. we replace each term of the form $\hat{v}_j\hat{u}_l$ by the commutator

$$\hat{v}_j\hat{u}_l = [\hat{v}_j, \hat{u}_l] + \hat{u}_l\hat{v}_j.$$

To simplify our notation, we summarise the commutators in a matrix $M_{l,j} := [\hat{u}_l, \hat{v}_j]$. Due to the commutator relation for the ladder operators in Lemma 4.1 it is clear that $M = M_t \in \mathbb{C}^{n\times n}$ is a time-dependent, complex matrix.

Moreover, we have for the commutator $[\hat{v}_j, \hat{u}_l^k] = -M_{l,j}k\hat{u}_l^{k-1} = -M_{l,j}\partial_{\hat{u}_l}\hat{u}_l^k$ and therefore for all polynomials $q(\hat{u})$,

$$[\hat{v}_j, q(\hat{u})] = -e_j^T M^T \nabla_{\hat{u}} q(\hat{u}).$$

We use this relation to show that the polynomials q_k indeed satisfy the recursion (9.3). We have

$$\begin{aligned} q_{k+e_j}(\hat{u})\varphi_0(Z_t) &= (\hat{u}_j + \hat{v}_j)q_k(\hat{u})\varphi_0(Z_t) = (\hat{u}_j q_k(\hat{u}) + [\hat{v}_j, q_k(\hat{u})] + q_k(\hat{u})\hat{v}_j)\,\varphi_0(Z_t) \\ &= \left(\hat{u}_j q_k(\hat{u}) - e_j^T M^T \nabla_{\hat{u}} q_k(\hat{u})\right)\varphi_0(Z_t) \end{aligned}$$

and it only remains to verify the form of M_t.

On the one hand, it follows from $Z_t = S_t Z_0 N_t^{-1/2}$ that

$$D_t^* = \tfrac{1}{2\mathrm{i}} Z_0^* S_t^T \Omega \mathcal{Z}_t = \tfrac{1}{2\mathrm{i}} Z_0^* S_t^T \Omega S_t Z_0 N_t^{-1/2} = N_t^{-1/2}.$$

For the matrix M_t on the other hand, the commutator relation from Lemma 4.1 implies

$$M_{l,j} = [\hat{A}^\dagger(Z_t D_t e_l), \hat{A}(Z_t \overline{C}_t e_j)] = \tfrac{1}{2\mathrm{i}}(Z_t \overline{C}_t e_j)^T \Omega \overline{Z}_t \overline{D}_t e_l = -e_j^T C_t^* \overline{D}_t e_l,$$

i.e. $M_t = -D_t^* \overline{C}_t$. Inserting C_t and D_t shows

$$-D_t^* \overline{C}_t = \tfrac{1}{4} Z_0^* S_t^T \Omega^T Z_t Z_t^* \Omega S_t \overline{Z}_0 = \tfrac{1}{4} Z_0^* S_t^T G_t S_t \overline{Z}_0,$$

or, equivalently,

$$-D_t^*\overline{C}_t = \tfrac{1}{2\mathrm{i}} N_t^{-1/2} Z_t^* \Omega S_t \overline{Z}_0 = \tfrac{1}{2\mathrm{i}} N_t^{-1} Z_0^* S_t^* \Omega S_t \overline{Z}_0.$$

From the first equality one can read off the symmetry of M_t, what finishes the proof. ■

This result nicely illustrates how the non-unitary time evolution activates lower order states. Equation (9.4) can be interpreted as an expansion of the propagated state into the basis defined by Z_t,

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0) = e^{\beta_t} \sum_{m\le k} \alpha_m \varphi_m(Z_t),$$

where the coefficients α_m can be computed in terms of N_t and the polynomial q_k. This emphasises the prominent role played by the matrices N_t and M_t. All the information about the effects of the non-Hermiticity on the propagation are encoded in those two matrices.

However, we can also interpret the application of $\hat{A}^\dagger(\overline{S}_t Z_0)$ to $\varphi_0(Z_t)$ as a generalised wave packet, generated via a non-normalised Lagrangian frame. We showed in the previous part that in both cases the overall structure of the wave packets, a multivariate polynomial times a Gaussian, is preserved. Hence, we expect a similar behaviour here.

Corollary 9.2 — Polynomial prefactor. Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ and $L_t := S_t L_0$ be positive Lagrangian subspaces for $t \in [0;T[$, $Z_t = S_t Z_0 N_t^{-1/2} \in F_n(L_t)$ and $G_t \in \mathrm{Sp}(n,\mathbb{R})$ denote the symplectic metric of L_t. We set

$$Z_t = \begin{pmatrix} P_t \\ Q_t \end{pmatrix}$$

and

$$M_t = \tfrac{1}{4}(S_t\overline{Z}_0)^T G_t (S_t \overline{Z}_0), \qquad \widetilde{M}_t = M_t + N_t^{-1/2} Q_t^{-1} \overline{Q}_t \overline{N}_t^{-1/2}.$$

We then have for any $k \in \mathbb{N}^n$

$$\widehat{\mathcal{U}}(t)\varphi_k(Z_0;x) = \tfrac{e^{\beta_t}}{\sqrt{2^{|k|}k!}}\, p_k^{\widetilde{M}_t}\left(\tfrac{1}{\sqrt{\varepsilon}} N_t^{-1/2} Q_t^{-1} x\right) \varphi_0(Z_t;x), \quad t\in[0;T[, \tag{9.5}$$

where the polynomials $p_k^{\widetilde{M}_t}$, satisfy the recursion relation (4.7).

Proof. This statement is also given in [LST15, Corollary 4.6]. Equivalently to the TTRR for the polynomials p_k^M, see Corollary 5.4, we find for the polynomials q_k from the previous theorem

$$\left(q_{k+e_j}(x)\right)_{j=1}^n = x q_k(x) - M_t \left(k_j q_{k-e_j}(x)\right)_{j=1}^n, \quad x\in\mathbb{R}^n.$$

We will use this relation and the ansatz

$$q_k(N_t^{-1/2}A^\dagger(Z_t))\varphi_0(Z_t;x) = \tfrac{1}{\sqrt{2^{|k|}}}\, p_k^{\widetilde{M}_t}(y_t)\,\varphi_0(Z_t;x), \quad y_t = \tfrac{1}{\sqrt{\varepsilon}} N_t^{-1/2} Q_t^{-1} x$$

that appears similarly as in Corollary 4.2 to show that (4.7) holds. We have

$$\begin{aligned}
&\left(q_{k+e_j}(N_t^{-1/2}A^\dagger(Z_t))\right)_{j=1}^n \varphi_0(Z_t;x)\\
&= \tfrac{1}{\sqrt{2^{|k|}}}\, N_t^{-1/2}A^\dagger(Z_t)\left(p_k^{\widetilde{M}_t}(y_t)\varphi_0(Z_t;x)\right) - M_t\left(\tfrac{k_j}{\sqrt{2^{|k|-1}}}p_{k-e_j}^{\widetilde{M}_t}(y_t)\varphi_0(Z_t;x)\right)_{j=1}^n\\
&= \tfrac{1}{\sqrt{2^{|k|+1}}}\left(\sqrt{2}N_t^{-1/2}A^\dagger(Z_t)\left(p_k^{\widetilde{M}_t}(y_t)\varphi_0(Z_t;x)\right) - M_t\nabla_{y_t}p_k^{\widetilde{M}_t}(y_t)\varphi_0(Z_t;x)\right)
\end{aligned}$$

where we used the gradient formula $\nabla_x p_k^M(x) = 2\left(k_j p_{k-e_j}^M(x)\right)_{j=1}^n$. Furthermore, with $A^\dagger(Z_t) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}(P_t^* x + \mathrm{i}\varepsilon Q_t^*\nabla_x)$ and $Q_t^* P_t - P_t^* Q_t = 2\mathrm{i}\mathrm{Id}$,

$$\begin{aligned}
&A^\dagger(Z_t)\left(p_k^{\widetilde{M}_t}(y_t)\varphi_0(Z_t;x)\right)\\
&= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}(P_t^* x p_k^{\widetilde{M}_t}(y_t) + \mathrm{i}\varepsilon Q_t^*(\tfrac{1}{\sqrt{\varepsilon}}Q_t^{-T}\overline{N}_t^{-1/2}\nabla_{y_t}p_k^{\widetilde{M}_t}(y_t) + \tfrac{\mathrm{i}}{\varepsilon}P_tQ_t^{-1}xp_k^{\widetilde{M}_t}(y_t)))\varphi_0(Z_t;x)\\
&= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}}((P_t^* - Q_t^*P_tQ_t^{-1})xp_k^{\widetilde{M}_t}(y_t) + \mathrm{i}\sqrt{\varepsilon}Q_t^*Q_t^{-T}\overline{N}_t^{-1/2}\nabla_{y_t}p_k^{\widetilde{M}_t}(y_t))\varphi_0(Z_t;x)\\
&= \tfrac{1}{\sqrt{2}}(2Q_t^{-1}xp_k^{\widetilde{M}_t}(y_t) - Q_t^{-1}\overline{Q}_t\overline{N}_t^{-1/2}\nabla_{y_t}p_k^{\widetilde{M}_t}(y_t))\varphi_0(Z_t;x),
\end{aligned}$$

since $N_t^{-1/2}$ is Hermitian and $Q_t^{-1}\overline{Q}_t$ symmetric. Inserting in the previous calculation yields the claim,

$$\begin{aligned}
&\left(q_{k+e_j}(N_t^{-1/2}A^\dagger(Z_t))\right)_{j=1}^n \varphi_0(Z_t;x)\\
&= \tfrac{1}{\sqrt{2^{|k|+1}}}\left(2N_t^{-1/2}Q_t^{-1}xp_k^{\widetilde{M}_t}(y_t) - (M_t + N_t^{-1/2}Q_t^{-1}\overline{Q}_t\overline{N}_t^{-1/2})\nabla_{y_t}p_k^{\widetilde{M}_t}(y_t)\right)\varphi_0(Z_t;x)\\
&= \tfrac{1}{\sqrt{2^{|k|+1}}}\left(2y_tp_k^{\widetilde{M}_t}(y_t) - \widetilde{M}_t\nabla_{y_t}p_k^{\widetilde{M}_t}(y_t)\right)\varphi_0(Z_t;x)\\
&= \tfrac{1}{\sqrt{2^{|k|+1}}}\left(p_{k+e_j}^{\widetilde{M}_t}(y_t)\right)_{j=1}^n \varphi_0(Z_t;x)
\end{aligned}$$

■

After determining the propagation of wave packets centred at the origin, we turn now to the evolution of wave packets centred at arbitrary phase space points $z \in \mathbb{R}^n \oplus \mathbb{R}^n$.

9.5. Dynamics of the centre

We assume that $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ and $L_t = S_tL_0$ are positive Lagrangian subspaces for $t \in [0;T[$ and consider the symplectic metric $G_t \in \mathrm{Sp}(n,\mathbb{R})$ and the complex structure $J_t \in \mathrm{Sp}(n,\mathbb{R})$ of the Lagrangian L_t. By repeating the calculations of Proposition 8.1 and Lemma 9.1, we obtain the dynamics of the centred ladder operators.

Lemma 9.2 — Ladder evolution. For all $l, z_0 \in \mathbb{C}^n \oplus \mathbb{C}^n$, we find

$$\widehat{\mathcal{U}}(t)\hat{A}(l,z_0)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}(S_tl, S_tz_0) \quad \text{and} \quad \widehat{\mathcal{U}}(t)\hat{A}^\dagger(l,z_0)\widehat{\mathcal{U}}(t)^{-1} = \hat{A}^\dagger(\overline{S}_tl, \overline{S}_tz_0).$$

Proof. Since a constant does not change the commutator properties, we find with a similar argumentation as in Lemma 9.1,

$$\begin{aligned}\hat{A}(l, z_0; S_t^{-1}z) &= \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T\Omega(S_t^{-1}z - z_0) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T\Omega S_t^{-1}(z - S_t z_0) = \tfrac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T S_t^T\Omega(z - S_t z_0)\\ &= \hat{A}(S_t l, S_t z_0; z),\\ \hat{A}^\dagger(l, z_0; S_t^{-1}z) &= \tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^*\Omega(S_t^{-1}z - \overline{z}_0) = \tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^T\Omega S_t^{-1}(z - S_t\overline{z}_0) = \tfrac{-\mathrm{i}}{\sqrt{2\varepsilon}} l^T S_t^*\Omega(z - S_t\overline{z}_0)\\ &= \hat{A}^\dagger(\overline{S}_t l, \overline{S}_t z_0; z),\end{aligned}$$

for all $z \in \mathbb{R}^n \oplus \mathbb{R}^n$. ■

Since S_t is complex, this implies that in contrast to the Hermitian dynamics we find here that even if we start with a real centre $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$, the time evolution will lead to a complex centre $S_t z_0$. However, we know by Theorem 4.4 that the projection P_{J_t} does not change the ladder operator if we parametrise by the Lagrangian L_t, that is,

$$A(S_t l, S_t z_0) = A(S_t l, P_{J_t}(S_t z_0))$$

for all $l \in L_0$ and $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$. The dynamics of the projected centres are easily inferred from the Riccati equations for the complex structure J_t in Theorem 9.1, see also [LST15, Corollary 4.7].

Corollary 9.3 — Projected dynamics. Let L_0 and $L_t = S_t L_0$ be positive Lagrangian subspaces for $t \in [0; T[$. Denote by $G_t, J_t \in \mathrm{Sp}(n, \mathbb{R})$ the symplectic metric and the complex structure of L_t, respectively. Let $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$. Then, $z_t := P_{J_t}(S_t z_0) \in \mathbb{R}^n \oplus \mathbb{R}^n$ satisfies

$$\dot{z}_t = \Omega\mathrm{Re}(H)z_t + G_t^{-1}\mathrm{Im}(H)z_t. \tag{9.6}$$

Proof. The same result can be found in [GS11]. We recall that the projection P_{J_t} was defined as

$$P_{J_t}(S_t z_0) = \mathrm{Re}(S_t z_0) + J_t\mathrm{Im}(S_t z_0).$$

With the equation for the linearised flow (8.12) and the Riccati equation for J_t,

$$\begin{aligned}\dot{z}_t &= \mathrm{Re}(\dot{S}_t z_0) + \dot{J}_t\mathrm{Im}(S_t z_0) + J_t\mathrm{Im}(\dot{S}_t z_0) = \mathrm{Re}(\Omega H S_t z_0) + \dot{J}_t\mathrm{Im}(S_t z_0) + J_t\mathrm{Im}(\Omega H S_t z_0)\\ &= \Omega\mathrm{Re}(H)\mathrm{Re}(S_t z_0) - \Omega\mathrm{Im}(H)\mathrm{Im}(S_t z_0) + \Omega\mathrm{Re}(H)J_t\mathrm{Im}(S_t z_0) - J_t\Omega\mathrm{Re}(H)\mathrm{Im}(S_t z_0)\\ &\quad + \Omega\mathrm{Im}(H)\mathrm{Im}(S_t z_0) + J_t\Omega\mathrm{Im}(H)J_t\mathrm{Im}(S_t z_0) + J_t\Omega\mathrm{Im}(H)\mathrm{Re}(S_t z_0) + J_t\Omega\mathrm{Re}(H)\mathrm{Im}(S_t z_0)\\ &= \Omega\mathrm{Re}(H)z_t + J_t\Omega\mathrm{Im}(H)z_t = \Omega\mathrm{Re}(H)z_t + G_t^{-1}\mathrm{Im}(H)z_t,\end{aligned}$$

since $J_t\Omega = \Omega^T G_t\Omega$ and G_t is symplectic. ■

The time evolution of coherent states with real projected centres resembles the one in Proposition 9.2, however, with an additional phase factor determined by the action integral of the Hamiltonian $\mathcal{H}$ along the real projected trajectory, see [LST15, Proposition 4.8] or Proposition 8.1.

Proposition 9.3 — Coherent state evolution. Let $L_0 \subset \mathbb{C}^n \oplus \mathbb{C}^n$ be a positive Lagrangian subspace, $Z_0 \in F_n(L_0)$ and $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$. If the Lagrangian $L_t = S_t L_0$ is positive for $t \in [0, T[$, then

$$\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0) = e^{\frac{i}{\varepsilon}\alpha_t(z_0)}\varphi_0(S_t Z_0, z_t) = e^{\frac{i}{\varepsilon}\alpha_t(z_0)+\beta_t}\varphi_0(Z_t, z_t)$$

for all $t \in [0; T[$, where $Z_t = S_t Z_0 N_t^{-1/2}$, $z_t =: (p_t, q_t) \in \mathbb{R}^n \oplus \mathbb{R}^n$ is defined by (9.6), β_t is the factor derived in Proposition 9.2 and

$$\alpha_t(z_0) := \int_0^t \left(p_\tau^T \dot{q}_\tau - \mathcal{H}_\tau(z_\tau)\right) d\tau \tag{9.7}$$

denotes the associated action integral of the Hamiltonian $\mathcal{H}_t$ along z_t.

Proof. With our standard approach, we find

$$0 = \widehat{\mathcal{U}}(t)\hat{A}(Z_0, z_0)\varphi_0(Z_0, z_0) = \hat{A}(S_t Z_0, S_t z_0)\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0) = \hat{A}(S_t Z_0, z_t)\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0)$$

and hence $\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0) = c_t \cdot \varphi_0(S_t Z_0, z_t)$ for $c_t \in \mathbb{C}$. The factor α_t emerges with an analogous computation as in Proposition 8.1. ■

Our previous results on excited state propagation, that is, Theorem 9.2 and Corollary 9.2, describe the time evolution of $\widehat{\mathcal{U}}(t)\varphi_k(Z_0, z_0)$, $k \in \mathbb{N}^n$, for the case $z_0 = 0$ in terms of multivariate polynomials. Essentially, these results stay the same when considering nonzero $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$. The ladder decomposition from Corollary 9.1 also holds true with phase space centres z_0,

$$\hat{A}^\dagger(\overline{S}_t Z_0, \overline{S}_t z_0) = D_t^* \hat{A}^\dagger(Z_t, \overline{S}_t z_0) + C_t^* \hat{A}(Z_t, S_t z_0) = D_t^* \hat{A}^\dagger(Z_t, z_t) + C_t^* \hat{A}(Z_t, z_t).$$

Hence, the propagated excited states can be constructed similar as in the previous section,

$$\begin{aligned}\widehat{\mathcal{U}}(t)\varphi_k(Z_0, z_0) &= \tfrac{1}{\sqrt{k!}}\,\hat{A}_k^\dagger(\overline{S}_t Z_0, S_t z_0)\widehat{\mathcal{U}}(t)\varphi_0(Z_0, z_0)\\ &= \tfrac{1}{\sqrt{k!}} e^{\frac{i}{\varepsilon}\alpha_t(z_0)+\beta_t}(D_t^* \hat{A}^\dagger(Z_t, z_t) + C_t^* \hat{A}(Z_t, z_t))^k \varphi_0(Z_t, z_t),\end{aligned}$$

and we only have to record the evolution of the centre and add the corresponding action integral.

Theorem 9.3 — Excited state evolution. Let L_0 and $L_t = S_t L_0$ be positive Lagrangian subspaces for $t \in [0; T[$, $z_0 \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $Z_t = S_t Z_0 N_t \in F_n(L_t)$. Set

$$Z_t = \begin{pmatrix} P_t \\ Q_t \end{pmatrix}$$

and denote by $G_t \in \mathrm{Sp}(n,\mathbb{R})$ the symplectic metric of L_t. Define

$$M_t = \tfrac{1}{4}(S_t\bar{Z}_0)^T G_t (S_t\bar{Z}_0) \quad \text{and} \quad \widetilde{M}_t = M_t + N_t^{-1/2} Q_t^{-1} \overline{Q}_t \overline{N}_t^{-1/2}.$$

Then, we have for any $k \in \mathbb{N}^n$ and $t \in [0;T[$

$$\begin{aligned}\widehat{\mathcal{U}}(t)\varphi_k(Z_0,z_0;x) &= \tfrac{1}{\sqrt{k!}}\, e^{\frac{\mathrm{i}}{\varepsilon}\alpha_t(z_0)+\beta_t}\, q_k(N_t^{-1/2}A^\dagger(Z_t,z_t))\,\varphi_0(Z_t,z_t;x)\\ &= \tfrac{1}{\sqrt{2^{|k|}k!}}\, e^{\frac{\mathrm{i}}{\varepsilon}\alpha_t(z_0)+\beta_t}\, p_k^{\widetilde{M}_t}\left(\tfrac{1}{\sqrt{\varepsilon}}\, N_t^{-1/2} Q_t^{-1}(x-q_t)\right)\varphi_0(Z_t,z_t;x)\end{aligned}$$

where $z_t = (p_t,q_t) \in \mathbb{R}^n \oplus \mathbb{R}^n$ is defined by (9.6) and $\alpha_t(z_0)$ is the action integral (9.7) of $\mathcal{H}_t$ along the trajectory z_t. The polynomials q_k satisfy the recursion (9.3) and $p_k^{\widetilde{M}_t}$ is defined as in Proposition 4.7.

9.6. Example: Davies-Swanson oscillator

As an example we investigate the dynamics of a one-dimensional quadratic non-Hermitian Hamiltonian, the Davies-Swanson oscillator

$$\widehat{\mathcal{H}} = \tfrac{\omega_0}{2}(\hat{p}^2+\hat{q}^2) - \tfrac{\mathrm{i}\delta}{2}(\hat{p}\hat{q}+\hat{q}\hat{p})$$

defined by the complex symmetric matrix

$$H = \begin{pmatrix} \omega_0 & -\mathrm{i}\delta \\ -\mathrm{i}\delta & \omega_0 \end{pmatrix}, \qquad \omega_0, \delta > 0.$$

For this particular Hamiltonian the spectrum and transition elements have been computed, see [Dav99a] and [Swa04], as well as the dynamics of coherent states, see [Gra+14]. It is our aim here to complement the picture by propagating excited wave packets.

We start with a positive Lagrangian

$$L_0 = \mathrm{span}\{l_0\}, \qquad l_0 = \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \in \mathbb{C}^2,$$

and first note that l_0 is normalised if $\mathrm{Im}(p_0\overline{q}_0) = 1$. To describe the propagation of the wave packets, we set $L_t = \mathrm{span}\{l_t\}$ with

$$l_t = \begin{pmatrix} p_t \\ q_t \end{pmatrix} = S_t l_0 n_t, \qquad n_t = h(S_t l_0, S_t l_0),$$

and only observe times $t \in \mathbb{R}$ with $n_t > 0$. As initial value we choose $l_0 = (1,-\mathrm{i})^T$, this means $\varphi_0(l_0)$ yields the standard coherent state.

Linearised flow

We calculate S_t as the solution of the Hamiltonian system (8.12) and obtain consequently $S_t = e^{t\Omega H}$. Since

$$(\Omega H)^{2k} = (-1)^k \omega^{2k} \mathrm{Id}_2 \,, \qquad (\Omega H)^{2k+1} = (-1)^k \omega^{2k} \Omega H \,, \qquad k \geq 0,$$

for $\omega^2 := \omega_0^2 + \delta^2$, we end up with

$$S_t = \sum_{k=0}^{\infty} (-1)^k \frac{t^{2k}}{(2k)!} \omega^{2k} \mathrm{Id}_2 + \sum_{k=0}^{\infty} (-1)^k \frac{t^{2k+1}}{(2k+1)!} \omega^{2k} \Omega H = \cos(t\omega) \mathrm{Id}_2 + \tfrac{1}{\omega} \sin(t\omega) \Omega H.$$

In particular, it holds

$$S_t^* \Omega S_t = \cos^2(t\omega) \mathrm{Id}_2 + \tfrac{1}{\omega^2} \sin^2(t\omega) \overline{H} \Omega H - \tfrac{2\mathrm{i}}{\omega} \cos(t\omega) \sin(t\omega) \mathrm{Im}(H),$$

where

$$\mathrm{Im}(H) = \begin{pmatrix} 0 & -\delta \\ -\delta & 0 \end{pmatrix} \quad \text{and} \quad \overline{H} \Omega H = \begin{pmatrix} 2\mathrm{i}\omega_0 \delta & \delta^2 - \omega_0^2 \\ \omega_0^2 - \delta^2 & -2\mathrm{i}\omega_0 \delta \end{pmatrix}.$$

Normalisation

The formula for S_t allows us to explicitly calculate the normalisation and derive times t such that our evolved Lagrangian is positive. A direct computation shows

$$n_t = \tfrac{1}{2\mathrm{i}} l_0^* S_t^* \Omega S_t l_0 = \cos^2(t\omega) + \tfrac{\omega_0^2 - \delta^2}{\omega_0^2 + \delta^2} \sin^2(t\omega),$$

since $l_0^* \overline{H} \Omega H l_0 = 2\mathrm{i}(\omega_0^2 - \delta^2)$ and $l_0^* \mathrm{Im}(H) l_0 = 0$. We can further rewrite this expression as

$$n_t = 1 - 2\tfrac{\delta^2}{\omega^2} \sin^2(t\omega) = 1 - \tfrac{\delta^2}{\omega^2}(1 - \cos(2t\omega)).$$

So, n_t is positive, if $\frac{\omega^2}{\delta^2} > 1 - \cos(2t\omega)$. This is true for all times t, if $\omega_0^2 > \delta^2$ or, for $t \in [0; T[$ with $T = \frac{1}{2\omega} \arccos(-\frac{\omega_0^2}{\delta^2})$.

Evolved coherent state

For all times t such that n_t is positive, we can parametrise the Lagrangian subspace L_t via the normalised Lagrangian frame

$$l_t = S_t l_0 n_t^{-1/2} = \begin{pmatrix} \cos(t\omega) + \mathrm{i}\frac{\omega_0 + \delta}{\omega} \sin(t\omega) \\ -\mathrm{i}\cos(t\omega) + \frac{\omega_0 - \delta}{\omega} \sin(t\omega) \end{pmatrix} n_t^{-1/2}.$$

Moreover, since we are handling a univariate setting, we may invoke $e^{\beta_t} = n_t^{-1/4}$ and directly state that

$$e^{\beta_t} = (1 - \tfrac{\delta^2}{\omega^2}(1 - \cos(2t\omega)))^{-1/4}.$$

With these two parameters the propagation of the coherent state $\mathcal{U}(t)\varphi_0(l_0)$ is entirely determined.

Evolved excited states

For our contribution on this example, the more excited state, we also have to examine the polynomial prefactor. For $m_t = n_t^{-1} h(S_t l_0, S_t \bar{l}_0)$, the formula for $S_t^* \Omega S_t$ provides

$$m_t = n_t^{-1} h(S_t l_0, S_t \bar{l}_0) = \tfrac{2\delta}{\omega} n_t^{-1} \sin(t\omega)(\tfrac{\omega_0}{\omega} \sin(t\omega) + \mathrm{i}\cos(t\omega)),$$

since $l_0^* \overline{H} \Omega H l_0 = 4\mathrm{i}\delta\omega_0$, $l_0^* \mathrm{Im}(H) l_0 = -2\mathrm{i}\delta$. The recursion matrix $\widetilde{m}_t$ exhibits the unpleasant form

$$\widetilde{m}_t = m_t + n_t^{-1} \frac{\frac{\omega_0 - \delta}{\omega} \sin(t\omega) + \mathrm{i}\cos(t\omega)}{\frac{\omega_0 - \delta}{\omega} \sin(t\omega) - \mathrm{i}\cos(t\omega)}.$$

The polynomials, by contrast, can in one dimension simply be written as scaled Hermite polynomials, see Section 5.1,

$$p_0^{\widetilde{m}_t}(x) = 1, \quad p_1^{\widetilde{m}_t}(x) = 2x, \quad p_2^{\widetilde{m}_t}(x) = 4x^2 - 2\widetilde{m}_t \quad p_3^{\widetilde{m}_t}(x) = 8x^3 - 12\widetilde{m}_t x.$$

Expansion in lower excited states

According to Theorem 9.2 we can also expand the evolved excited states in terms of lower excited states, what is more convenient when we calculate the norm. The polynomials q_k are scaled Hermite polynomials,

$$q_0(x) = 1, \quad q_1(x) = x, \quad q_2(x) = x^2 - m_t \quad q_3(x) = x^3 - 3m_t x$$

and we obtain for the propagated wave packets

$$\begin{aligned}
\widehat{\mathcal{U}}(t)\varphi_0(l_0) &= e^{\beta_t}\varphi_0(l_t),\\
\widehat{\mathcal{U}}(t)\varphi_1(l_0) &= e^{\beta_t}\left(n_t^{-1/2}\hat{A}^\dagger(l_t)\right)\varphi_0(l_t) = e^{\beta_t} n_t^{-1/2}\varphi_1(l_t),\\
\widehat{\mathcal{U}}(t)\varphi_2(l_0) &= \tfrac{e^{\beta_t}}{\sqrt{2}}\left(n_t^{-1}\hat{A}_2^\dagger(l_t) - m_t\right)\varphi_0(l_t) = e^{\beta_t}\left(n_t^{-1}\varphi_2(l_t) - \tfrac{m_t}{\sqrt{2}}\varphi_0(l_t)\right),\\
\widehat{\mathcal{U}}(t)\varphi_3(l_0) &= \tfrac{e^{\beta_t}}{\sqrt{3!}} n_t^{-1/2}\left(n_t^{-1}\hat{A}_3^\dagger(l_t) - 3m_t\hat{A}^\dagger(l_t)\right)\varphi_0(l_t) = e^{\beta_t} n_t^{-1/2}\left(n_t^{-1}\varphi_3(l_t) - \tfrac{\sqrt{6}}{2} m_t\varphi_1(l_t)\right).
\end{aligned}$$

Since $(\varphi_k(l_t))_{k\in\mathbb{N}}$ forms an orthonormal basis set, this implies for the norms

$$\begin{aligned}
\|\widehat{\mathcal{U}}(t)\varphi_0(l_0)\| &= e^{\beta_t}, & \|\widehat{\mathcal{U}}(t)\varphi_2(l_0)\| &= e^{\beta_t}\sqrt{n_t^{-2} + \tfrac{1}{2}|m_t|^2}\\
\|\widehat{\mathcal{U}}(t)\varphi_1(l_0)\| &= e^{\beta_t} n_t^{-1/2}, & \|\widehat{\mathcal{U}}(t)\varphi_3(l_0)\| &= e^{\beta_t} n_t^{-1/2}\sqrt{n_t^{-2} + \tfrac{3}{2}|m_t|^2}.
\end{aligned}$$

The time evolution of these norms is displayed in Figure 15. One can recognise that all norms significantly differ from one, the higher the excited state, the larger the deviation.

Dynamics of the centre

For the dynamic of the centre we first state the time-evolved metric G_t of L_t. A direct calculation using l_t shows

$$G_t = n_t^{-1}\begin{pmatrix} 1 - 2\frac{\delta\omega_0}{\omega^2}\sin^2(t\omega) & 2\frac{\delta}{\omega}\cos(t\omega)\sin(t\omega) \\ 2\frac{\delta}{\omega}\cos(t\omega)\sin(t\omega) & 1 + 2\frac{\delta\omega_0}{\omega^2}\sin^2(t\omega) \end{pmatrix}$$

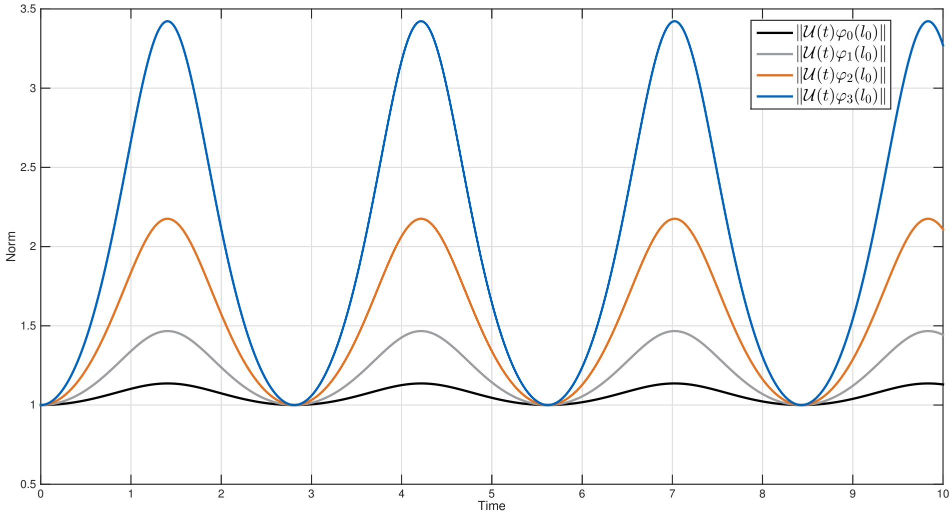

Figure 15.: Time evolution of $\|\mathcal{U}(t)\varphi_k(l_0)\|$ for $k = 0, \ldots, 3$ with $\omega_0 = 1$ and $\delta = 0.5$.

Hence, z_t is determined by the initial value z_0 and the differential equation

$$\dot{z}_t = n_t^{-1} \begin{pmatrix} 2\frac{\delta^2}{\omega}\cos(t\omega)\sin(t\omega) & -(\delta + \omega_0) \\ \omega_0 - \delta & 2\frac{\delta^2}{\omega}\cos(t\omega)\sin(t\omega) \end{pmatrix} z_t$$

that was solved numerically to obtain the trajectories in Figure 16. We find that the circular trajectory of the harmonic oscillator, see Figure 14, is converted to an ellipsoid due to the imaginary part.

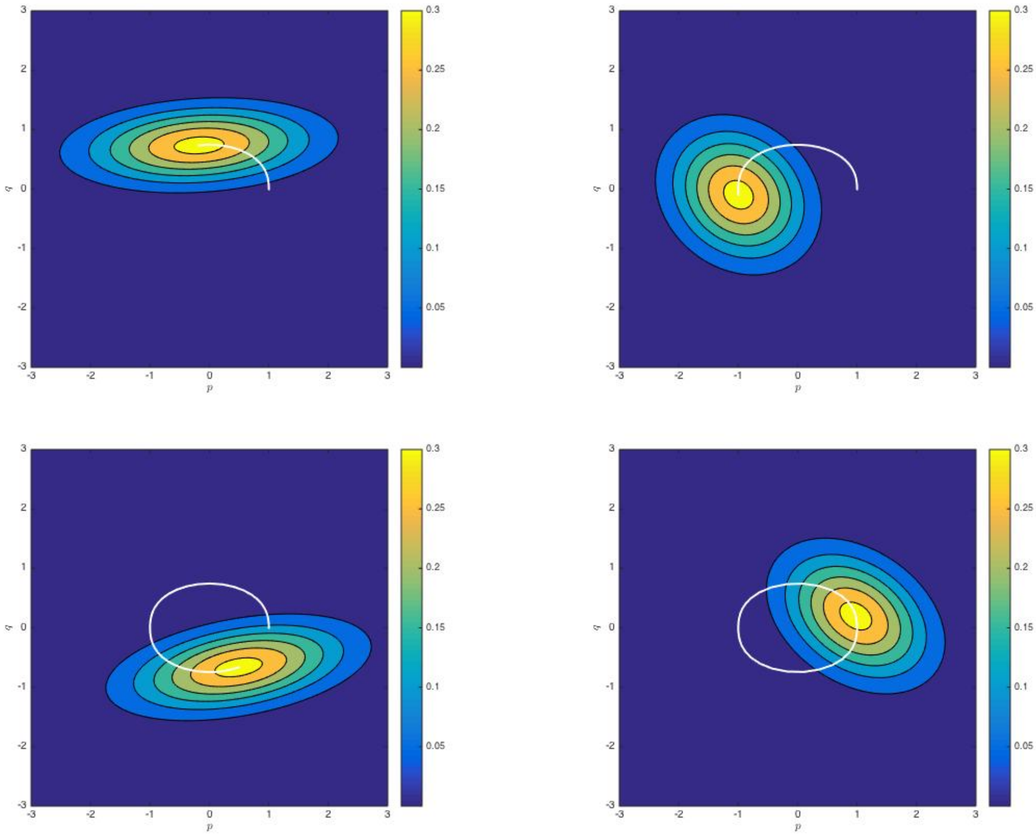

Figure 16.: Trajectory of the centre z_t starting from $z_0 = (1, 0)$ and contour plot of the absolute value of $\mathcal{W}_0(\mathcal{Z}_t, z_t)$ at time $t = 1.5$ (upper left), $t = 3$ (upper right), $t = 4.5$ (lower left) and $t = 6$ (lower right) for $\varepsilon = 1$

10. Lindblad dynamics

In the standard description of quantum mechanics via a Hermitian Hamiltonian we investigate the time evolution of closed systems. By allowing for non-Hermitian Hamiltonians we relax this aspect. As we have seen in the previous example we can now also model diffusion, i.e. an interaction between our quantum system and its environment. Such interactions will in practical situation always occur to some extent and are thus worth a closer study.

A more general characterisation of open quantum system is given by the Lindblad equation. Analogously to the derivation of the Schrödinger equation in Section 8.1 via the generator of a continuous semigroup, we now represent the state of an open system by a density matrix $\hat{\rho}$. For simplicity, we skipped in the previous chapters that the representation via a wave function is only suitable in the special case of a pure quantum system, see [Gos10, §13.1]. A *density matrix* or *density operator* is a positive trace class operator with trace one, i.e.

$$\hat{\rho} : L^2(\mathbb{R}^n) \mapsto L^2(\mathbb{R}^n) \quad \text{such that} \quad \hat{\rho}^* = \hat{\rho}, \quad \hat{\rho} \geq 0, \quad \operatorname{tr}(\hat{\rho}) = 1. \tag{10.1}$$

Lindblad assumed that the time evolution in an open system is governed by a quantum dynamical semigroup $\{\mathcal{U}(t)\,;\, t \geq 0\}$, see Definition 8.1 and (8.4) and derived the generator of an arbitrary contraction semigroup. Analogously to Lemma 8.1 he obtained the *Lindblad master equation*

$$\mathrm{i}\varepsilon\, \partial_t \hat{\rho} = \left[\widehat{\mathcal{H}}, \hat{\rho}\right] + \tfrac{\mathrm{i}}{2} \sum_{j=1}^{m} 2\hat{\mathcal{L}}_j \hat{\rho} \hat{\mathcal{L}}_j^* - \hat{\mathcal{L}}_j^* \hat{\mathcal{L}}_j \hat{\rho} - \hat{\rho} \hat{\mathcal{L}}_j^* \hat{\mathcal{L}}_j, \tag{10.2}$$

see [Lin76b]. The Hamiltonian $\widehat{\mathcal{H}}$ thereby describes the internal system, the Lindblad operators $\hat{\mathcal{L}}_j$ the coupling to the environment. If $\hat{\mathcal{L}}_j = 0$ we find the classical Liouville-von-Neumann equation, otherwise the time evolution will be non-unitary even if $\widehat{\mathcal{H}}$ and $\hat{\mathcal{L}}_j$, $j = 1, \ldots, m$, are self-adjoint operators.

In this thesis we will discuss the time evolution under the Lindblad equation if $\widehat{\mathcal{H}}$ is a self-adjoint, quadratic Hamiltonian and the Lindblad terms $\hat{\mathcal{L}}_j$, $j = 1, \ldots, m$, are linear, this means

$$\mathcal{H}(z) = \tfrac{1}{2} z^T H z, \; H = H^T \in \mathbb{R}^{2n \times 2n} \quad \text{and} \quad \mathcal{L}_j(z) = \ell_j^T z, \; \ell_j \in \mathbb{C}^{2n} \tag{10.3}$$

for $1 \leq j \leq m$. We show in the first section that in this case we can rewrite (10.2) as a Schrödinger equation of doubled dimension with non-Hermitian Hamiltonian. Since density operators are closely related to Wigner functions, we can combine our findings from Chapter 6 and Chapter 9 and handle the Lindblad equation as a complex

Schrödinger equation on phase space. To illustrate our results we review two different examples, a damped harmonic oscillator and as a theoretical approach a system without internal Hamiltonian at the end of this chapter.

10.1. Lindblad equation

The idea to use Wigner functions as ansatz for the Lindblad equation has been carried out before, see for example [Alm02, §1, §3]. In their work the authors used Gaussians as ansatz functions as their Wigner functions are again Gaussians. Due to our findings for the Wigner transform of Hagedorn's wave packets in Chapter 6, we are again able to generalise these results to more excited states. The basic principle is to utilise that Weyl-operators of any symmetric Wigner function form density operators.

Proposition 10.1 — Density operators. Let $\hat{\rho}$ be a density operator satisfying (10.1). Then, there exists a function $\psi \in L^2(\mathbb{R}^n)$ such that $\hat{\rho}$ can be written as

$$(\hat{\rho}\varphi)(x) = \psi\langle\varphi, \psi\rangle = \int_{\mathbb{R}^n} \psi(x)\overline{\psi}(y)\varphi(y)\, dy.$$

The Weyl symbol of $\hat{\rho}$ and the Wigner transform $\mathcal{W}^\varepsilon(\psi)$ are related by

$$\rho = (2\pi\varepsilon)^n \mathcal{W}^\varepsilon(\psi).$$

Proof. This result is a combination of [Gos10, Proposition 291] and [Gos10, Proposition 296]. The integral formula is obtained if one notices that $\hat{\rho}$ must be a projection on a one-dimensional subspace of $L^2(\mathbb{R}^n)$, i.e.

$$\hat{\rho} : L^2(\mathbb{R}^n) \mapsto \operatorname{span}\{\psi\}$$

for some $\psi \in L^2(\mathbb{R}^n)$. For the Weyl symbol we first state that similar to Lemma A.2 one can show that the kernel of a Weyl-operator $\hat{a}$ is given by

$$K_a(x, y) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)} a(\xi, \frac{1}{2}(x+y))\, d\xi.$$

A detailed proof for this equality can be found in [Gos10, Proposition 205] or Proposition A.1. The integral formula on the other hand directly implies $K_\rho(x, y) = \psi(x)\overline{\psi}(y)$ and thus,

$$\psi(x - \frac{y}{2})\overline{\psi}(x + \frac{y}{2}) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}\xi^T y} \rho(\xi, x)\, d\xi = (2\pi\varepsilon)^{-n/2} (\mathcal{F}_\xi^\varepsilon \rho)(y, x)$$

where $\mathcal{F}_\xi^\varepsilon$ denotes the Fourier transform in the first component. Applying the inverse Fourier transform then yields the result,

$$\rho(\xi, x) = \int_{\mathbb{R}^n} \psi(x - \frac{y}{2})\overline{\psi}(x + \frac{y}{2}) e^{\frac{\mathrm{i}}{\varepsilon}\xi^T y}\, dy = (2\pi\varepsilon)^n \mathcal{W}^\varepsilon(\psi)(\xi, x).$$

■

Mixed Wigner functions $\mathcal{W}^\varepsilon(\varphi,\psi)$ then emerge as the deviation between symmetric Wigner functions

$$\mathcal{W}^\varepsilon(\varphi,\psi) + \mathcal{W}^\varepsilon(\psi,\varphi) = \mathcal{W}^\varepsilon(\varphi+\psi) - \mathcal{W}^\varepsilon(\varphi) - \mathcal{W}^\varepsilon(\psi).$$

Our aim now is to deduce an equivalent formalism of the Lindblad equation for the symbol ρ and then insert the Wigner transform of Hagedorn's wave packets, that are wave packets on phase space, as ansatz functions. An easy approach is to first write (10.2) in commutator form,

$$\mathrm{i}\varepsilon\,\partial_t\hat{\rho} = \left[\widehat{\mathcal{H}},\hat{\rho}\right] + \tfrac{\mathrm{i}}{2}\sum_{j=1}^m\left(\left[\hat{\mathcal{L}}_j\hat{\rho},\hat{\mathcal{L}}_j^*\right] + \left[\hat{\mathcal{L}}_j,\hat{\rho}\hat{\mathcal{L}}_j^*\right]\right) \tag{10.4}$$

and then use the Weyl calculus from Appendix A to proceed a semiclassical expansion up to second order.

Lemma 10.1 — Dynamics of the symbol. We denote by $\widehat{\mathcal{H}}$ and $\hat{\mathcal{L}}_j$ the Weyl-operators of $\mathcal{H}$ and $\mathcal{L}_j$, $j=1,\dots,m$, as defined in (10.3). Then, a density operator $\hat{\rho}$ is a solution of the Lindblad-equation (10.2) if its symbol ρ satisfies

$$\partial_t\rho = \{\mathcal{H},\rho\} + \tfrac{\mathrm{i}}{2}\sum_{j=1}^m\{\mathcal{L}_j\rho,\mathcal{L}_j^*\} + \{\mathcal{L}_j,\rho\mathcal{L}_j^*\} - \tfrac{\varepsilon}{4}\sum_{j=1}^m\{\{\mathcal{L}_j,\rho\},\mathcal{L}_j^*\} + \{\mathcal{L}_j,\{\rho,\mathcal{L}_j^*\}\}.$$

Proof. Since $\mathcal{H}$ and $\mathcal{L}_j$ are for all $j=1,\dots,m$ at most quadratic operators, we can invoke (A.2) and find $\left[\hat{\mathcal{H}},\hat{\rho}\right] = \mathrm{i}\varepsilon\{\mathcal{H},\rho\}$ and

$$\begin{aligned}\left[\hat{\mathcal{L}}_j\hat{\rho},\hat{\mathcal{L}}_j^*\right] &= \mathrm{i}\varepsilon\,\mathrm{op}_\varepsilon[\{\mathcal{L}_j\#\rho,\mathcal{L}_j^*\}] = \mathrm{i}\varepsilon\,\mathrm{op}_\varepsilon[\{\mathcal{L}_j\rho,\mathcal{L}_j^*\} + \tfrac{\mathrm{i}\varepsilon}{2}\{\{\mathcal{L}_j,\rho\},\mathcal{L}_j^*\}]\\ \left[\hat{\mathcal{L}}_j,\hat{\rho}\hat{\mathcal{L}}_j^*\right] &= \mathrm{i}\varepsilon\,\mathrm{op}_\varepsilon[\{\mathcal{L}_j,\rho\#\mathcal{L}_j^*\}] = \mathrm{i}\varepsilon\,\mathrm{op}_\varepsilon[\{\mathcal{L}_j,\rho\mathcal{L}_j^*\} + \tfrac{\mathrm{i}\varepsilon}{2}\{\mathcal{L}_j,\{\rho,\mathcal{L}_j^*\}\}]\end{aligned}$$

for all $j=1,\dots,m$. ■

Since the Poisson bracket involves only first derivatives of the symbols, we see that the equation for the symbol contains at most second derivatives and we can thus rewrite it as a complex Schrödinger equation of doubled dimension.

We moreover utilise Proposition 10.1 and identify the symbol ρ with a symmetric Wigner function $\mathcal{W}^\varepsilon(\psi)$. In Chapter 6 we introduced the Wigner transform only for Schwartz functions since this was sufficing for our further proceeding. We also restrict ourselves to Schwartz functions ψ in the next proposition, as we want to insert Hagdorn's wave packets anyway. However, we refer to [Gos10, Proposition 183] for an extension of the Wigner transform to general L^2-functions.

Proposition 10.2 — Schrödinger formalism. Let $\mathcal{H}$ and $\mathcal{L}_j$, $1\le j\le m$, be defined as in (10.3) and $\mathcal{W} = \mathcal{W}^\varepsilon(\psi)$ denote the Wigner transform of an arbitrary Schwartz function $\psi\in\mathcal{S}(\mathbb{R}^n)$.

The density matrix $(2\pi\varepsilon)^n\widehat{\mathcal{W}}$ is a solution of the Lindblad equation (10.2) if $\mathcal{W}$ solves

$$\mathrm{i}\varepsilon\,\partial_t\mathcal{W} = (\widehat{\mathcal{H}}_S + \mathrm{i}\varepsilon\gamma)\mathcal{W} \tag{10.5}$$

where $\mathcal{H}_S$ is a quadratic function on $\mathbb{C}^{2n}\oplus\mathbb{C}^{2n}$ with Hessian matrix

$$H_S = \begin{pmatrix} \mathrm{i}\mathrm{Re}(L) & \Omega H + \mathrm{Im}(L)\Omega \\ -H\Omega + \Omega\mathrm{Im}(L) & 0 \end{pmatrix}, \quad L = \sum_{j=1}^m \Omega\ell_j\ell_j^*\Omega \tag{10.6}$$

and $\gamma = \sum_{j=1}^m \mathrm{Re}(\ell_j)^T\Omega\mathrm{Im}(\ell_j)$ the dissipation coefficient.

Before we start with the proof let us briefly note that the Hamiltonian satisfies

$$\mathrm{Im}(H_S) = \begin{pmatrix} \mathrm{Re}(L) & 0 \\ 0 & 0 \end{pmatrix}$$

and $\mathrm{Re}(L)$ is negative semidefinite, since $z^*\mathrm{Re}(L)z = -\frac{1}{2}\sum_{j=1}^m |\ell_j^*\Omega z|^2 + |\ell_j^T\Omega z|^2$ for all $z\in\mathbb{R}^n\oplus\mathbb{R}^n$. So, Proposition 9.1 implies that our approach for the Lindblad equation is well-defined for all times $t\geq 0$.

Proof. The idea is to rewrite the Poisson brackets in Lemma 10.1 in terms of the gradient, $\{a,b\} = \nabla a^T\Omega\nabla b$, and compare our findings to the formula for general quadratic Hamiltonians in Lemma 8.2. Since

$$\begin{aligned}
\{\mathcal{L}_j\mathcal{W},\mathcal{L}_j^*\} + \{\mathcal{L}_j,\mathcal{W}\mathcal{L}_j^*\} &= 2\{\mathcal{L}_j,\mathcal{L}_j^*\}\mathcal{W} + \{\mathcal{W},\mathcal{L}_j^*\}\mathcal{L}_j + \{\mathcal{L}_j,\mathcal{W}\}\mathcal{L}_j^* \\
&= \left(-2\ell_j^*\Omega\ell_j - z^T\ell_j\ell_j^*\Omega\nabla_z + z^T\overline{\ell}_j\ell_j^T\Omega\nabla_z\right)\mathcal{W} \\
&= -2\left(\ell_j^*\Omega\ell_j + \mathrm{i}z^T\mathrm{Im}(\ell_j\ell_j^*)\Omega\nabla_z\right)\mathcal{W},
\end{aligned}$$

and

$$\{\{\mathcal{L}_j,\mathcal{W}\},\mathcal{L}_j^*\} = \{\mathcal{L}_j^*,\{\mathcal{W},\mathcal{L}_j\}\} = \ell_j^*\Omega D^2\mathcal{W}\Omega\ell_j, \quad \{\mathcal{L}_j,\{\rho,\mathcal{L}_j^*\}\} = \ell_j^T\Omega D^2\mathcal{W}\Omega\overline{\ell}_j$$

for all $j=1,\dots,m$, where $D^2\mathcal{W}$ denotes the Hessian matrix of $\mathcal{W}$, the Wigner transform $\mathcal{W}$ satisfies

$$\partial_t\mathcal{W} = z^T(H + \sum_{j=1}^m \mathrm{Im}(\ell_j\ell_j^*))\Omega\nabla_z\mathcal{W} - \mathrm{i}\sum_{j=1}^m \ell_j^*\Omega\ell_j\mathcal{W}(z) - \tfrac{\varepsilon}{4}\sum_{j=1}^m \ell_j^*\Omega D^2\mathcal{W}\Omega\ell_j + \ell_j^T\Omega D^2\mathcal{W}\Omega\overline{\ell}_j.$$

Introducing the notation

$$H_S = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \in \mathbb{C}^{4n\times 4n}$$

we can directly conclude that $H_{22} = 0$ and $H_{21} = -(H + \sum_{j=1}^m \mathrm{Im}(\ell_j\ell_j^*))\Omega$. For H_{11} we stress that

$$\ell_j^*\Omega D^2\mathcal{W}\Omega\ell_j + \ell_j^T\Omega D^2\mathcal{W}\Omega\overline{\ell}_j = -\sum_{s,r=1}^{2n}\left((\Omega\overline{\ell}_j)_s(\Omega\ell_j)_r + (\Omega\ell_j)_s(\Omega\overline{\ell}_j)_r\right)\partial_{z_s}\partial_{z_r}\mathcal{W}(z)$$

So, $(H_{11})_{s,r} = -\frac{\mathrm{i}}{2}\sum_{j=1}^m (\Omega\bar{\ell}_j)_s(\Omega\ell_j)_r + (\Omega\ell_j)_s(\Omega\bar{\ell}_j)_r$, i.e.

$$H_{11} = -\tfrac{\mathrm{i}}{2}\sum_{j=1}^m (\Omega\bar{\ell}_j)(\Omega\ell_j)^T + (\Omega\ell_j)(\Omega\bar{\ell}_j)^T = \mathrm{i}\sum_{j=1}^m \Omega\mathrm{Re}(\ell_j\ell_j^*)\Omega$$

By denoting $L := \sum_{j=1}^m \Omega\ell_j\ell_j^*\Omega$, we find that $H_{11} = \mathrm{i}\mathrm{Re}(L)$ and $H_{21} = -H\Omega + \Omega\mathrm{Im}(L)$.

It remains to calculate $\mathrm{tr}(H_{21})$. Since H is symmetric,

$$-\tfrac{\mathrm{i}\varepsilon}{2}\mathrm{tr}\left(H_{21}\right) = \tfrac{\mathrm{i}\varepsilon}{2}\mathrm{tr}\left(\sum_{j=1}^m \mathrm{Im}(\ell_j\ell_j^*)\Omega\right) = \tfrac{\mathrm{i}\varepsilon}{2}\sum_{j=1}^m \mathrm{Im}\left(\mathrm{tr}\left(\ell_j\ell_j^*\Omega\right)\right) = \tfrac{\mathrm{i}\varepsilon}{2}\sum_{j=1}^m \mathrm{Im}\left(\ell_j^*\Omega\ell_j\right).$$

Furthermore,

$$\ell_j^*\Omega\ell_j = \mathrm{i}\left(\mathrm{Re}(\ell_j)^T\Omega\mathrm{Im}(\ell_j) - \mathrm{Im}(\ell_j)^T\Omega\mathrm{Re}(\ell_j)\right) = 2\mathrm{i}\mathrm{Re}(\ell_j)^T\Omega\mathrm{Im}(\ell_j)$$

and thus, $-\frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(H_{21}) = \mathrm{i}\varepsilon\sum_{j=1}^m \mathrm{Re}(\ell_j)^T\Omega\mathrm{Im}(\ell_j)$. All in all, we find

$$\mathrm{i}\varepsilon\,\partial_t\mathcal{W} = \widehat{\mathcal{H}}_S\mathcal{W} + \mathrm{i}\varepsilon\sum_{j=1}^m \mathrm{Re}(\ell_j)^T\Omega\mathrm{Im}(\ell_j)\mathcal{W}$$

what completes the proof. ■

In the study of open quantum systems one is usually interested in three effects that may occur: *decoherence*, i.e. vanishing off-diagonal terms in the density matrix, *dissipation*, the loss or gain of energy in the system and *diffusion* that can be found in all open system, see [AB11, §1].

The matrix L given in (10.6) comprises dissipation and diffusion of our open system. If the Lindblad terms L_j are Hermitian, i.e. $\mathrm{Im}(\ell_j) = 0$ for $j = 1, \ldots, m$, what corresponds to a non-dissipative system, see for example [BA04a, §3], then our constant part vanishes, $\gamma = 0$, and the Hamiltonian can be written as

$$\widehat{\mathcal{H}}_S = \tfrac{1}{2}\hat{z}^T\begin{pmatrix}\mathrm{i}\mathrm{Re}(L) & \Omega H\\ -H\Omega & 0\end{pmatrix}\hat{z}.$$

This means the remaining diffusion is described by the real part of L. Therefore, we link the imaginary part of L to the dissipation and the real part of L to the diffusion of the system. This interpretation can also be underpinned by the relation

$$\mathrm{tr}\left(\mathrm{Im}(L)\Omega\right) = -2\gamma.$$

To sum up, we deduced a Schrödinger equation on phase space that is equivalent to the Lindblad equation and since the Wigner transform of Hagedorn's wave packets are Hagedorn wave packets on phase space, we can directly transmit our results for non-Hermitian Hamiltonians.

10.2. Coherent state evolution

We start with two positive Lagrangian subspaces L_1 and L_2 and the corresponding frames $Z_1 \in F_n(L_1)$ resp. $Z_2 \in F_n(L_2)$. We use the Wigner transform

$$\mathcal{W}_0(\mathcal{Z}; z) := \mathcal{W}^\varepsilon(\varphi_0(Z_1), \varphi_0(Z_2))(z),$$

where $\mathcal{Z}$ denotes the phase space frame of Z_1 and Z_2 as ansatz function and insert into Equation (10.5). Moreover, we denote by $\mathcal{L} = \mathrm{range}(\mathcal{Z}) \subset \mathbb{C}^{2n} \oplus \mathbb{C}^{2n}$ the positive Lagrangian subspace determined in Proposition 6.1.

We note here that we can not consider an arbitrary positive Lagrangian subspace $\mathcal{L} \subset \mathbb{C}^{2n} \oplus \mathbb{C}^{2n}$, because not all wave packets $\Phi(\mathcal{Z})$ on phase space can be written as Wigner functions.

The time evolution operator $\widehat{\mathcal{U}}(t)$ exists since $\mathrm{Im}(H_S) \leq 0$ and solves the formal equation

$$\mathrm{i}\varepsilon\, \partial_t \widehat{\mathcal{U}}(t) = (\widehat{\mathcal{H}}_S + \mathrm{i}\varepsilon\, \hat{\gamma})\widehat{\mathcal{U}}(t), \quad \widehat{\mathcal{U}}(0) = \mathrm{Id}.$$

For the propagation of the wave packets it again suffices to calculate the dynamics of the centre z_t and the linearisation $S_t \in \mathbb{C}^{2n\times 2n}$ of the classical flow around it. Although, we add a constant factor γ_S to the quadratic Hamiltonian $\mathcal{H}_S$, we will see later that S_t still describes the exact propagation of our wave packets.

Lemma 10.2 — Linearised Flow. The solution S_t of the system $\dot{S}_t = \Omega_2 H_S S_t$ and $S_0 = \mathrm{Id}_{2n}$ with H_S as defined in (10.6) can be written as

$$S_t = \begin{pmatrix} e^{(H\Omega - \Omega\mathrm{Im}(L))t} & 0 \\ \mathrm{i}e^{(\Omega H + \mathrm{Im}(L)\Omega)t} I_t & e^{(\Omega H + \mathrm{Im}(L)\Omega)t} \end{pmatrix} \tag{10.7}$$

with the symmetric matrix integral

$$I_t = \int_0^t e^{-(\Omega H + \mathrm{Im}(L)\Omega)\tau} \mathrm{Re}(L) e^{(H\Omega - \Omega\mathrm{Im}(L))\tau}\, d\tau \in \mathbb{R}^{n\times n}.$$

Moreover, S_t satisfies

$$S_t^* \Omega S_t = \begin{pmatrix} -2\mathrm{i}I_t & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}. \tag{10.8}$$

Proof. We can write S_t as a block matrix containing four $n \times n$-matrices and solve differential equations for these four entries,

$$\begin{pmatrix} \dot{S}_{11}(t) & \dot{S}_{12}(t) \\ \dot{S}_{21}(t) & \dot{S}_{22}(t) \end{pmatrix} = \begin{pmatrix} H\Omega - \Omega\mathrm{Im}(L) & 0 \\ \mathrm{i}\,\mathrm{Re}(L) & \Omega H + \mathrm{Im}(L)\Omega \end{pmatrix} \begin{pmatrix} S_{11}(t) & S_{12}(t) \\ S_{21}(t) & S_{22}(t) \end{pmatrix}$$

with initial values $S_{11}(0) = S_{22}(0) = \mathrm{Id}$ and $S_{12}(0) = S_{21}(0) = 0$. We only present the calculation of the third entry S_{21} here, the remaining entries follow directly from the properties of exponential matrices. We have

$$\dot{S}_{21}(t) = \mathrm{i}\mathrm{Re}(L) e^{(H\Omega - \Omega\mathrm{Im}(L))t} + (\Omega H + \mathrm{Im}(L)\Omega) S_{21}(t).$$

The solution to the homogeneous problem reads $S_{21}(t) = e^{(\Omega H + \mathrm{Im}(L)\Omega)t}c(t)$. Thus, with variation of constants

$$\dot{c}(t) = \mathrm{i}e^{-(\Omega H + \mathrm{Im}(L)\Omega)t}\mathrm{Re}(L)e^{(H\Omega - \Omega\mathrm{Im}(L))t}$$

and

$$c(t) = \mathrm{i}\int_0^t e^{-(\Omega H + \mathrm{Im}(L)\Omega)\tau}\mathrm{Re}(L)e^{(H\Omega - \Omega\mathrm{Im}(L))\tau}\, d\tau.$$

The formula for $S_t^*\Omega S_t$ follows by a direct computation. ∎

We stress here that for a Hermitian Hamiltonian we find $S_t^*\Omega S_t = \Omega$. Thus, the integral term I_t can be nicely interpreted as the deviation from the unitary evolution.

Once more, we evolve the Lagrangian subspace $\mathcal{L}$ along the flow and obtain a positive Lagrangian subspace $\mathcal{L}_t := S_t\mathcal{L}$ for all times t such that the normalisation

$$N_t = \tfrac{1}{2\mathrm{i}}\mathcal{Z}^* S_t^*\Omega S_t\mathcal{Z} = \frac{1}{2\mathrm{i}}\begin{pmatrix}\mathcal{P}^* & \mathcal{Q}^*\end{pmatrix}\begin{pmatrix}-2\mathrm{i}I_t & -\mathrm{Id}\\ \mathrm{Id} & 0\end{pmatrix}\begin{pmatrix}\mathcal{P}\\ \mathcal{Q}\end{pmatrix} = \mathrm{Id}_{2n} - \mathcal{P}^* I_t\mathcal{P}$$

is positive definite. The fact that $\mathrm{Im}(H_S) \leq 0$ already predicts that N_t is positive for all $t \geq 0$ and we summarise the evolution of the Lagrangian subspace in the following proposition.

Proposition 10.3 — Evolved phase space frame. Let $\mathcal{L}$ be a positive Lagrangian subspace and $\mathcal{Z} \in F_n(\mathcal{L})$. Then, the evolved Lagrangian subspace $\mathcal{L}_t = S_t\mathcal{L}$ is a positive for all times $t \geq 0$ and can be parametrised by the normalised Lagrangian frame

$$\mathcal{Z}_t = S_t\mathcal{Z}N_t^{-1/2} = \begin{pmatrix} e^{(H\Omega - \Omega\mathrm{Im}(L))t}\mathcal{P}\\ e^{(\Omega H + \mathrm{Im}(L)\Omega)t}(\mathrm{Id}_{2n} - 2I_tG)\mathcal{Q}\end{pmatrix} N_t^{-1/2}. \tag{10.9}$$

Proof. Due to Lemma 2.5, $\mathcal{L}_t$ is positive if N_t is a positive definite matrix. Let $v \in \mathbb{C}^{2n}$, then

$$v^* N_t v = v^*(\mathrm{Id}_{2n} - \mathcal{P}^* I_t\mathcal{P})v = |v|^2 - \int_0^t w_\tau^*\mathrm{Re}(L)w_\tau\, d\tau$$

for $w_\tau = e^{(H\Omega - \Omega\mathrm{Im}(L))\tau}\mathcal{P}v$. Since $e^{(H\Omega - \Omega\mathrm{Im}(L))\tau}$ and $\mathcal{P}$ are invertible for all $\tau \geq 0$, it suffices to consider $\mathrm{Re}(L)$. We find

$$w_\tau^*\mathrm{Re}(L)w_\tau = \frac{1}{2}w_\tau^*\Omega\left(\ell\ell^* + \bar{\ell}\ell^T\right)\Omega w_\tau = -\frac{1}{2}\left(|\ell^*\Omega w_\tau|^2 + |\ell^T\Omega w_\tau|^2\right) \leq 0.$$

and hence $N_t > 0$. A short calculation using (10.7) and $\mathcal{P}\mathcal{Q}^{-1} = 2\mathrm{i}G$ further yields

$$\mathcal{Z}_t = \begin{pmatrix} e^{(H\Omega - \Omega\mathrm{Im}(L))t}\mathcal{P}\\ e^{(\Omega H + \mathrm{Im}(L)\Omega)t}(\mathrm{i}I_t\mathcal{P}\mathcal{Q}^{-1} + \mathrm{Id}_{2n})\mathcal{Q}\end{pmatrix} N_t^{-1/2} = \begin{pmatrix} e^{(H\Omega - \Omega\mathrm{Im}(L))t}\mathcal{P}\\ e^{(\Omega H + \mathrm{Im}(L)\Omega)t}(\mathrm{Id}_{2n} - 2I_tG)\mathcal{Q}\end{pmatrix} N_t^{-1/2}.$$

∎

As shown in Chapters 8 and 9 the evolved metric G_t completely determines the gain or loss in the open system. For the Lindblad equation we can replace the Riccati equation from Theorem 9.1 by an equivalent expression using the integral term I_t.

Lemma 10.3 — Evolved metric. We consider positive Lagrangian subspaces $L_1, L_2 \subset \mathbb{C}^{2n}$ with $Z_1 \in F_n(L_1)$ and $Z_2 \in F_n(L_2)$. We denote by G the generalised metric of Z_1 and Z_2 and define the propagation of Z_1 and Z_2 via their phase space frame

$$\mathcal{Z}_t = \begin{pmatrix} \mathcal{P}_t \\ \mathcal{Q}_t \end{pmatrix} = S_t \mathcal{Z} N_t^{-1/2}.$$

Then, the propagated generalised metric $G_t = \frac{1}{2\mathrm{i}} \mathcal{P}_t \mathcal{Q}_t^{-1}$ satisfies

$$G_t = e^{(H\Omega - \Omega \mathrm{Im}(L))t} (G^{-1} - 2I_t)^{-1} e^{-(\Omega H + \mathrm{Im}(L)\Omega)t}$$

and the deviation of G_t and the time evolved symplectic metrics $G_{1,t}$ resp. $G_{2,t}$ is singular for all times $t \geq 0$.

Proof. The first statement follows directly from (10.9),

$$\begin{aligned} G_t &= \tfrac{1}{2\mathrm{i}} e^{(H\Omega - \Omega \mathrm{Im}(L))t} \mathcal{P} \mathcal{Q}^{-1} (\mathrm{Id}_{2n} - 2I_t G)^{-1} e^{-(\Omega H + \mathrm{Im}(L)\Omega)t} \\ &= e^{(H\Omega - \Omega \mathrm{Im}(L))t} G (\mathrm{Id}_{2n} - 2I_t G)^{-1} e^{-(\Omega H + \mathrm{Im}(L)\Omega)t}. \end{aligned}$$

For the singularity, we first note that the same result holds true for the propagation of G_1, i.e.

$$G_{1,t} = e^{(H\Omega - \Omega \mathrm{Im}(L))t} G_1 (\mathrm{Id}_{2n} - 2I_t G_1)^{-1} e^{-(\Omega H + \mathrm{Im}(L)\Omega)t}$$

if both metrics are evolved along the same flow S_t. Thus,

$$\begin{aligned} &e^{-(H\Omega - \Omega \mathrm{Im}(L))t} (G_t - G_{1,t}) e^{(\Omega H + \mathrm{Im}(L)\Omega)t} = (G^{-1} - 2I_t)^{-1} - (G_1^{-1} - 2I_t)^{-1} \\ &= (G^{-1} - 2I_t)^{-1} \left(G_1^{-1} - G^{-1}\right) (G_1^{-1} - 2I_t)^{-1} = (G^{-1} - 2I_t)^{-1} \Omega^T \left(G_1 - G\right) \Omega (G_1^{-1} - 2I_t)^{-1} \end{aligned}$$

and the singularity follows from the singularity of the G and G_1, see Corollary 2.6. ■

In particular, the above result emphasises that if we start with a real symplectic metric G, what corresponds to a symmetric Wigner function, also the time evolved metric G_t will stay real-valued, i.e. the evolved wave packet can still be written as a symmetric Wigner function.

The evolution of the ladder operators in Lemma 8.5 and Lemma 9.1, respectively, was based on the relation

$$\mathrm{i}\varepsilon\, \partial_t \hat{A}_t(l) = [\hat{\mathcal{H}}, \hat{A}_t(l)], \qquad l \in \mathbb{C}^n \oplus \mathbb{C}^n.$$

Since adding a constant does not change the commutator properties, we can directly infer

$$\widehat{\mathcal{U}}(t) \hat{A}(\mathcal{Z}) \widehat{\mathcal{U}}(t)^{-1} = \hat{A}(S_t \mathcal{Z}) \quad \text{and} \quad \widehat{\mathcal{U}}(t) \hat{A}^\dagger(\mathcal{Z}) \widehat{\mathcal{U}}(t)^{-1} = \hat{A}^\dagger(\overline{S}_t \mathcal{Z})$$

where $\mathcal{Z} \in \mathbb{C}^{4n \times 2n}$ is an isotropic matrix and S_t the linearised flow defined in (10.7). Thus, we can adopt the strategy for propagation of coherent states from the previous chapter. However, we have to be careful, the constant factor might not change the evolution of the ladder operators, but it will affect the norm of the evolved coherent state.

Proposition 10.4 — Coherent state evolution. Let $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ denote two normalised Lagrangian frames, $\mathcal{Z} \in \mathbb{C}^{4n\times 2n}$ their phase space frame and

$$\mathcal{W}_0(\mathcal{Z}) := \mathcal{W}^\varepsilon(\varphi_0(Z_1), \varphi_0(Z_2))$$

the Wigner transform of the corresponding coherent states. Then, the time evolution of $\mathcal{W}_0(\mathcal{Z})$ is given by

$$\widehat{\mathcal{U}}(t)\mathcal{W}_0(\mathcal{Z}) = e^{\beta_t+\gamma t} \cdot \mathcal{W}_0(\mathcal{Z}_t)$$

with $\mathcal{Z}_t$ as defined in (10.9), $\gamma \in \mathbb{R}$ the dissipation coefficient from Proposition 10.2 and

$$\beta_t = \int_0^t \operatorname{tr}(\operatorname{Re}(L)(\tfrac{1}{4}\mathcal{P}_\tau\mathcal{P}_\tau^* + \mathrm{i}\operatorname{Im}(G_t))\, d\tau.$$

If $Z_1^T\Omega Z_2 = 0$, this factor simplifies to $\beta_t = \int_0^t \operatorname{tr}(\operatorname{Re}(L)G_\tau)\, d\tau + \gamma t$.

Proof. We start with the special case $Z_1^T\Omega Z_2 = 0$. In this setting the metric G_t is real and we choose as ansatz similar to Proposition 9.2

$$\mathcal{W}_0(t) := c_t \cdot \mathcal{W}_0(\mathcal{Z}_t) = (\pi\varepsilon)^{-n} c_t \cdot e^{-z^T G_t z/\varepsilon}.$$

We insert into Equation (10.5) and use that $\operatorname{tr}(\Omega\operatorname{Im}(L)) = -2\gamma$. For the time derivative we find

$$\partial_t\mathcal{W}_0(t) = \left(\frac{\dot c_t}{c_t} - \tfrac{1}{\varepsilon}z^T\dot G_t z\right)\cdot\mathcal{W}_0(t).$$

The formula for quadratic Hamiltonians from Lemma 8.2 and the form of H_S in (10.6) moreover implies

$$\begin{aligned}(-\tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}_S + \gamma)\mathcal{W}_0(t) &= (-\tfrac{\varepsilon}{2}\nabla_z^T\operatorname{Re}(L)\nabla_z + z^T(H\Omega - \Omega\operatorname{Im}(L))\nabla_z + 2\gamma)\mathcal{W}_0(t)\\ &= \left(\operatorname{tr}(\operatorname{Re}(L)G_t) + 2\gamma - \tfrac{\varepsilon}{2}z^T\left(G_t\operatorname{Re}(L)G_t + (H\Omega - \Omega\operatorname{Im}(L))G_t\right)z\right)\mathcal{W}_0(t)\end{aligned}$$

Thus, $\mathcal{W}_0(t)$ is a solution of (10.5) if

$$\frac{\dot c_t}{c_t} = \operatorname{tr}(\operatorname{Re}(L)G_t) + 2\gamma$$

and

$$\dot G_t = 2G_t\operatorname{Re}(L)G_t + (H\Omega - \Omega\operatorname{Im}(L))G_t - G_t(\Omega H + \operatorname{Im}(L)\Omega).$$

The first equation yields the form of β_t if $Z_1^T\Omega Z_2 = 0$. It can easily be shown that the second equation is equivalent to the previous lemma if one uses that

$$\dot I_t = e^{-(\Omega H + \operatorname{Im}(L)\Omega)t}\operatorname{Re}(L)\, e^{(H\Omega - \Omega\operatorname{Im}(L))t}.$$

In the general case, we also have to consider $\mathrm{Re}(G_t)$, since

$$\mathcal{W}_0(\mathcal{Z}_t) = (\pi\varepsilon)^{-n}\det(\mathrm{Re}(G_t))^{1/4}e^{-z^T G_t z/\varepsilon}.$$

Fortunately, this concerns only the time derivative. We denote again $\mathcal{W}_0(t) := c_t \cdot \mathcal{W}_0(\mathcal{Z}_t)$. Then,

$$\partial_t \mathcal{W}_0(t) = \left(\frac{\dot{c}_t}{c_t} + \tfrac{1}{4}\mathrm{tr}(\partial_t \mathrm{Re}(G_t)\mathrm{Re}(G_t)^{-1}) - \tfrac{1}{\varepsilon} z^T \dot{G}_t z\right) \cdot \mathcal{W}_0(t).$$

The evolution equation of G_t furthermore implies

$$\begin{aligned}\partial_t \mathrm{Re}(G_t) = {} & 2\left(\mathrm{Re}(G_t)\mathrm{Re}(L)\mathrm{Re}(G_t) - \mathrm{Im}(G_t)\mathrm{Re}(L)\mathrm{Im}(G_t)\right) + (H\Omega - \Omega\mathrm{Im}(L))\mathrm{Re}(G_t) \\ & - \mathrm{Re}(G_t)(\Omega H + \mathrm{Im}(L)\Omega)\end{aligned}$$

and hence with $\mathrm{tr}(\Omega H) = \mathrm{tr}(H\Omega) = 0$,

$$\mathrm{tr}(\partial_t \mathrm{Re}(G_t)\mathrm{Re}(G_t)^{-1}) = 2 \cdot \mathrm{tr}\left(\mathrm{Re}(G_t)\mathrm{Re}(L) - \mathrm{Re}(L)\mathrm{Im}(G_t)\mathrm{Re}(G_t)^{-1}\mathrm{Im}(G_t) - \Omega\mathrm{Im}(L)\right).$$

If we regard $G_t = \frac{1}{2\mathrm{i}}\mathcal{P}_t\mathcal{Q}_t^{-1}$ and Corollary 2.3, we find

$$\mathrm{Im}(G_t)\mathrm{Re}(G_t)^{-1}\mathrm{Im}(G_t) = \tfrac{1}{2}\mathcal{P}_t\mathcal{P}_t^* - \mathrm{Re}(G_t).$$

Since $\mathrm{Re}(G_t)$ and $\mathrm{Re}(L)$ are symmetric, we end up with

$$\mathrm{tr}(\partial_t \mathrm{Re}(G_t)\mathrm{Re}(G_t)^{-1}) = 4 \cdot \mathrm{tr}(\mathrm{Re}(G_t)\mathrm{Re}(L)) - \mathrm{tr}(\mathcal{P}_t^*\mathrm{Re}(L)\mathcal{P}_t) - 2 \cdot \mathrm{tr}(\Omega\mathrm{Im}(L)).$$

Comparing again the constant terms shows,

$$\begin{aligned}\mathrm{tr}(\mathrm{Re}(L)G_t) + 2\gamma &= \frac{\dot{c}_t}{c_t} + \mathrm{tr}(\mathrm{Re}(L)\mathrm{Re}(G_t)) - \tfrac{1}{4}\mathrm{tr}(\mathcal{P}_t^*\mathrm{Re}(L)\mathcal{P}_t) + \gamma, \\ \frac{\dot{c}_t}{c_t} &= \mathrm{i} \cdot \mathrm{tr}(\mathrm{Re}(L)\mathrm{Im}(G_t)) + \tfrac{1}{4}\mathrm{tr}(\mathcal{P}_t^*\mathrm{Re}(L)\mathcal{P}_t) + \gamma.\end{aligned}$$

■

In Proposition 9.2 we deduced for the damping or growth factor

$$\beta_t = \tfrac{1}{4}\int_0^t \mathrm{tr}(G_\tau^{-1}\mathrm{Im}(H))\,d\tau,$$

here we find for the phase space metric and the Hamiltonian $\mathcal{H}_S$

$$\mathrm{tr}(\mathcal{G}_t^{-1}\mathrm{Im}(H_S)) = \mathrm{tr}\left(\begin{pmatrix}\mathcal{P}_t\mathcal{P}_t^* & \mathcal{P}_t\mathcal{Q}_t^* - \mathrm{iId} \\ \mathcal{Q}_t\mathcal{P}_t^* + \mathrm{iId} & \mathcal{Q}_t\mathcal{Q}_t^*\end{pmatrix}\begin{pmatrix}\mathrm{Re}(L) & 0 \\ 0 & 0\end{pmatrix}\right) = \mathrm{tr}(\mathcal{P}_t^*\mathrm{Re}(L)\mathcal{P}_t).$$

Hence, the additional terms induced by the dissipation are $e^{\gamma t}$ and a phase factor

$$e^{\mathrm{i}\int_0^t \mathrm{tr}(\mathrm{Re}(L)\mathrm{Im}(G_\tau))\,d\tau}.$$

Our approach for the evolution of the coherent state was adapted from our study of non-Hermitian Hamiltonians. However, in the context of the Lindblad equation we could also use the trace preservation to determine the coefficient c_t as we will present in the following corollary.

Corollary 10.1 — Trace preservation. Let $\mathcal{W}_0(t,z) := e^{\beta_t+\gamma t}\cdot \mathcal{W}_0(\mathcal{Z}_t;z)$ be defined as in the previous Proposition 10.4. Then, we have for all $t \geq 0$,

$$\int_{\mathbb{R}^{2n}} \mathcal{W}_0(t,z)\, dz = 1.$$

Proof. Since G_t is an invertible matrix with positive definite real part for all $t \geq 0$, it holds

$$(\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} e^{-z^T G_t z/\varepsilon}\, dz = \det(G_t)^{-1/2}.$$

Hence, $\mathcal{W}_0(t,z) := (\pi\varepsilon)^{-n}\det(G_t)^{1/2} e^{-z^T G_t z/\varepsilon}$ is L^1-normalised and it remains to determine the determinant. Again, with Jacobi's determinant formula,

$$\partial_t(\det(G_t)^{1/2}) = \tfrac{1}{2}\det(G_t)^{1/2}\mathrm{tr}(\dot{G}_t G_t^{-1})$$

and with our findings from the previous proof for $\dot{G}_t$,

$$\mathrm{tr}(\dot{G}_t G_t^{-1}) = 2\cdot \mathrm{tr}(G_t \mathrm{Re}(L) - \Omega \mathrm{Im}(L)) = 2\cdot \mathrm{tr}(G_t\mathrm{Re}(L)) + 4\gamma$$

where we again used that $\mathrm{tr}(\Omega H) = \mathrm{tr}(H\Omega) = 0$. Thus, we find

$$\mathcal{W}_0(t,z) := (\pi\varepsilon)^{-n} e^{\int_0^t \mathrm{tr}(G_\tau \mathrm{Re}(L))\, d\tau + 2\gamma t} e^{-z^T G_t z/\varepsilon}.$$

Taking into account our definition of $\mathcal{W}_0(\mathcal{Z}_t)$ in Proposition 6.2, we need to extract $\det(\mathrm{Re}(G_t))^{1/4}$. With a similar calculation

$$\partial_t(\det(\mathrm{Re}(G_t))^{1/4}) = \tfrac{1}{4}\det(\mathrm{Re}(G_t))^{1/4}\mathrm{tr}(\mathrm{Re}(\dot{G}_t)\mathrm{Re}(G_t)^{-1})$$

what we already identified as

$$\tfrac{1}{4}\mathrm{tr}(\mathrm{Re}(\dot{G}_t)\mathrm{Re}(G_t)^{-1}) = \mathrm{tr}(\mathrm{Re}(L)\mathrm{Re}(G_t)) - \tfrac{1}{4}\mathrm{tr}(\mathcal{P}_t^*\mathrm{Re}(L)\mathcal{P}_t) + \gamma.$$

Hence $\mathcal{W}_0(t,z)$ can be written as $\mathcal{W}_0(t,z) = e^{\beta_t+\gamma t}\cdot \mathcal{W}_0(\mathcal{Z}_t;z)$ with β_t as in Proposition 10.4. ■

The propagation of excited states now follows similarly as for the non-Hermitian Hamiltonians in Corollary 9.2. However, we are able to give a simplified relation for the appearing polynomials in the case of symmetric Wigner functions.

10.3. Excited state evolution

Let again $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ denote two positive Lagrangian frames and $\mathcal{Z} \in \mathbb{C}^{4n\times 2n}$ their corresponding phase space frame. We are now interested in the evolution of Wigner functions of the form

$$\mathcal{W}_{(k,l)}(\mathcal{Z}; z) := \mathcal{W}^{\varepsilon}(\varphi_k(Z_1), \varphi_l(Z_2))(z),$$

for $k, l \in \mathbb{N}$.

Theorem 10.1 — Excited state evolution. The propagated Wigner function is given by

$$\widehat{\mathcal{U}}(t)\mathcal{W}_{(k,l)}(\mathcal{Z}; z) = \frac{e^{\beta_t + \gamma t}}{\sqrt{2^{|k|+|l|}k!l!}} p_{(k,l)}^{\mathcal{M}_t}\left(\tfrac{1}{\sqrt{\varepsilon}} N_t^{-1/2} \mathcal{Q}_t^{-1} z\right) \mathcal{W}_0(\mathcal{Z}_t; z)$$

where the polynomials $p_{(k,l)}^{\mathcal{M}_t}$ are defined by the recursion (4.7) with

$$\mathcal{M}_t = \mathcal{Q}^{-1}\left(2\mathrm{i}\mathcal{Q}\mathcal{P}^* I_t \overline{G} + (\mathrm{Id}_{2n} - 2I_t G)^{-1}(\mathrm{Id}_{2n} - 2I_t\overline{G})\right)\overline{\mathcal{Q}N_t^{-1}}, \tag{10.10}$$

the damping or growth factor β_t as in Proposition 10.4 and the dissipation coefficient γ as in Proposition 10.2.

Proof. The proof follows directly from Corollary 9.2, we only have to simplify the recursion matrix

$$M_t = \tfrac{1}{2\mathrm{i}} N_t^{-1}(S_t\mathcal{Z})^*\Omega_2 S_t\overline{\mathcal{Z}} + N_t^{-1/2} Q_t^{-1}\overline{Q}_t \overline{N}_t^{-1/2}.$$

For the first term we find with the same approach as for the normalisation

$$\tfrac{1}{2\mathrm{i}} N_t^{-1}\mathcal{Z}^* S_t^*\Omega_2 S_t\overline{\mathcal{Z}} = \tfrac{1}{2\mathrm{i}} N_t^{-1}\left(-2\mathrm{i}\mathcal{P}^* I_t\overline{\mathcal{P}} + \overline{\mathcal{Q}^T\mathcal{P} - \mathcal{P}^T\mathcal{Q}}\right) = -N_t^{-1}\mathcal{P}^* I_t\overline{\mathcal{P}}.$$

and since $\mathcal{M}_t$ is symmetric, $N_t^{-1}\mathcal{P}^* I_t\overline{\mathcal{P}} = \mathcal{P}^* I_t\overline{\mathcal{P}N_t^{-1}}$.

For the second term we can deduce from Equation (10.9) that

$$N_t^{-1/2}\mathcal{Q}_t^{-1}\overline{\mathcal{Q}}_t\overline{N}_t^{-1/2} = \mathcal{Q}^{-1}(\mathrm{Id}_{2n} - 2I_t G)^{-1}(\mathrm{Id}_{2n} - 2I_t\overline{G})\overline{\mathcal{Q}N_t^{-1}}.$$

Summing up the two terms leads to

$$\begin{aligned} M_t &= \left(-\mathcal{P}^* I_t\overline{\mathcal{P}} + \mathcal{Q}^{-1}(\mathrm{Id}_{2n} - 2I_t G)^{-1}(\mathrm{Id}_{2n} - 2I_t\overline{G})\overline{\mathcal{Q}}\right)\overline{N_t^{-1}} \\ &= \mathcal{Q}^{-1}\left(-\mathcal{Q}\mathcal{P}^* I_t\overline{\mathcal{P}\mathcal{Q}^{-1}} + (\mathrm{Id}_{2n} - 2I_t G)^{-1}(\mathrm{Id}_{2n} - 2I_t\overline{G})\right)\overline{\mathcal{Q}N_t^{-1}} \end{aligned}$$

and the claim follows since $\mathcal{P}\mathcal{Q}^{-1} = 2\mathrm{i}G$. ■

If we consider Wigner functions of the form

$$\mathcal{W}^{\varepsilon}(\varphi_k(Z), \varphi_l(Z)),$$

for $k, l, \mathbb{N}^n$, i.e. of wave packets that are parametrised by the same Lagrangian subspace, the phase space wave packet is not described by the generalised metric, but by the real symplectic metric introduced in Section 2.4. Since we have more information in this case about the symplectic metric and the phase space frame $\mathcal{Z}$, we can simplify our findings further.

Corollary 10.2 — Symmetric Wigner functions. If $Z_1, Z_2 \in \mathbb{C}^{2n\times n}$ are two normalised Lagrangian frames defining the same subspace, i.e. $Z_1^T \Omega Z_2 = 0$, the recursion matrix in (10.10) simplifies to

$$\mathcal{M}_t = (2N_t^{-1} - \mathrm{Id}_{2n})\mathcal{Q}^{-1}\overline{\mathcal{Q}}$$

with $\mathcal{Q}^{-1}\overline{\mathcal{Q}} = \begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}$.

Proof. If $Z_1^T \Omega Z_2 = 0$, the matrix G is real and we have $\mathcal{Q}\mathcal{P}^* = -\mathrm{i}\mathrm{Id}_{2n}$, see Remark 2.4 and 2.2. This simplifies $\mathcal{M}_t$ to

$$\mathcal{M}_t = \mathcal{Q}^{-1}\left(\mathrm{Id}_{2n} + 2I_t G\right)\overline{\mathcal{Q}N_t^{-1}}.$$

Moreover, we find in this case $\mathcal{Q}N_t\mathcal{Q}^{-1} = \mathcal{Q}(\mathrm{Id}_{2n} - \mathcal{P}^* I_t \mathcal{P})\mathcal{Q}^{-1} = \mathrm{Id}_{2n} - 2I_t G$. Replacing $2I_t G = \mathrm{Id}_{2n} - \mathcal{Q}N_t\mathcal{Q}^{-1}$ leads to

$$\mathcal{M}_t = \mathcal{Q}^{-1}\left(2\mathrm{Id}_{2n} - \mathcal{Q}N_t\mathcal{Q}^{-1}\right)\overline{\mathcal{Q}N_t^{-1}} = \left(2\mathrm{Id}_{2n} - N_t\right)\mathcal{Q}^{-1}\overline{\mathcal{Q}N_t^{-1}}.$$

It remains to show that $\mathcal{Q}^{-1}\overline{\mathcal{Q}N_t^{-1}} = N_t^{-1}\mathcal{Q}^{-1}\overline{\mathcal{Q}}$, but this follows from

$$\begin{aligned} N_t\mathcal{Q}^{-1}\overline{\mathcal{Q}} - \mathcal{Q}^{-1}\overline{\mathcal{Q}N_t} &= \mathcal{Q}^{-1}\overline{\mathcal{Q}}\mathcal{P}^T I_t \overline{\mathcal{P}} - \mathcal{P}^* I_t \mathcal{P}\mathcal{Q}^{-1}\overline{\mathcal{Q}} \\ &= \mathcal{Q}^{-1}\left(\overline{\mathcal{Q}\mathcal{P}^*} I_t \overline{\mathcal{P}\mathcal{Q}^{-1}} - \mathcal{Q}\mathcal{P}^* I_t \mathcal{P}\mathcal{Q}^{-1}\right)\overline{\mathcal{Q}} = 0 \end{aligned}$$

since $\mathcal{Q}\mathcal{P}^*$ and $\mathcal{P}\mathcal{Q}^{-1}$ are both purely imaginary in this case. ■

10.4. Evolution of the Chord function

Before we discuss some examples, we want to present a small linkup to another approach that is often used for the study of Lindblad dynamics, the Chord functions.

The basic idea is to describe the evolution of a Wigner function by a pair of phase space trajectories and combine them in double phase space, see [BA06].

We start with recalling that the Heisenberg-Weyl translation operator can be written as

$$T(z) = e^{-\frac{\mathrm{i}}{\varepsilon} z^T \Omega \hat{z}}$$

for any phase space point $z \in \mathbb{R}^n \oplus \mathbb{R}^n$, see also Appendix A. We then expand an arbitrary operator $\hat{a} = \mathrm{op}_\varepsilon[a]$ with an admissible symbol a as superposition of translation operators

$$\hat{a} = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} T(z)\chi_a(z)\,dz,$$

see [ABMR09, §2]. The function χ_a is called the *Chord symbol* of $\hat{a}$. One can further show that the symbol a and the Chord symbol χ_a are related via

$$\chi_a(z) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} a(\zeta)e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega z}\,d\zeta.$$

This transform can be generally defined as a Fourier transform on phase space.

Definition 10.1 — Symplectic Fourier transform. Let $\Phi \in L^2(\mathbb{R}^{2n})$. We define the symplectic Fourier transform of Φ by

$$\mathcal{F}_S^\varepsilon \Phi(z) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \Phi(\zeta) e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega z} \, d\zeta$$

for all $\zeta \in \mathbb{R}^{2n}$.

If moreover the operator $\hat{\rho}$ is a density operator, i.e. $\rho(z) = (2\pi\varepsilon)^n \mathcal{W}^\varepsilon(\psi)$ for some $\psi \in L^2(\mathbb{R}^n)$, see Proposition 10.1, we call the corresponding symbol $\chi = \chi_\rho$ a *Chord function*. In quantum optics, the function χ is also known as (quantum) characteristic function. The Lindblad dynamics for the Chord function reduces to a Fokker-Planck equation and is thus solvable. Furthermore, caustics that are induced by decoherence can be projected either to the space of the Wigner functions or to the space of the Chord function. Hence, this approach may help to avoid caustics, see [BA04a].

As we use Hagedorn's wave packets as ansatz functions, the next reasonable step is to determine their symplectic Fourier transform.

Proposition 10.5 — Symplectic Fourier transform of Hagedorn's wavepackets. Let $\kappa \in \mathbb{N}^{2n}$, $\mathcal{Z} = (\mathcal{P}; \mathcal{Q}) \in \mathbb{C}^{4n \times 2n}$ be a normalised Lagrangian frame and $\Phi_\kappa(\mathcal{Z})$ denote the κ-th Hagedorn wavepacket on phase space. Then,

$$\mathcal{F}_S^\varepsilon \Phi_\kappa(\mathcal{Z}) = \Phi_\kappa(\tilde{\mathcal{Z}}) \quad \text{with} \quad \tilde{\mathcal{Z}} = \begin{pmatrix} \Omega \mathcal{Q} \\ \Omega^T \mathcal{P} \end{pmatrix}.$$

In particular, this implies for the coherent state

$$\mathcal{F}_S^\varepsilon \Phi_0(\mathcal{Z}; z) = 2^{-n} \Phi_0(\mathcal{Z}; z/2), \qquad z \in \mathbb{R}^{2n}.$$

Proof. We first note that for a general $\Phi \in L^2(\mathbb{R}^{2n})$,

$$\begin{aligned}
\mathcal{F}_S^\varepsilon(\mathcal{F}_S^\varepsilon \Phi)(z) &= (2\pi\varepsilon)^{-2n} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \Phi(z') e^{-\frac{\mathrm{i}}{\varepsilon} z'^T \Omega \zeta} \, dz' e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega z} \, d\zeta \\
&= (2\pi\varepsilon)^{-2n} \int_{\mathbb{R}^{4n}} \Phi(z') e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega (z - z')} \, dz' d\zeta = \int_{\mathbb{R}^{4n}} \Phi(z') \delta_{z'=z} \, dz' = \Phi(z)
\end{aligned}$$

and thus $(\mathcal{F}_S^\varepsilon)^{-1} = \mathcal{F}_S^\varepsilon$. We now apply the same strategy as for the standard Fourier transform and utilise that

$$0 = \hat{A}(\mathcal{Z}) \Phi_0(\mathcal{Z}) = \mathcal{F}_S^\varepsilon \hat{A}(\mathcal{Z}) (\mathcal{F}_S^\varepsilon)^{-1} \mathcal{F}_S^\varepsilon \Phi_0(\mathcal{Z}).$$

For the position and momentum operator on phase space, it holds

$$\begin{aligned}
\mathcal{F}_S^\varepsilon \hat{z} \mathcal{F}_S^\varepsilon \Phi(z) &= (2\pi\varepsilon)^{-2n} \int_{\mathbb{R}^{4n}} \Phi(z') \zeta e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega (z - z')} \, dz' d\zeta \\
&= (2\pi\varepsilon)^{-2n} \int_{\mathbb{R}^{4n}} \Phi(z') (-\mathrm{i}\varepsilon \Omega \nabla_{z'} e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega (z - z')}) \, dz' d\zeta \\
&= (2\pi\varepsilon)^{-2n} \int_{\mathbb{R}^{4n}} \mathrm{i}\varepsilon \Omega \nabla_{z'} \Phi(z') e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T \Omega (z - z')} \, dz' d\zeta = -\mathrm{i}\varepsilon \Omega^T \nabla_z \Phi(z)
\end{aligned}$$

and

$$\begin{aligned}\mathcal{F}_S^\varepsilon(-\mathrm{i}\varepsilon\nabla_z)\mathcal{F}_S^\varepsilon\Phi(z) &= (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} -\mathrm{i}\varepsilon\nabla_\zeta\mathcal{F}_S^\varepsilon\Phi(\zeta)e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T\Omega z}\,d\zeta\\ &= (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} \mathcal{F}_S^\varepsilon\Phi(\zeta)(\mathrm{i}\varepsilon\nabla_\zeta e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T\Omega z})\,d\zeta\\ &= (2\pi\varepsilon)^{-2n}\Omega z\int_{\mathbb{R}^{2n}} \mathcal{F}_S^\varepsilon\Phi(\zeta)e^{-\frac{\mathrm{i}}{\varepsilon}\zeta^T\Omega z}\,d\zeta = \Omega z\Phi(z).\end{aligned}$$

Hence, we find for the phase space operator $\hat{v} = \begin{pmatrix}-\mathrm{i}\varepsilon\nabla_z\\ \hat{z}\end{pmatrix}$,

$$\mathcal{F}_S^\varepsilon\hat{v}\mathcal{F}_S^\varepsilon = \begin{pmatrix}0 & \Omega\\ \Omega^T & 0\end{pmatrix}\hat{v}$$

and thus $\mathcal{F}_S^\varepsilon\hat{A}(\mathcal{Z})\mathcal{F}_S^\varepsilon = \hat{A}(\tilde{\mathcal{Z}})$ resp. $\mathcal{F}_S^\varepsilon\hat{A}^\dagger(\mathcal{Z})\mathcal{F}_S^\varepsilon = \hat{A}^\dagger(\tilde{\mathcal{Z}})$ with

$$\tilde{\mathcal{Z}} = \begin{pmatrix}\tilde{\mathcal{P}}\\ \tilde{\mathcal{Q}}\end{pmatrix} = \begin{pmatrix}0 & \Omega\\ \Omega^T & 0\end{pmatrix}\mathcal{Z} = \begin{pmatrix}\Omega\mathcal{Q}\\ \Omega^T\mathcal{P}\end{pmatrix}.$$

This proves the claim for the general wave packets. For the coherent state we moreover note that since $G := \frac{1}{2\mathrm{i}}\mathcal{P}\mathcal{Q}^{-1}$ is symplectic

$$\tilde{\mathcal{P}}\tilde{\mathcal{Q}}^{-1} = \Omega\mathcal{Q}\mathcal{P}^{-1}\Omega = -\tfrac{1}{2\mathrm{i}}G \quad\text{and}\quad \det(\tilde{\mathcal{Q}}) = \det(\mathcal{P}) = (2\mathrm{i})^{2n}\det(\mathcal{Q}).$$

Besides that, the symplectic Fourier transform $\mathcal{F}_S^\varepsilon$ is a unitary transform, see for example [Fei+08, §6], and therefore $\|\mathcal{F}_S^\varepsilon\Phi_0(\mathcal{Z})\| = 1$. Lemma 4.2 then implies

$$\mathcal{F}_S^\varepsilon\Phi_0(\mathcal{Z};z) = (\pi\varepsilon)^{-n/2}2^{-n}\det(\mathcal{Q})^{-1/2}e^{-\frac{1}{4\varepsilon}z^TGz} = 2^{-n}\Phi_0(\mathcal{Z};z/2).$$

■

The previous proposition shows that the Chord function of a coherent state equals just a rescaling of this state. Thus, if we restrict ourselves to coherent states as ansatz functions, our evolution equation given in (10.5) describes also the evolution of the corresponding Chord function.

This setting, with a general Hamiltonian function, was already investigated in a series of publications by Ozorio de Almeida and Brodier, see [BA04a], [BA04b], [BA06] and [BA10]. They deduced the propagation of the Chord function $\chi(z,t)$ via a double Hamiltonian given by

$$\mathcal{H}_C(z,\zeta) = \mathcal{H}(z-\tfrac{1}{2}\Omega\zeta) - \mathcal{H}(z+\tfrac{1}{2}\Omega\zeta) - \gamma z^T\zeta - \tfrac{\mathrm{i}}{2}\left((\Omega\mathrm{Re}(\ell)\zeta)^2 + (\Omega\mathrm{Im}(\ell)\zeta)^2\right)$$

where γ denotes the dissipation coefficent, $\mathcal{H}$ the internal Hamiltonian and $\mathcal{L}(z) = \ell^T z$ the Lindblad term. For simplicity we consider only one Lindblad term here.

The Chord function is then the solution of the non-Hermitian Schrödinger equation

$$\mathrm{i}\varepsilon\,\partial_t\chi(z,t) = \mathcal{H}_C(z,-\mathrm{i}\varepsilon\nabla_z)\chi(z,t), \tag{10.11}$$

see [BA10, Eq. (13), (14)]. If we take $\mathcal{H}$ to be quadratic, then $\mathcal{H}_C$ is also a quadratic Hamiltonian and we can show that this result is equivalent to our approach for coherent states in one dimension.

Corollary 10.3 — Evolution equation in one dimension. For $n = 1$, we can write Equation (10.5) as

$$\mathrm{i}\varepsilon\partial_t\mathcal{W} = \left(-\tfrac{\mathrm{i}\varepsilon^2}{2}\nabla_z^T\mathrm{Re}(L)\nabla_z + \mathrm{i}\varepsilon x^T(H\Omega + \gamma\cdot\mathrm{Id}_2)\nabla_z\right)\mathcal{W}$$

what matches exactly with the evolution equation for the Chord function (10.11).

Proof. Let $\ell = \begin{pmatrix}\ell_p\\ \ell_q\end{pmatrix}$ with $\ell_p, \ell_q \in \mathbb{C}$. Then, $\gamma = \mathrm{Re}(\ell)^T\Omega\mathrm{Im}(\ell) = \mathrm{Im}(\ell_p\bar{\ell}_q)$ and

$$\mathrm{Im}(L) = \Omega\mathrm{Im}(\ell\ell^*)\Omega = \Omega\begin{pmatrix}0 & \mathrm{Im}(\ell_p\bar{\ell}_q)\\ -\mathrm{Im}(\ell_p\bar{\ell}_q) & 0\end{pmatrix}\Omega = \mathrm{Im}(\ell_p\bar{\ell}_q)\cdot\mathrm{Id}_2 = \gamma\cdot\mathrm{Id}_2.$$

Hence, we can rewrite (10.5) in the specified form. On the other hand we find for the double Hamiltonian with $\mathcal{H}(z) = \frac{1}{2}z^THz$,

$$\mathcal{H}(z - \tfrac{1}{2}\Omega\zeta) - \mathcal{H}(z + \tfrac{1}{2}\Omega\zeta) = \tfrac{1}{2}\left(-z^TH\Omega\zeta + \zeta^T\Omega Hz\right) = -z^TH\Omega\zeta$$

and

$$\begin{aligned}(\Omega\mathrm{Re}(\ell)\zeta)^2 + (\Omega\mathrm{Im}(\ell)\zeta)^2 &= \zeta^T\Omega\mathrm{Re}(\ell)\mathrm{Re}(\ell)^T\Omega\zeta + \zeta^T\Omega\mathrm{Im}(\ell)\mathrm{Im}(\ell)^T\Omega\zeta\\ &= \zeta^T\Omega\mathrm{Re}(\ell\ell^T)\Omega\zeta = \zeta^T\mathrm{Re}(L)\zeta.\end{aligned}$$

This yields a double Hamiltonian of the form

$$\mathcal{H}_C(z,\zeta) = -z^T(H\Omega + \gamma\cdot\mathrm{Id}_2)\zeta - \tfrac{\mathrm{i}}{2}\zeta^T\mathrm{Re}(L)\zeta$$

what verifies our result. ■

10.5. Example: Damped harmonic oscillator

For the examples we again only consider the one dimensional case such that we can visualise the time evolution of our Wigner transform. We start with the damped harmonic oscillator as it appears in the context of electromagnetic fields, see [BH02, §2, §5]. This model is a standard simple example in quantum dynamics to show decoherence effects. We take the harmonic oscillator as Hamiltonian,

$$\widehat{\mathcal{H}} = \tfrac{1}{2}(\hat{p}^2 + \hat{q}^2), \qquad H = \mathrm{Id}_2$$

and a single coupling to the environment that is proportional to Dirac's ladder operators,

$$\hat{\mathcal{L}}_1 = (\hat{q} + \mathrm{i}\hat{p}), \qquad \ell_1 = \begin{pmatrix}\mathrm{i}\\ 1\end{pmatrix}.$$

We stress that due to the form of the matrix $L = \Omega \sum_{j=1}^{m} \ell_j \ell_j^* \Omega$ it suffices for a mathematical study to consider only one Lindblad term. We find

$$L = \Omega \ell_1 \ell_1^* \Omega = \begin{pmatrix} -1 & -\mathrm{i} \\ \mathrm{i} & -1 \end{pmatrix} = -\mathrm{Id}_2 + \mathrm{i}\Omega \quad \text{and} \quad \gamma = \mathrm{Re}(\ell)^T \Omega \mathrm{Im}(\ell) = 1.$$

We will investigate two cases here, the dynamics of a symmetric Wigner transform $\mathcal{W}^\varepsilon(\varphi_k(l), \varphi_m(l))$ and of a non-symmetric Wigner transform $\mathcal{W}^\varepsilon(\varphi_k(l_1), \varphi_m(l_2))$.

For a start we again consider the standard coherent state,

$$L_0 = \mathrm{span}\{l_0\}, \qquad l_0 = \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \in \mathbb{C}^2,$$

with the symplectic metric $G = \mathrm{Id}_2$. The corresponding phase space frame $\mathcal{Z}$ is of the form

$$\mathcal{Z} = \begin{pmatrix} \mathcal{P} \\ \mathcal{Q} \end{pmatrix}, \quad \text{where} \quad \mathcal{P} = \begin{pmatrix} \mathrm{i} & \mathrm{i} \\ -1 & 1 \end{pmatrix}, \; \mathcal{Q} = \tfrac{1}{2} \begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix}.$$

and we denote $\mathcal{L} := \mathrm{span}\{\mathcal{Z}\}$.

Linearised flow

For the linearised flow that is independent of our initial wave packets, and thus equal for the symmetric and the non-symmetric Wigner function, we find $\mathrm{Re}(L) = -\mathrm{Id}_2$, $\mathrm{Im}(L) = \Omega$ and

$$\begin{aligned} I_t &= \int_0^t e^{-(\Omega H + \mathrm{Im}(L)\Omega)\tau} \,\mathrm{Re}(L)\, e^{(H\Omega - \Omega \mathrm{Im}(L))\tau} \, d\tau = -\int_0^t e^{-(\Omega - \mathrm{Id}_2)\tau} e^{(\Omega + \mathrm{Id}_2)\tau} \, d\tau \\ &= -\int_0^t e^{2\tau} \, d\tau \cdot \mathrm{Id}_2 = \tfrac{1}{2}(1 - e^{2t}) \mathrm{Id}_2. \end{aligned}$$

This implies

$$S_t = \begin{pmatrix} e^{(\Omega + \mathrm{Id}_2)t} & 0 \\ \mathrm{i}e^{(\Omega - \mathrm{Id}_2)t} I_t & e^{(\Omega - \mathrm{Id}_2)t} \end{pmatrix} \quad \text{with} \quad S_t^* \Omega S_t = \begin{pmatrix} -2\mathrm{i}I_t & -\mathrm{Id}_2 \\ \mathrm{Id}_2 & 0 \end{pmatrix}.$$

and the integral term I_t includes the deviation from the Hermitian case.

Normalisation

Since

$$\mathcal{P}^* \mathcal{P} = \begin{pmatrix} -\mathrm{i} & -1 \\ -\mathrm{i} & 1 \end{pmatrix} \begin{pmatrix} \mathrm{i} & \mathrm{i} \\ -1 & 1 \end{pmatrix} = 2 \cdot \mathrm{Id}_2$$

we obtain for the normalisation

$$N_t = \mathrm{Id}_2 - \mathcal{P}^* I_t \mathcal{P} = \mathrm{Id}_2 - (1 - e^{2t})\mathrm{Id}_2 = e^{2t}\, \mathrm{Id}_2.$$

what displays that N_t is positive for all times $t \geq 0$ due to Proposition 10.3.

Evolved coherent state

Proposition 10.3 moreover implies that the time evolved phase space frame is given by

$$\mathcal{Z}_t = \begin{pmatrix} e^{(H\Omega-\Omega\mathrm{Im}(L))t}\mathcal{P} \\ e^{(\Omega H+\mathrm{Im}(L)\Omega)t}(\mathrm{Id}_{2n} - 2I_t G)\mathcal{Q} \end{pmatrix} N_t^{-1/2} = \begin{pmatrix} e^{-t}e^{(\Omega+\mathrm{Id}_2)t}\mathcal{P} \\ e^{t}e^{(\Omega-\mathrm{Id}_2)t}\mathcal{Q} \end{pmatrix},$$

what is equivalent to a simple unitary rotation,

$$\mathcal{P}_t = \begin{pmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{pmatrix} \mathcal{P}, \quad \mathcal{Q}_t = \begin{pmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{pmatrix} \mathcal{Q}.$$

In particular, the symplectic metric G_t is constant over time, $G_t = \mathrm{Id}_2$. The gain or loss factor of the system is then easily computed as

$$\beta_t + \gamma t = \int_0^t \mathrm{tr}(\mathrm{Re}(L)G_\tau)\, d\tau + 2\gamma t = -2t + 2t = 0.$$

Hence, the coherent state is time invariant, $\widehat{\mathcal{U}}(t)\mathcal{W}_0(\mathcal{Z}) = \mathcal{W}_0(\mathcal{Z})$, what matches with the results in [BH02, §5.2.1]. This behaviour can also be explained since $\mathcal{W}_0$ is an eigenstate of $\mathcal{H}_S$ in this case.

Evolved excited states

As we are considering the case of a symmetric Wigner function, we can for the excited states invoke the shortened formula for the recursion matrix $\mathcal{M}_t$,

$$\mathcal{M}_t = (2N_t^{-1} - \mathrm{Id}_2)\mathcal{Q}^{-1}\overline{\mathcal{Q}} = (2e^{-2t} - 1)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and the circular structure of the excited states is preserved over time, see Section 5.3. In particular, we see

$$\mathcal{M}_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{M}_t \to \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{as } t \to \infty.$$

However, we evaluate the polynomial prefactor at $\frac{1}{\sqrt{\varepsilon}} N_t^{-1/2}\mathcal{Q}_t^{-1} z$ and

$$N_t^{-1/2}\mathcal{Q}_t^{-1} = e^{-t}\mathcal{Q}\begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix} \to 0$$

for $t \to \infty$. This means, excited states with $k = m$, i.e. density operators, tend to the coherent state $\mathcal{W}_0(\mathcal{Z})$, while excited states with $k \neq m$, i.e. the differences between the density operator, vanish, see Figures 17 and 18.

For the non-symmetric Wigner transform $\mathcal{W}^\varepsilon(\varphi_k(l_1), \varphi_m(l_2))$ we choose $L_1 = \mathrm{span}\{l_1\}$ and $L_2 = \mathrm{span}\{l_2\}$ with

$$l_1 = \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}, \qquad l_2 = \begin{pmatrix} \mathrm{i} \\ 1 - 2\mathrm{i} \end{pmatrix}.$$

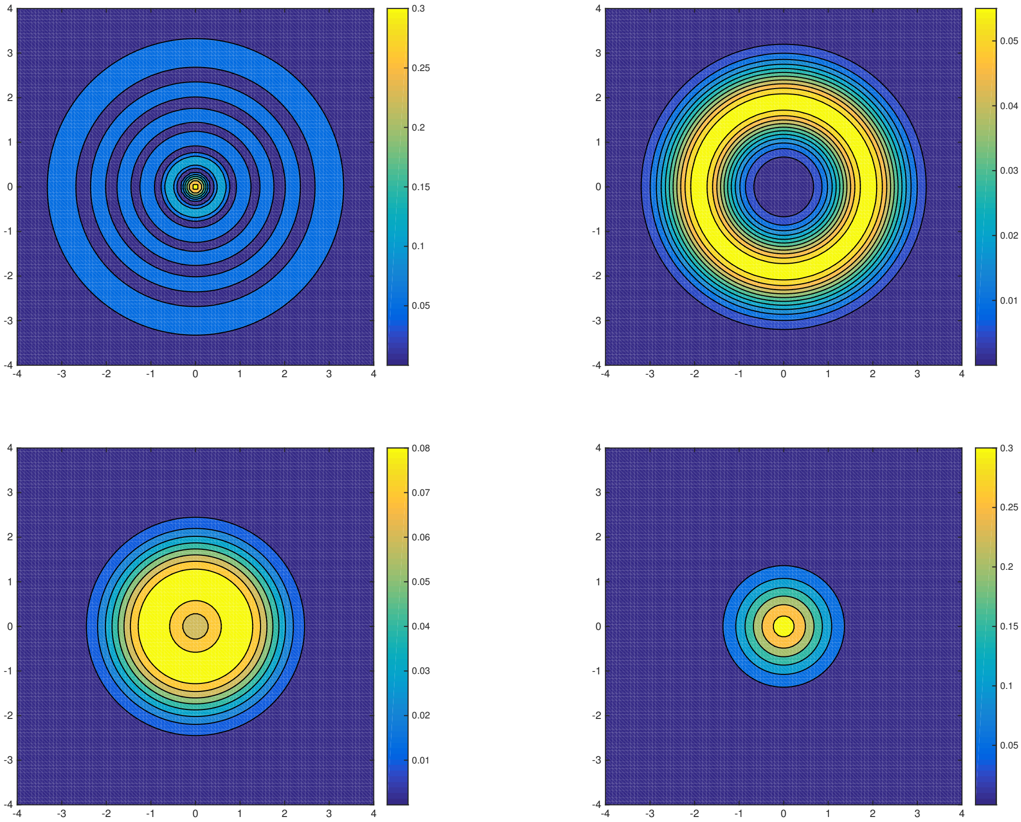

Figure 17.: Contour plots of the absolute values of $\mathcal{U}(t)\mathcal{W}_{(5,5)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.5$ (upper right), $t = 1$ (lower left) and $t = 4$ (lower right) for $\varepsilon = 1$

The phase space frame $\mathcal{Z}$ of l_1 and l_2 is then given by

$$\mathcal{Z} = \begin{pmatrix} \mathcal{P} \\ \mathcal{Q} \end{pmatrix}, \quad \text{where} \quad \mathcal{P} = \begin{pmatrix} \mathrm{i} & -1+2\mathrm{i} \\ -1 & \mathrm{i} \end{pmatrix}, \; \mathcal{Q} = \tfrac{1}{2}\begin{pmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1-2\mathrm{i} \end{pmatrix}$$

and the generalised metric G of l_1 and l_2 is complex-valued,

$$G = \tfrac{1}{2}\begin{pmatrix} 3-\mathrm{i} & 1+\mathrm{i} \\ 1+\mathrm{i} & 1+\mathrm{i} \end{pmatrix}.$$

Normalisation

For the normalisation we obtain similar as in the first case

$$N_t = \mathrm{Id}_2 - \mathcal{P}^* I_t \mathcal{P} = \mathrm{Id}_2 - \tfrac{1}{2}(1-e^{2t})\mathcal{P}^*\mathcal{P} = \begin{pmatrix} e^{2t} & e^{2t}-1 \\ e^{2t}-1 & 3e^{2t}-2 \end{pmatrix}.$$

Our calculations for coherent and excited states get more involved.

Evolved coherent state

For the propagation of the coherent state we omit $\mathcal{P}_t$ and $\mathcal{Q}_t$ and determine the evolved

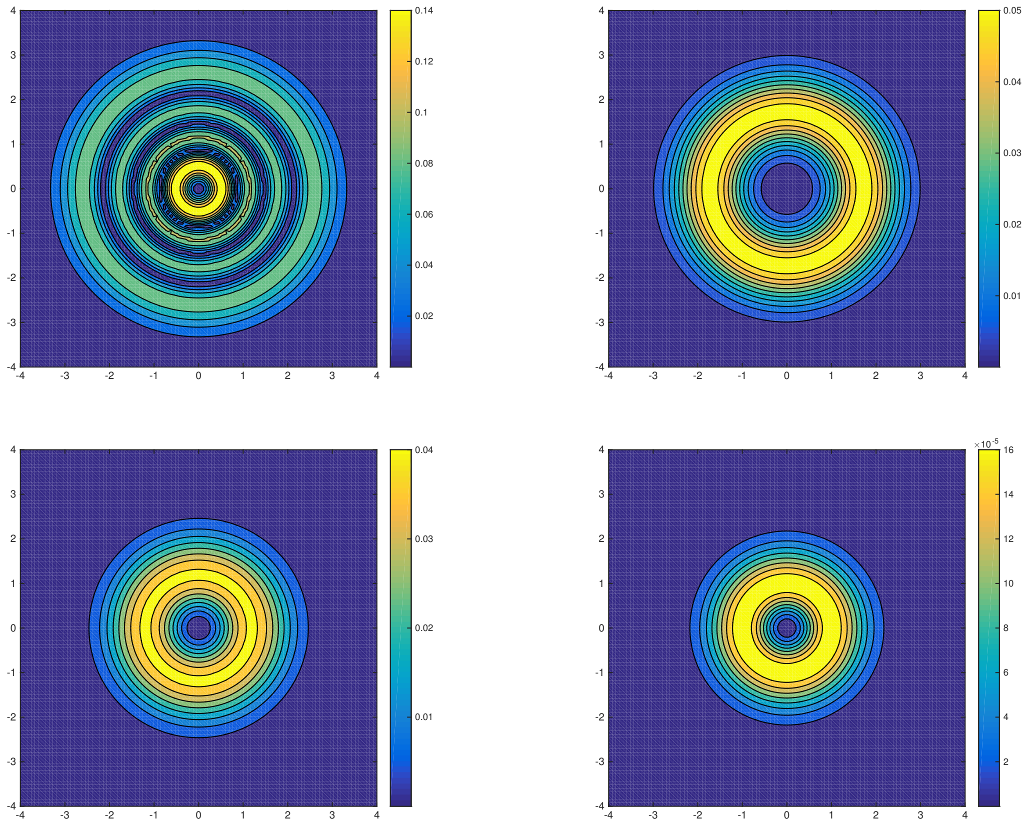

Figure 18.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\mathcal{W}_{(5,3)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.5$ (upper right), $t = 1$ (lower left) and $t = 4$ (lower right) for $\varepsilon = 1$

metric by means of Lemma 10.3,

$$G_t = e^{(\Omega+\mathrm{Id}_2)t} G(\mathrm{Id}_2 - 2I_t G)^{-1} e^{-(\Omega-\mathrm{Id}_2)t} = \mathrm{Id}_2 + \tfrac{1}{2} e^{-(2+2\mathrm{i})t} \begin{pmatrix} 1-\mathrm{i} & 1+\mathrm{i} \\ 1+\mathrm{i} & -1+\mathrm{i} \end{pmatrix}$$

what nicely addresses the second statement of Lemma 10.3, we recover the metric from the symmetric case with an additional singular matrix. For the gain or loss in the system we find

$$\beta_t + \gamma t = \int_0^t \mathrm{tr}(\mathrm{Re}(L)(\tfrac{1}{4}\mathcal{P}_\tau\mathcal{P}_\tau^* + \mathrm{i}\mathrm{Im}(G_\tau))\, d\tau + \gamma t = -\int_0^t \mathrm{tr}(\tfrac{1}{4}\mathcal{P}_\tau\mathcal{P}_\tau^* + \mathrm{i}\mathrm{Im}(G_\tau))\, d\tau + t,$$

$\mathrm{tr}(\mathrm{Im}(G_\tau)) = 0$ and

$$\begin{aligned} \mathcal{P}_\tau\mathcal{P}_\tau^* &= e^{(\Omega+\mathrm{Id}_2)\tau}\mathcal{P}N_\tau^{-1}\mathcal{P}^* e^{(-\Omega+\mathrm{Id}_2)\tau} \\ &= \tfrac{e^{2t}}{2e^{4t}-1}\left(4e^{2t}\cdot\mathrm{Id}_2 + 2\begin{pmatrix} \cos(2t)-\sin(2t) & \cos(2t)+\sin(2t) \\ \cos(2t)+\sin(2t) & -\cos(2t)+\sin(2t) \end{pmatrix}\right). \end{aligned}$$

So, β_t emerges as

$$\beta_t = -\int_0^t \tfrac{2e^{4\tau}}{2e^{4\tau}-1}\, d\tau = -\tfrac{1}{4}\ln(2e^{4t}-1), \quad e^{\beta_t+\gamma t} = \frac{e^t}{(2e^{4t}-1)^{1/4}},$$

and the coherent state tend to constant multiple of the coherent state in the symmetric case.

Evolved excited states

For the excited states we have to utilise formula (10.10) for the recursion matrix and obtain

$$\mathcal{M}_t = \frac{1-\mathrm{i}}{2}(2e^{-2t}-1)\begin{pmatrix} 2e^{-2t}-1 & 1 \\ 1 & -(2e^{-2t}-1)^{-1} \end{pmatrix}.$$

with

$$\mathcal{M}_0 = \frac{1-\mathrm{i}}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad \text{and} \quad \mathcal{M}_t \to \frac{1-\mathrm{i}}{2}\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}$$

for $t \to \infty$. Due to the substitution $\frac{1}{\sqrt{\varepsilon}}N_t^{-1/2}\mathcal{Q}_t^{-1}z$ we find a similar picture for the propagation as in the first example. Excited states with $k = m$ approach the coherent state, excited states with $k \neq m$ disappear, see Figure 19. This behaviour is again consistent with the one found in [BH02, §5.2.1].

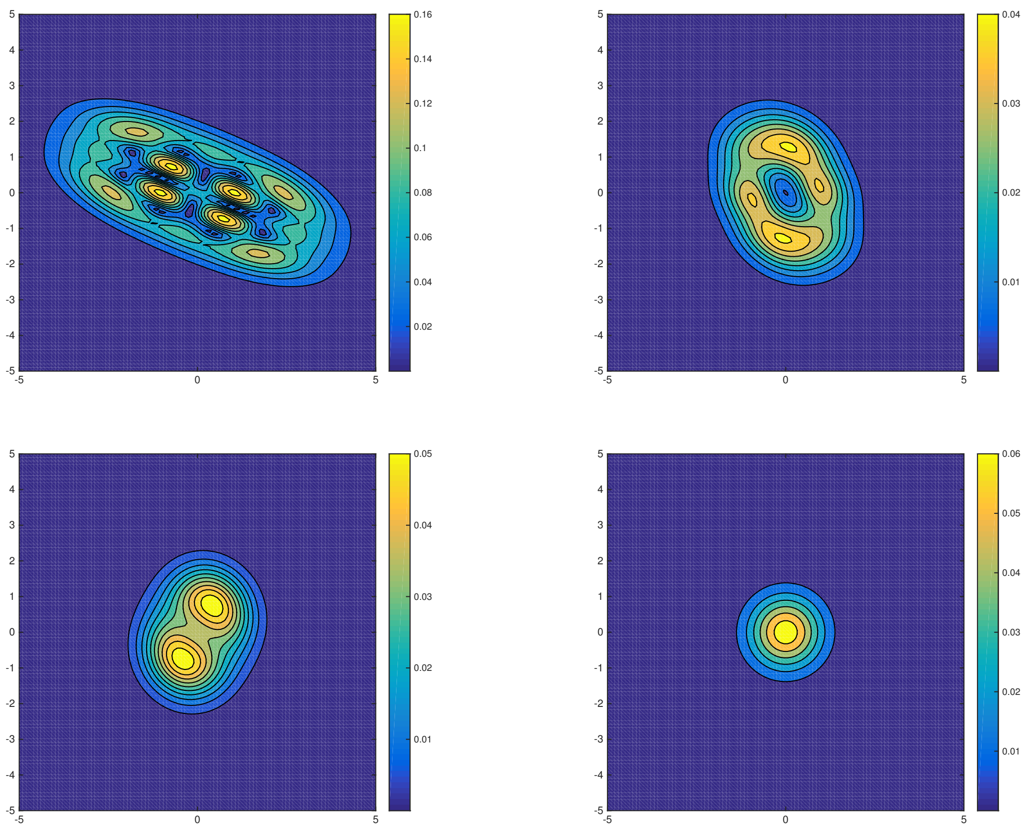

Figure 19.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\mathcal{W}_{(2,2)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.5$ (upper right), $t = 1$ (lower left) and $t = 4$ (lower right) for $\varepsilon = 1$

10.6. Example Pure Lindblad dynamics

As second example we investigate the effect of the Lindblad operators by neglecting the Hamiltonian, i.e. we take

$$H = 0,$$

and choose the most general one-dimensional setting for the Lindblad operators,

$$\hat{\mathcal{L}}_1 = \ell_1^T \hat{z}, \qquad \ell_1 = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathbb{C}^2.$$

Then,

$$L = \begin{pmatrix} -|\alpha|^2 & \mathrm{Re}(\alpha\overline{\beta}) \\ \mathrm{Re}(\alpha\overline{\beta}) & -|\beta|^2 \end{pmatrix} + \mathrm{i} \begin{pmatrix} 0 & -\mathrm{Im}(\alpha\overline{\beta}) \\ \mathrm{Im}(\alpha\overline{\beta}) & 0 \end{pmatrix}, \qquad \gamma = \mathrm{Im}(\alpha\overline{\beta})$$

and we distinguish the two cases $\mathrm{Im}(\overline{\alpha}\beta) = 0$ and $\mathrm{Im}(\overline{\alpha}\beta) \neq 0$. The first example describes the evolution in a non-dissipative system, the second includes dissipation.

In both examples we start from the standard coherent state,

$$L_0 = \mathrm{span}\{l_0\}, \qquad l_0 = \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \in \mathbb{C}^2, \qquad G = \mathrm{Id}_2$$

with symmetric Wigner functions of the form $\mathcal{W}_{k,m} = \mathcal{W}(\varphi_k(l_0), \varphi_m(l_0))$.

Linearised flow

If $\mathrm{Im}(\overline{\alpha}\beta) = 0$, we find $\mathrm{Im}(L) = 0$ and an easy calculation yields

$$I_t = \int_0^t \mathrm{Re}(L)\, d\tau = t\,\mathrm{Re}(L).$$

and $S_t = \begin{pmatrix} \mathrm{Id} & 0 \\ \mathrm{i}t\mathrm{Re}(L) & \mathrm{Id} \end{pmatrix}$.

Normalisation

The normalisation is then given by

$$N_t = \mathrm{Id}_2 - \mathcal{P}^* I_t \mathcal{P} = \mathrm{Id}_2 + t \begin{pmatrix} |\alpha|^2 + |\beta|^2 & -(\alpha - \mathrm{i}\beta)(\overline{\alpha} - \mathrm{i}\overline{\beta}) \\ -(\alpha + \mathrm{i}\beta)(\overline{\alpha} + \mathrm{i}\overline{\beta}) & |\alpha|^2 + |\beta|^2 \end{pmatrix}$$

and we denote again the determinant of N_t as $d_t = 1 + 2(|\alpha|^2 + |\beta|^2)t$.

Evolved coherent state

For the evolved symplectic metric we once more refer to Lemma 10.3,

$$G_t = \frac{1}{d_t} \begin{pmatrix} 1 + 2|\beta|^2 t & 2\alpha\overline{\beta}t \\ 2\alpha\overline{\beta}t & 1 + 2|\alpha|^2 t \end{pmatrix}.$$

Thus, we find a notably nice long term behaviour: for $t \to \infty$ it holds

$$G_t \to \frac{1}{|\alpha|^2 + |\beta|^2} \begin{pmatrix} |\beta|^2 & \overline{\alpha}\beta \\ \overline{\alpha}\beta & |\alpha|^2 \end{pmatrix}.$$

For the deduction of β_t, we kept things simple, since we are investigating symmetric Wigner functions and in this case $\gamma = 0$. Thus

$$\beta_t = \int_0^t \mathrm{tr}(\mathrm{Re}(L)G_\tau)\, d\tau = \int_0^t \frac{-(|\alpha|^2 + |\beta|^2)}{1 + 2(|\alpha|^2 + |\beta|^2)t}\, d\tau = -\tfrac{1}{2}\ln(d_t), \qquad e^{\beta_t} = \sqrt{\tfrac{1}{d_t}}.$$

Hence, we find a loss factor and the pure coherent state $\mathcal{W}_0$ is slowly damped.

Evolved excited states

For excited states $\mathcal{W}_{k,m}$, $k, m \in \mathbb{N}$, we note that

$$M_t = \frac{1}{d_t} \begin{pmatrix} 2(\alpha - \mathrm{i}\beta)(\overline{\alpha} - \mathrm{i}\overline{\beta})t & 1 \\ 1 & 2(\alpha + \mathrm{i}\beta)(\overline{\alpha} + \mathrm{i}\overline{\beta})t \end{pmatrix}$$

and the circular structure is preserved if and only if $\alpha = \mathrm{i}\beta$ or $\alpha = -\mathrm{i}\beta$. However, since we assume $\mathrm{Im}(\overline{\alpha}\beta) = 0$ this implies $\alpha = \beta = 0$. For the polynomial prefactor we furthermore find

$$N_t^{-1/2}\mathcal{Q}_t^{-1}z = \mathcal{Q}^{-1}(\mathrm{Id}_2 - 2I_tG)^{-1}z \quad \text{with} \quad (\mathrm{Id} - 2I_tG)^{-1} = \frac{1}{d_t}\begin{pmatrix} 1 + 2|\beta|^2 t & 2\overline{\alpha}\beta t \\ 2\overline{\alpha}\beta t & 1 + 2|\alpha|^2 t \end{pmatrix},$$

the damping of the excited states is only caused by β_t, see Figure 20. Since we investigate a non-dissipative system, we will not converge to a steady-state what is confirmed by the illustrations.

If we consider the case $\gamma = \mathrm{Im}(\alpha\overline{\beta}) \neq 0$ the calculations get more extensive.

Linearised flow

We have $e^{-\Omega \mathrm{Im}(L)t} = e^{\mathrm{Im}(\alpha\overline{\beta})t} \cdot \mathrm{Id}_2 = e^{\gamma t} \cdot \mathrm{Id}_2$ and thus

$$I_t = \tfrac{1}{2\gamma}(e^{2\gamma t} - 1)\mathrm{Re}(L)$$

and $S_t = \begin{pmatrix} e^{\gamma t}\,\mathrm{Id}_2 & 0 \\ \mathrm{i}e^{-\gamma t} I_t & e^{-\gamma t}\,\mathrm{Id}_2 \end{pmatrix}$.

Normalisation

The normalisation in this case reads

$$N_t = \mathrm{Id}_2 + \frac{e^{2\gamma t} - 1}{2\gamma}\begin{pmatrix} |\alpha|^2 + |\beta|^2 & -|\alpha|^2 + |\beta|^2 + 2\mathrm{i}\mathrm{Re}(\overline{\alpha}\beta) \\ -|\alpha|^2 + |\beta|^2 - 2\mathrm{i}\mathrm{Re}(\overline{\alpha}\beta) & |\alpha|^2 + |\beta|^2 \end{pmatrix}$$

with determinant $d_t = 1 + \frac{|\alpha|^2 + |\beta|^2}{\gamma}(e^{2\gamma t} - 1) + (e^{2\gamma t} - 1)^2$.

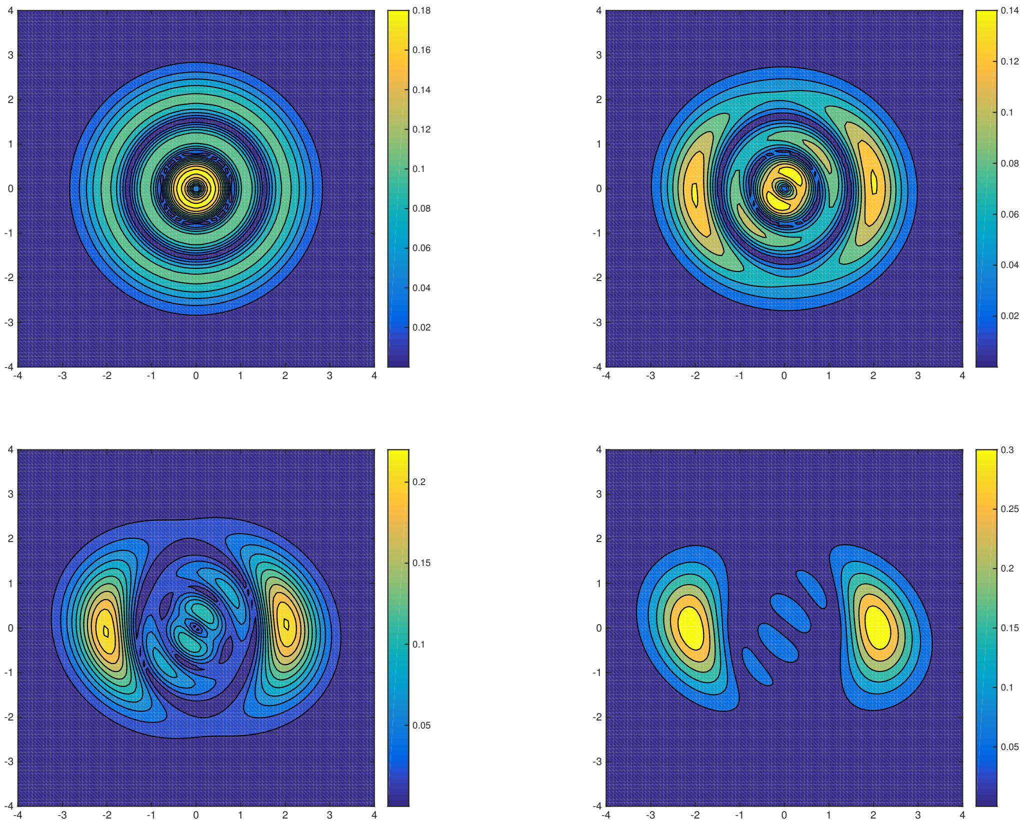

Figure 20.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\mathcal{W}_{(3,2)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.01$ (upper right), $t = 0.03$ (lower left) and $t = 0.06$ (lower right) for $\alpha = 1$, $\beta = 2$ and $\varepsilon = 1$

Evolved coherent state

The propagation of the symplectic metric is then described by

$$G_t = \frac{e^{2\gamma t}}{d_t}\left(\mathrm{Id}_2 + \frac{e^{2\gamma t}-1}{\gamma}\begin{pmatrix} |\alpha|^2 & \mathrm{Re}(\overline{\alpha}\beta) \\ \mathrm{Re}(\overline{\alpha}\beta) & |\beta|^2 \end{pmatrix}\right)$$

For the gain or loss factor β_t, we first stress that

$$\mathrm{tr}(\mathrm{Re}(L)G_t) = -\frac{e^{2\gamma t}}{d_t}\left(|\alpha|^2 + |\beta|^2 + 2\gamma(e^{2\gamma t}-1)\right) = -\frac{d_t'}{2d_t}.$$

Therefore, $\beta_t = -\frac{1}{2}\ln(d_t) + \gamma t$ and $e^{\beta_t + \gamma t} = \frac{e^{2\gamma t}}{\sqrt{d_t}}$.

Evolved excited states

Finally, the propagation of the excited states is determined by

$$M_t = \frac{1}{d_t}\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + (1 - e^{-2\mathrm{Im}(\overline{\alpha}\beta)t})\begin{pmatrix} \frac{|\alpha|^2 - |\beta|^2 - 2\mathrm{i}\mathrm{Re}(\overline{\alpha}\beta)}{\mathrm{Im}(\overline{\alpha}\beta)} & e^{-2\mathrm{Im}(\overline{\alpha}\beta)t} - 1 \\ e^{-2\mathrm{Im}(\overline{\alpha}\beta)t} - 1 & \frac{|\alpha|^2 - |\beta|^2 + 2\mathrm{i}\mathrm{Re}(\overline{\alpha}\beta)}{\mathrm{Im}(\overline{\alpha}\beta)} \end{pmatrix}\right)$$

what pleasantly illustrates the circular structure that is only preserved if

$$|\alpha|^2 - |\beta|^2 - 2\mathrm{i}\mathrm{Re}(\overline{\alpha}\beta) = 0.$$

This was for example satisfied for the damped harmonic oscillator, where we investigated $\alpha = \mathrm{i}$, $\beta = 1$. Moreover, we see that the sign of γ is characteristic for the dynamics, for $\gamma > 0$ we expect a contraction of the wavepacket, see [BA04b, §2] and for $\gamma < 0$ an expansion. We visualise the time evolution for $\alpha = 1$, $\beta = \mathrm{i}$ in Figure 21 and $\alpha = 1$, $\beta = -\mathrm{i}$ in Figure 22.

In both settings we have $|\alpha|^2 - |\beta|^2 = 0$ and the circular structure is preserved. For our first choice with $\gamma < 0$ our wave packet spreads, while in the second case with $\gamma > 0$, the wave packet is concentrated and tends to the coherent state what matches with the findings in [BA04b]. For the substitution

$$N_t^{-1/2}\mathcal{Q}_t^{-1}z = \mathcal{Q}^{-1}(\mathrm{Id}_2 - 2I_tG)^{-1}e^{-\mathrm{Im}(L)\Omega t}z$$

we moreover note

$$(\mathrm{Id} - 2I_tG)^{-1}e^{-\mathrm{Im}(L)\Omega t} = \frac{e^{\gamma t}}{d_t}\left(\mathrm{Id} + \frac{e^{2\gamma t} - 1}{\gamma}\begin{pmatrix} |\alpha|^2 & \mathrm{Re}(\overline{\alpha}\beta) \\ \mathrm{Re}(\overline{\alpha}\beta) & |\beta|^2 \end{pmatrix}\right).$$

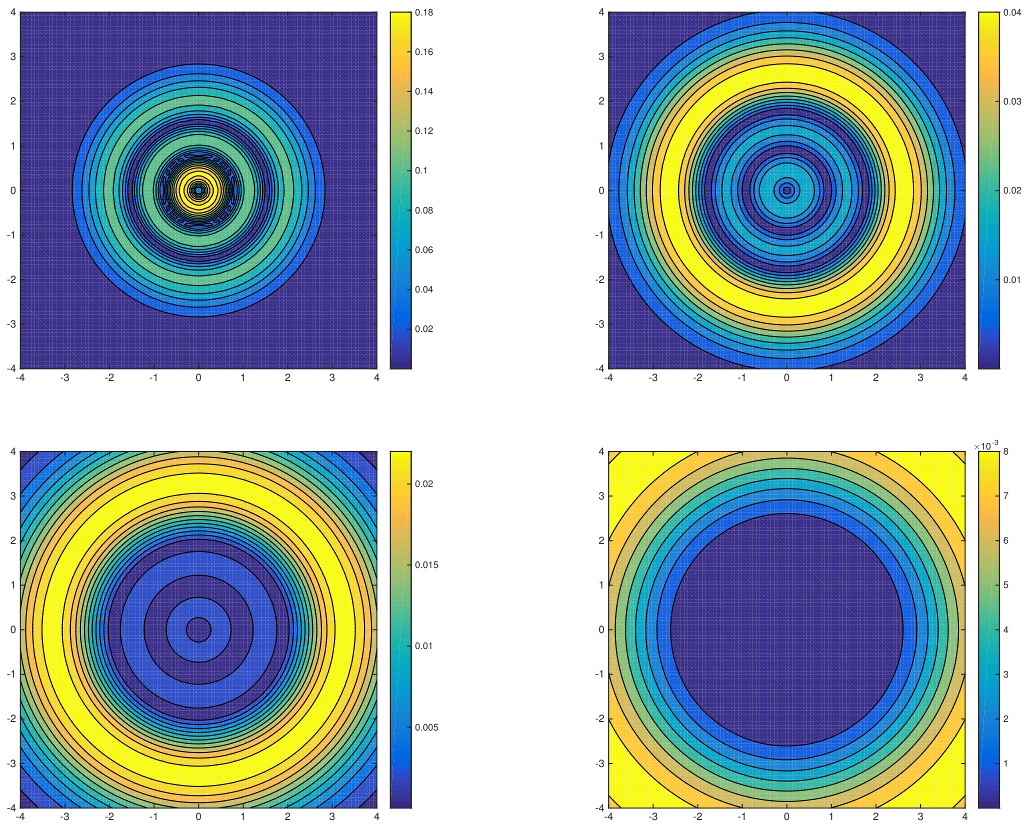

Figure 21.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\mathcal{W}_{(3,2)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.2$ (upper right), $t = 0.4$ (lower left) and $t = 0.08$ (lower right) for $\alpha = 1$, $\beta = \mathrm{i}$ and $\varepsilon = 1$

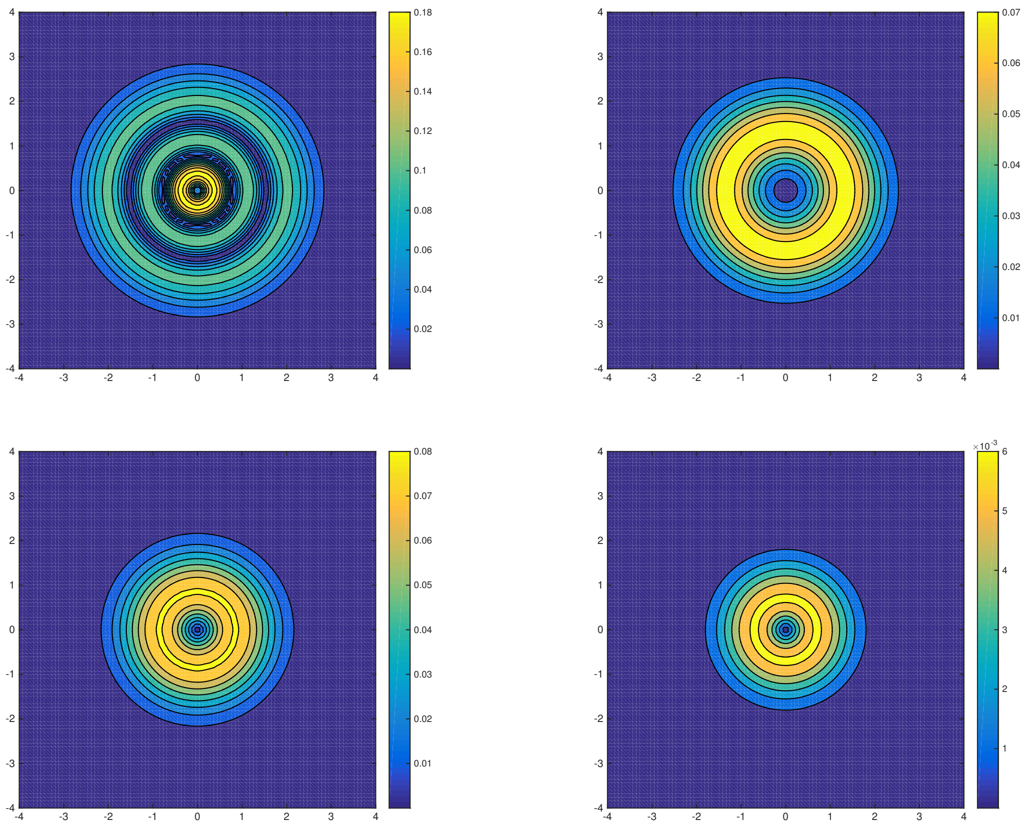

Figure 22.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\mathcal{W}_{(3,2)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.5$ (upper right), $t = 1$ (lower left) and $t = 2$ (lower right) for $\alpha = 1$, $\beta = -\mathrm{i}$ and $\varepsilon = 1$

11. Further applications

In the last chapter of this thesis we want to present further areas of application for non-Hermitian quadratic Hamiltonians. We will shortly introduce three different differential equations that are closely connected to each other, namely the diffusion equation, the Langevin equation and the Fokker-Planck equation, and show that under certain assumptions they can be rewritten as Schrödinger equation with quadratic, non-Hermitian Hamiltonian. Thus, we can apply our findings from the second part and specify wave packets that are solutions to those equations.

The diffusion equation is probably the most natural extension of our findings. We will give a brief recap of its deduction in the first section and show that the corresponding Hamiltonian is of the form $\widehat{\mathcal{H}} = \frac{1}{2}\hat{z}^T H \hat{z}$ with

$$H_{Diff} = -2\mathrm{i}\delta \cdot \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

where δ denotes the diffusion coefficient. We will investigate all examples in the univariate case here. By also allowing for complex values of d we can nicely compare the dynamics of the diffusion equation to the free Schrödinger equation.

The relation of Brownian motion to open quantum systems was already investigated in several works, see for example [Sze11] or [BA04a]. We will present the approach of [Lin76a] here, where the joined distribution of position and momentum of a Brownian particle is described by a Lindblad equation with quadratic Hamiltonian and two linear Lindblad terms determined by

$$H_{Br} = \begin{pmatrix} \frac{1}{m} & \frac{\gamma}{2} \\ \frac{\gamma}{2} & m\omega^2 \end{pmatrix}, \quad \ell_1 = -\begin{pmatrix} \gamma \\ m\omega^2 \end{pmatrix}, \quad \ell_2 = \begin{pmatrix} \frac{1}{m} \\ 0 \end{pmatrix},$$

where m denotes the mass of the particle, γ the friction coefficient and ω^2 an external force or potential. As an explicit example we choose the simplified Brownian motion from [BH02, §5.3.3] assuming that there is no potential acting on the system.

Since it is known that the evolution of the distribution $\rho(p, q)$ of a Brownian particle is governed by a Fokker-Planck equation, this moreover shows the relation of the Fokker-Planck and the Lindblad equation. In one dimension, i.e. if we consider the Fokker-Planck equation for a distribution $\rho(x)$, $x \in \mathbb{R}$, we can also write a general Fokker-Planck equation with drift α and diffusion δ as Schrödinger equation with

$$H_{FP} = \begin{pmatrix} \mathrm{i}\delta & \alpha \\ \alpha & 0 \end{pmatrix}.$$

and a constant term $\frac{1}{2}\alpha$. This ansatz can be seen as an alteration of [Ris84, p. 5.4], where the Fokker-Planck equation is interpreted as an Schrödinger equation with complex time scale. Since Fokker-Planck equations do not only play a role in physics, but also in statistics we present as example the Black and Scholes model, see [BS73]. In our calculations we explicitly highlight how the constant term effects the time evolution.

11.1. Diffusion equation

The diffusion equation describes the time evolution of a density $\rho \in L^2(\mathbb{R}^n)$ of some quantity such as heat or a chemical concentration for example, see [Eva98, §2.3]. The diffusion is thereby a result of random molecular motions. This matter was first picked up by Fourier studying the distribution of heat in [Fou22] what lead to the well-known heat equation. Some years later Fick recognised the analogy to general diffusion and adopted Fourier's mathematical description of the heat conduction in [Fic55], see [Cra75, §1].

The derivation of the diffusion equations is based on the hypothesis that the transfer rate of the diffusing substance is proportional to the gradient of the concentration, i.e.

$$F = -\delta \nabla_x \rho, \tag{11.1}$$

where $\delta > 0$ is called *diffusion coefficient*. In our study we take δ to be a constant, what is reasonable for dilute solutions, but we stress that in other examples the diffusion coefficient markedly relies on the concentration, see [Cra75, §1].

If we then consider a smooth region $V \subset \mathbb{R}^n$, the rate of change of the total quantity within V is given by transfer rate through the boundary ∂V,

$$\partial_t \int_V \rho(x)\, dx = -\int_{\partial V} F \cdot \nu \, dS.$$

Since V was arbitrary this yields $\partial_t \rho = -\mathrm{div}(F)$ and with assumption (11.1) we find the diffusion equation

$$\partial_t \rho = \delta \Delta \rho, \tag{11.2}$$

see [Eva98, §2.3]. Equation (11.1) is also called *Fick's first law of diffusion*, while (11.2) is known as *Fick's second law of diffusion*. In particular, taking $\delta = 1$ yields the heat equation.

11.2. Example: Diffusion equation

Accordingly to the previous deduction we will apply our results now to the differential equation

$$\mathrm{i}\, \partial_t \rho = (\mathrm{i}\delta) \partial_x^2 \rho.$$

For simplicity, we restrict ourselves to one dimension, however, the calculations can be directly lifted to multi-dimensions.

To be able to compare directly the dynamics of the diffusion equation with the free Schrödinger equation, see [Lub08, §I.2], we allow for $\delta \in \mathbb{C}$. Then again, $\delta = 1$ corresponds to the heat equation, $\delta > 0$ to a standard diffusion equation and $\delta = -\mathrm{i}$ to Schrödinger's equation.

To start with our analysis, we consider a positive Lagrangian subspace $L_0 = \mathrm{range}(l_0)$ and its propagation $L_t = \mathrm{range}(l_t)$ defined via

$$l_0 = \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \in \mathbb{C}^2 \quad \text{and} \quad l_t = \begin{pmatrix} p_t \\ q_t \end{pmatrix} = S_t l_0 n_t^{-1/2} \in \mathbb{C}^2.$$

The dynamics in this case governed by the quadratic Hamiltonian $\mathcal{H}(z) = \frac{1}{2} z^T H z$ with

$$H = -2\mathrm{i}\delta \cdot \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{C}^{2\times 2},$$

compare to Lemma 8.2. We note that $\mathrm{Im}(H) \leq 0$ if and only if $\mathrm{Re}(\delta) \geq 0$ what is satisfied in the practical situation mentioned before.

Linearised flow

Taking into account that $(\Omega H)^2 = 0$, we can easily deduce $S_t = e^{t\Omega H}$ as the sum

$$S_t = \mathrm{Id}_2 + t\Omega H = \begin{pmatrix} 1 & 0 \\ -2\mathrm{i}\delta t & 1 \end{pmatrix}.$$

We directly augment the relation for $S_t^* \Omega S_t$ here, so we can draw back on it in the following calculations,

$$S_t^* \Omega S_t = \begin{pmatrix} 1 & 2\mathrm{i}\bar{\delta} t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 2\mathrm{i}\delta t & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 4\mathrm{i}\mathrm{Re}(\delta) t & -1 \\ 1 & 0 \end{pmatrix}.$$

Besides that, this formula also gives a nice intuition for the "non-Hermiticity" of the example. For a real Hamiltonian, S_t satisfies $S_t^* \Omega S_t = \Omega$. Hence, the first entry $4\mathrm{i}\mathrm{Re}(\delta)t$ measures the deviation from unitary evolution. Here, this interpretation is particularly pleasant: if δ is purely imaginary we are in the setting of the free Schrödinger equation, the evolution is unitary. The larger the real part of δ, the more we deviate from the Hermitian evolution.

Normalisation

The normalisation of $S_t l_0$ is then given by

$$n_t = \frac{1}{2\mathrm{i}} l_0^* S_t^* \Omega S_t l_0 = \frac{1}{2\mathrm{i}} \begin{pmatrix} p_0^* & q_0^* \end{pmatrix} \begin{pmatrix} 4\mathrm{i}\mathrm{Re}(\delta) t & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = 1 + 2\mathrm{Re}(\delta)|p_0|^2 t.$$

We observe that the normalisation is only required if $\mathrm{Re}(\delta) \neq 0$. Beyond that we distinguish the cases $\mathrm{Re}(\delta) > 0$, what corresponds to the diffusion equation and $\mathrm{Re}(\delta) < 0$, what describes only a theoretical example. In the first case our propagation is well-defined for all times $t \geq 0$, while in the second case can only consider times $t \in [0; T[$ with $T = (-2\mathrm{Re}(\delta)|p_0|^2)^{-1}$.

Evolved coherent state

We restrict ourselves to times t such that n_t is positive. Then, the Lagrangian subspace L_t can be parametrised by

$$l_t = S_t l_0 n_t^{-1/2} = n_t^{-1/2} \begin{pmatrix} p_0 \\ q_0 - 2\mathrm{i}\delta p_0 t \end{pmatrix}.$$

For the gain or loss factor β_t, we know that in the univariate setting, it holds $e^{\beta_t} = n_t^{-1/4}$.

Evolved excited states

For the evolution of excited state, it only remains to compute the recursion matrices M_t and $\widetilde{M}_t$, respectively. We have

$$\begin{aligned} M_t &= \tfrac{1}{2\mathrm{i}} n_t^{-1} (S_t l_0)^* \Omega S_t \bar{l}_0 = \tfrac{1}{2\mathrm{i}} n_t^{-1} \begin{pmatrix} p_0^* & q_0^* \end{pmatrix} \begin{pmatrix} 4\mathrm{i}\mathrm{Re}(\delta)t & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \overline{p}_0 \\ \overline{q}_0 \end{pmatrix} \\ &= 2n_t^{-1}\mathrm{Re}(\delta)\overline{p}_0^2 t. \end{aligned}$$

Moreover, since n_t is a real number in one dimension,

$$n_t^{-1/2} q_t^{-1} \overline{q}_t \overline{n}_t^{-1/2} = n_t^{-1} \frac{\overline{q}_0 + 2\mathrm{i}\overline{\delta p_0} t}{q_0 - 2\mathrm{i}\delta p_0 t}$$

and

$$\widetilde{M}_t = M_t + n_t^{-1/2} q_t^{-1} \overline{q}_t \overline{n}_t^{-1/2} = n_t^{-1} \left(\mathrm{Re}(\delta)\overline{p}_0^2 t + \frac{\overline{q}_0 + 2\mathrm{i}\overline{\delta p_0} t}{q_0 - 2\mathrm{i}\delta p_0 t} \right)$$

We illustrate the dynamics of the heat equation, i.e. $\delta = 1$, in one dimension. The fundamental solution of the heat equation is known to be a normalised Gaussian given by

$$\varphi(x,t) = (4\pi t)^{-n/2} e^{-|x|^2/(4t)},$$

for $t > 0$ and $\varphi(x,t) = 0$ otherwise.

Hence, we take the standard Gaussian, i.e. $l_0 = (\mathrm{i}, 1)^T$ as initial value and compare the dynamics of the coherent state $\widehat{\mathcal{U}}(t)\varphi_0(l_0)$ and the excited state $\widehat{\mathcal{U}}(t)\varphi_2(l_0)$ in Figure 23. We find that the coherent state φ_0 is slowly spreading over time, while the excited state tends to the coherent state.

11.3. Brownian motion

In this section we will have a closer look at the random motion of particles that causes diffusion. We concern a large particle, the Brownian particle, that is surrounded by a medium containing smaller particles, the classical example R. Brown studied in 1827 are pollen in a liquid. Due to collisions with small particles the Brownian particle

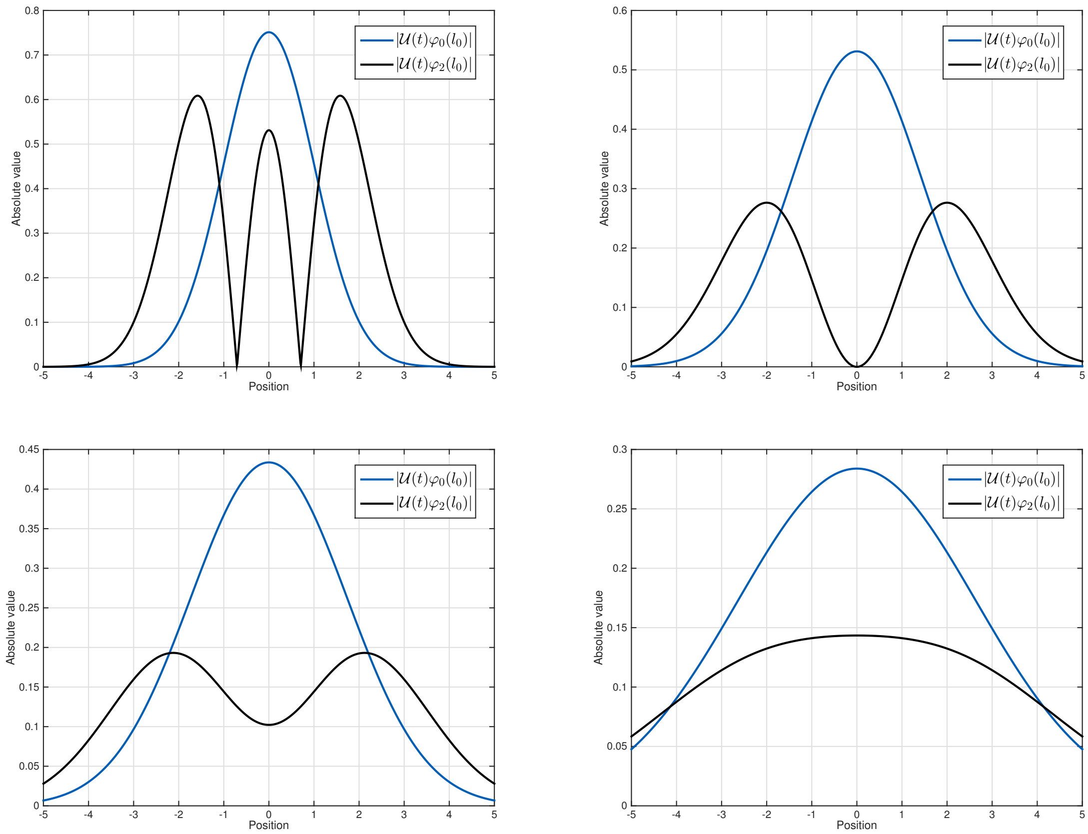

Figure 23.: Absolute values of the wave packets $\widehat{\mathcal{U}}(t)\varphi_0(l_0)$ and $\widehat{\mathcal{U}}(t)\varphi_2(l_0)$ starting from $l_0 = (\mathrm{i}, 1)^T$ at time $t = 0$ (upper left), $t = 0.5$ (upper right), $t = 1$ (lower left) and $t = 3$ (lower right) for $\delta = 1$.

moves, however, one cannot predict the exact trajectory of the particle since the interaction is random, we obtain a stochastic process, see [Hid80, §2].

The first to describe this phenomena mathematically was Einstein in 1905, see [Ein05]. Let $q \in \mathbb{R}^n$ denote the position of the particle and $m \in \mathbb{R}$ its mass, then the motion of the particle is described by

$$m\ddot{q} + m\gamma\dot{q} + V'(q) = \sigma^2 W(t),$$

see [BH02, p. 5.2.1]. This equation is obtained if we assume that the force acting on the particle is on one hand given by an external potential V and on the other hand caused by the friction with the environment that is proportional to the momentum $p = m\dot{q} \in \mathbb{R}^n$. A particle that is for example moving to the right will be hit by more particles from the right than from the left, see [UO30, §1].

The uncertainty is modelled by a Wiener process $W(t)$ and the *diffusion coefficient*,

$$\sigma^2 = 2m\gamma k_B T,$$

where k_B denotes the Boltzmann constant and T the temperature in the system, see [Lin76a, §].

Definition 11.1 — Wiener process. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. A map

$$W : \mathbb{R}_0^+ \mapsto [0;1]$$

is called a *Wiener process* if

1. $W(0) = 0$,
2. $t \to W(t)$ is continuous,
3. for all $0 \leq t_0 < t_1 < \ldots < t_l$ the differences $W(t_l) - W(t_{l-1})$, $W(t_{l-1}) - W(t_{l-2}), \ldots$ are independent and normally distributed with

$$\mathbb{E}(W(t_j) - W(t_{j-1})) = 0 \quad \text{and} \quad \mathbb{E}(W(t_j) - W(t_{j-1}))^2 = t_j - t_{j-1},$$

see [BS96, §4.1].

Using Newton's second law of motion $p = m\dot{q}$, we can split the second-order differential equation into two first order equations. The motion of the particle is governed by the *Langevin equations*, see also [BH02, §5.2.1],

$$\begin{aligned} \partial_t p &= -\gamma p - V'(q) + \sigma^2 W(t), \\ \partial_t q &= \tfrac{1}{m} p. \end{aligned} \tag{11.3}$$

The density of a Brownian particle then satisfies the diffusion equation discussed in the previous sections parametrised by the *friction coefficient* γ. Denoting a Hamiltonian

$$\mathcal{H}(p,q) = \tfrac{1}{2m} p^2 + V(q), \tag{11.4}$$

we can rewrite the Langevin equations as

$$\begin{aligned} \partial_t p &= -\partial_q \mathcal{H}(p,q) - \gamma p + \sigma^2 W(t), \\ \partial_t q &= \partial_p \mathcal{H}(p,q). \end{aligned}$$

We will reproduce the idea of Lindblad in [Lin76a] here who used that the phase space volume is due to the friction not preserved and thus modelled a quantum Brownian particle with an open system and obtained a type of Lindblad master equation we discussed in Chapter 10.

Analogously to [UO30] Lindblad takes expectation values of (11.3) and therefore deduced for the average position and momentum

$$\begin{aligned} \partial_t p &= -\gamma p - V'(q), \\ \partial_t q &= \tfrac{1}{m} p, \end{aligned}$$

where he formally replaced p by $\mathbb{E}(p)$ and q by $\mathbb{E}(q)$. If the potential V is at most linear in q, these equations can be rewritten as a first order differential equation and associated with a Lindblad equation. Analogously to [Lin76a] we assume that

$$V(q) = \tfrac{m\omega^2}{2} q^2$$

for some $\omega \in R$. By invoking his previous findings for the generators of quantum dynamical semigroups in [Lin76b], Lindblad was able to show that the propagation of the probability density $\rho = \rho(p, q, t)$ of p and q can be described by an Lindblad equation,

$$\mathrm{i}\varepsilon\, \partial_t \hat{\rho} = \left[\widehat{\mathcal{H}}, \hat{\rho}\right] + \tfrac{\mathrm{i}}{2} \sum_{j=1}^{2} 2\hat{\mathcal{L}}_j \hat{\rho} \hat{\mathcal{L}}_j^* - \hat{\mathcal{L}}_j^* \hat{\mathcal{L}}_j \hat{\rho} - \hat{\rho} \hat{\mathcal{L}}_j^* \hat{\mathcal{L}}_j,$$

with quadratic, internal Hamiltonian

$$\mathcal{H}(p, q) = \tfrac{1}{2}\left(\tfrac{1}{m}|p|^2 + \tfrac{\gamma}{2}(p^T q + q^T p) + m\omega^2 |q|^2\right),$$

and two linear Lindblad terms,

$$\mathcal{L}_1(p, q) = -\gamma p - m\omega^2 q, \qquad \mathcal{L}_2(p, q) = \tfrac{1}{m} p,$$

see [Lin76a, §3]. It is a well-known result that considering the density phase space probability distribution $\rho(p, q, t)$ of a Brownian particle leads to a Fokker-Planck equation. After examining the dynamics of a Brownian particle in a simple system in the next chapter, we will study the relation between the Lindblad equation and the Fokker-Planck equation in more detail.

11.4. Example: Simplified Brownian motion

Since an explicit computation of the Brownian motion gets very extensive due to the exponential matrices, we only examine a special case stated also in [BH02, §5.3.3]. We stress that although the explicit calculations are involving, one can easily solve the general case numerically with the formulas introduced in Chapter 10.

We assume that the Brownian particle has mass $m = 1$ and is free, i.e. there is no potential V. Moreover, we neglect the friction, i.e. $\gamma = \omega = 0$. Even though this model seems very simple, the calculations are still illustrative. Due to Lindblad's findings we consider in the univariate case the Hamiltonian

$$\widehat{\mathcal{H}} = \tfrac{1}{2}\hat{p}^2, \qquad H = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

and the Lindblad coupling

$$\hat{\mathcal{L}}_1 = \hat{p}, \quad \ell_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad L = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}.$$

Since the Lindblad terms are real, we will find a non-dissipative system and thus the wavepackets will not tend to steady state.

As initial state we choose the standard coherent state,

$$L_0 = \operatorname{span}\{l_0\}, \qquad l_0 = \begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} \in \mathbb{C}^2,$$

with symplectic metric $G = \mathrm{Id}_2$.

Linearised flow

The integral term here contains polynomials. We have

$$-\Omega H = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad e^{-\Omega H t} = \mathrm{Id}_2 - \Omega H t = \begin{pmatrix} 1 & 0 \\ -t & 1 \end{pmatrix}.$$

and $e^{H\Omega t} = (e^{-\Omega H t})^R$. Since $\operatorname{Im}(L) = 0$,

$$I_t = \int_0^t e^{-\Omega H \tau} \operatorname{Re}(L)\, e^{H\Omega\tau}\, d\tau = \int_0^t \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} d\tau = \begin{pmatrix} 0 & 0 \\ 0 & -t \end{pmatrix}$$

and the linearised flow is given by

$$S_t = \begin{pmatrix} e^{H\Omega t} & 0 \\ \mathrm{i} e^{\Omega H t} I_t & e^{\Omega H t} \end{pmatrix}.$$

Normalisation

Moreover, a direct computation yields for phase space frame

$$\mathcal{P} = \begin{pmatrix} -\Omega \bar{l}_0 & \Omega l_0 \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ \mathrm{i} & \mathrm{i} \end{pmatrix}$$

and accordingly for the normalisation

$$N_t = \mathrm{Id}_2 - \mathcal{P}^* I_t \mathcal{P} = \begin{pmatrix} 1+t & t \\ t & 1+t \end{pmatrix}.$$

The eigenvalues of N_t are 1 and $1+2t$, what displays that N_t is positive for all $t \geq 0$. We denote the determinant of N_t with $d_t = 1 + 2t$.

Evolved coherent state

For the evolved metric we revert to Lemma 10.3 and find

$$G_t = e^{H\Omega t} (\mathrm{Id}_2 - 2 I_t)^{-1} e^{-\Omega H t} = \frac{1}{d_t} \begin{pmatrix} (1+t)^2 & -t \\ -t & 1 \end{pmatrix}.$$

As we are considering a symmetric Wigner function, we can furthermore utilise for the gain or loss factor β_t,

$$\beta_t = \int_0^t \operatorname{tr}(\operatorname{Re}(L) G_\tau)\, d\tau + \gamma t = -\int_0^t \frac{1}{d_\tau}\, d\tau = -\tfrac{1}{2} \ln(1+2t),$$

and we receive a damping, $e^{\beta_t+\gamma t} = \sqrt{\frac{1}{1+2t}}$. Hence, our coherent state is slowly absorbed.

Evolved excited states

For the recursion matrix we can also draw back on the simpler formula and find that it can similarly as the metric be expressed in terms of d_t,

$$\mathcal{M}_t = (2N_t^{-1} - \mathrm{Id}_2)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{d_t}\begin{pmatrix} -2t & 1 \\ 1 & -2t \end{pmatrix},$$

So, we can state for the behaviour of the recursion matrix,

$$\mathcal{M}_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{M}_t \to \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

as $t \to \infty$. Comparing these findings to the results in Chapter 5 shows that we move from a factorisation in Laguerre polynomials to a complex-scaled factorisation into Hermite polynomials. Additionally, we also have keep track of the rotation. We evaluate the polynomials at the grid $N_t^{-1/2}\mathcal{Q}_t^{-1}z = \mathcal{Q}^{-1}(\mathrm{Id}_2 - 2I_tG)^{-1}e^{-\Omega Ht}z$ where

$$(\mathrm{Id}_2 - 2I_tG)^{-1}e^{-\Omega Ht} = \frac{1}{d_t}\begin{pmatrix} 1+2t & 0 \\ -t & 1 \end{pmatrix}.$$

Figure 24 displays the evolution of $\mathcal{W}_{(3,2)}(\mathcal{Z})$. One can nicely see that the circular structure that comes from the Laguerre polynomials vanishes and develops more to a grid. Along that way, the wave packet is damped and due to the rotation the portion in p-direction decreases, the wave packet is stretch in the direction of q.

11.5. Fokker-Planck equation

Let us again regard a Brownian particle whose motions is determined by the Langevin equations (11.3) and the Hamiltonian $\mathcal{H}$ defined in (11.4). Then, the probability density $\rho = \rho(p, q, t)$ satisfies

$$\partial_t\rho = \{\mathcal{H}, \rho\} + \gamma\partial_p(p\rho) + \tfrac{\sigma^2}{2}\partial_p^2\rho,$$

see [BH02, Eq. (5.41)]. If we once more take $V(q) = \frac{m\omega^2}{2}q^2$ and replace the Poisson bracket by derivatives, we find that

$$\partial_t\rho = \tfrac{\sigma^2}{2}\partial_p^2\rho + \begin{pmatrix} p & q \end{pmatrix}\begin{pmatrix} \gamma & -\frac{1}{m} \\ m\omega^2 & 0 \end{pmatrix}\begin{pmatrix} \partial_p\rho \\ \partial_q\rho \end{pmatrix} + \gamma\rho.$$

Comparing these equations with the general quadratic Weyl-operator given in Lemma 8.2 and the Hamiltonian that defines Lindblad equation in Proposition 10.2 emphasises Lindblad's choice

$$\mathcal{H}(p, q) = \tfrac{1}{2}\left(\tfrac{1}{m}|p|^2 + \tfrac{\gamma}{2}(p^Tq + q^Tp) + m\omega^2|q|^2\right),$$

however, as he takes averages the coefficient σ^2 does not appear in his calculations.

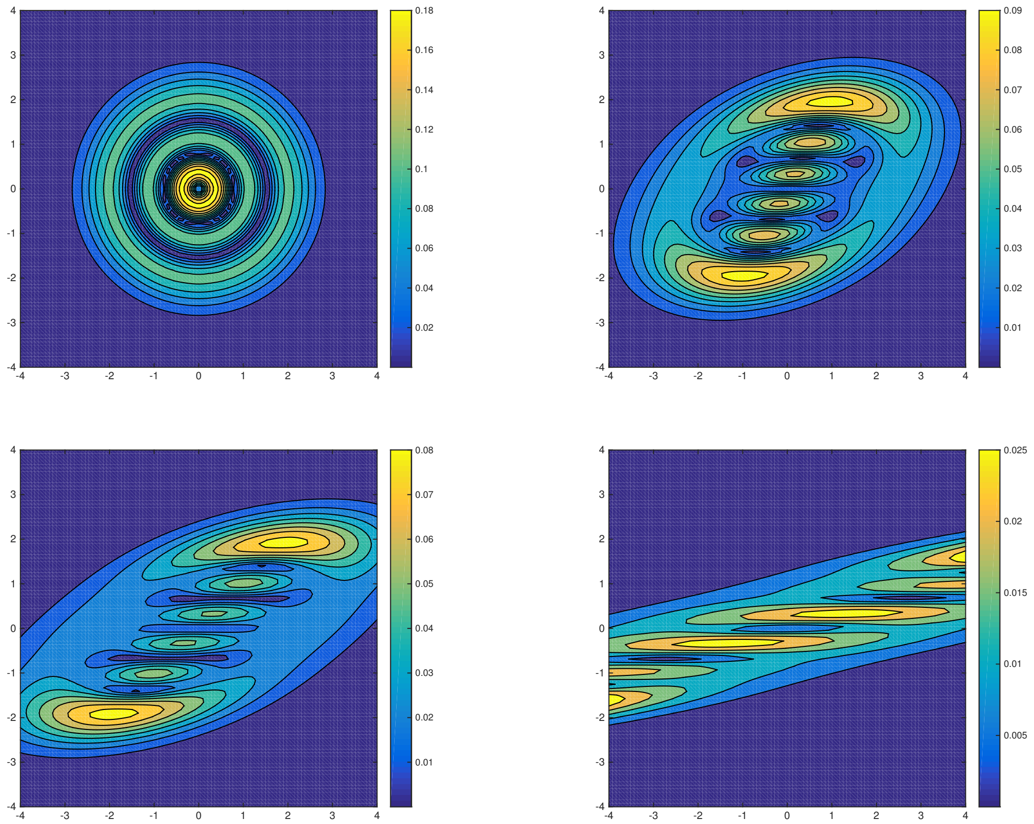

Figure 24.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\mathcal{W}_{(3,2)}(\mathcal{Z})$ at time $t = 0$ (upper left), $t = 0.5$ (upper right), $t = 1$ (lower left) and $t = 4$ (lower right)

In this section we want to take a more general point of view and consider a one-dimensional Fokker-Planck equation for a distribution function $\rho = \rho(x,t)$ of the form

$$\partial_t \rho(x,t) = -\partial_x \left(a(x,t)\rho(x,t)\right) + \partial_x^2 \left(d(x,t)\rho(x,t)\right), \tag{11.5}$$

where $x \in \mathbb{R}$ and $a, d : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ are two twice differentiable functions , see [Ris84, §1.2.2]. The function a thereby models the drift, d the diffusion. This abstract equation was introduced by Fokker in [Fok14] and proven by Planck in [Pla17]. For a historical overview see also [Kam97].

It is known that in one dimension, the Fokker-Planck equation can be written as a Schrödinger equation with complex time-scaling resp. complex Hamiltonian if the diffusion is constant, see [Ris84, §5.4]. To obtain moreover a quadratic operator, we need in addition a linear drift a, i.e.

$$a(x,t) = \alpha x, \quad d(x,t) = \delta \qquad \alpha, \delta \in \mathbb{R}.$$

Then, we can rewrite the Fokker-Planck equation (11.5) as

$$\begin{aligned}\partial_t \rho(x,t) &= -\alpha\rho(x,t) - \alpha x \partial_x \rho(x,t) + \delta \partial_x^2 \rho(x,t) \\ &= -\delta \hat{p}^2 \rho(x,t) + \tfrac{\mathrm{i}}{2}\alpha(\hat{p}\hat{q} + \hat{q}\hat{p})\rho(x,t) - \tfrac{1}{2}\alpha\rho(x,t).\end{aligned}$$

Hence, we found a Schrödinger equation with a complex, quadratic Hamiltonian and a constant term,

$$\mathrm{i}\partial_t \rho(x,t) = \left(\widehat{\mathcal{H}} + \hat{\gamma}\right)\rho(x,t), \qquad \widehat{\mathcal{H}} = \tfrac{1}{2}\hat{z}^T \begin{pmatrix} -2\mathrm{i}\delta & \alpha \\ \alpha & 0 \end{pmatrix} \hat{z}$$

and $\gamma = -\frac{\mathrm{i}}{2}\alpha$. This approach can be easily generalised to multi-dimensions, again if we consider a constant diffusion and a linear drift.

11.6. Example: Black & Scholes model

To finish our chapter about further applications we choose an example from a completely different area and investigate the Black and Scholes model from financial mathematics, see [Pas05, §1] or [BS73].

The price of an option $\rho = \rho(x,t)$ depending on the stock price $x \in \mathbb{R}$ and the time $t \in \mathbb{R}$ can, in a given area, be derived as the solution to

$$\partial_t \rho = -\tfrac{1}{2}\sigma^2 \partial_x^2 \rho - rx\partial_x \rho + r\rho \tag{11.6}$$

where $r \in \mathbb{R}$ denotes the interest rate and σ the standard deviation of the stock. We stress here that this equation can not exactly be written in the form (11.5), since it requires an additional constant term, but can be solved with equivalent methods.

We first bring (11.6) in the form of a Schrödinger equation with quadratic Hamiltonian,

$$\begin{aligned}\mathrm{i}\partial_t \rho &= -\tfrac{\mathrm{i}}{2}\left(\sigma^2\partial_x^2 + rx\partial_x + r\partial_x x - 3r\right)\rho = \tfrac{1}{2}\left(\mathrm{i}\sigma^2\hat{p}^2 + r\hat{q}\hat{p} + r\hat{p}\hat{q} - 3\mathrm{i}r\right)\rho \\ &= \left(\tfrac{1}{2}\hat{z}^T H\hat{z} + \hat{\gamma}\right)\rho\end{aligned}$$

with the constant term $\gamma = \frac{3\mathrm{i}}{2}r$ and the complex, symmetric matrix

$$H = \begin{pmatrix} \mathrm{i}\sigma^2 & r \\ r & 0 \end{pmatrix}.$$

The above matrix obviously has a positive semi-definite imaginary part, however, we assume that the time evolution operator exists for times $0 \le t < T$, due to its close connection to the Fokker-Planck equation. We use again the standard Hermite functions parametrised by

$$L_0 = \operatorname{span}\{l_0\}, \qquad l_0 = \begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} \in \mathbb{C}^2,$$

as ansatz functions. The corresponding symplectic metric is $G = \mathrm{Id}_2$.

Linearised flow

For $S_t = e^{\Omega H t}$ we use that

$$\Omega H = \begin{pmatrix} -r & 0 \\ \mathrm{i}\sigma^2 & r \end{pmatrix}$$

satisfies $(\Omega H)^{2k} = r^{2k}\mathrm{Id}_2$ and $(\Omega H)^{2k+1} = r^{2k}\Omega H$ for all $k \geq 0$. Hence, if $r \neq 0$,

$$S_t = \sum_{k=0}^{\infty} \tfrac{1}{(2k)!}(rt)^{2k} \cdot \mathrm{Id}_2 + \tfrac{1}{r}\sum_{k=0}^{\infty} \tfrac{1}{(2k+1)!}(rt)^{2k+1} \cdot \Omega H = \cosh(rt) \cdot \mathrm{Id}_2 + \tfrac{1}{r}\sinh(rt) \cdot \Omega H.$$

and

$$\begin{aligned} S_t^* \Omega S_t &= \left(\cosh(rt) \cdot \mathrm{Id}_2 + \tfrac{1}{r}\sinh(rt) \cdot \overline{H}\Omega^T\right)\Omega\left(\cosh(rt) \cdot \mathrm{Id}_2 + \tfrac{1}{r}\sinh(rt) \cdot \Omega H\right) \\ &= \cosh^2(rt) \cdot \Omega - \tfrac{2\mathrm{i}}{r}\cosh(rt)\sinh(rt) \cdot \mathrm{Im}(H) + \tfrac{1}{r^2}\sinh^2(rt) \cdot \overline{H}\Omega H. \end{aligned}$$

Normalisation

Calculating $l_0^* \mathrm{Im}(H) l_0 = \sigma^2$ and

$$l_0^* \overline{H}\Omega H l_0 = \begin{pmatrix} -\mathrm{i} & 1 \end{pmatrix} \begin{pmatrix} 2\mathrm{i}r\sigma^2 & r^2 \\ -r^2 & 0 \end{pmatrix} \begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} = 2\mathrm{i}r(\sigma^2 - r)$$

we find for the normalisation

$$\begin{aligned} n_t = \tfrac{1}{2\mathrm{i}} l_0^* S_t^* \Omega S_t l_0 &= \cosh^2(rt) - \tfrac{\sigma^2}{r}\sinh(rt)\cosh(rt) + \tfrac{1}{r}(\sigma^2 - r)\sinh^2(rt) \\ &= 1 + \tfrac{\sigma^2}{r}\sinh(rt)\left(\sinh(rt) - \cosh(rt)\right) \\ &= 1 + \tfrac{\sigma^2}{2r}\left(e^{-2rt} - 1\right). \end{aligned}$$

In particular, the normalisation is positive for all times $t \geq 0$ if $2r > \sigma^2$ and otherwise for all times $t \in [0; T[$ with $T = -\frac{1}{2r}\ln(1 - \frac{2r}{\sigma^2})$.

Evolved coherent state

So far, we didn't need to take the constant γ into account, this changes if we determine the damping factor β_t. For the evolved Lagrangian frame we first note that

$$l_t = \begin{pmatrix} p_t \\ q_t \end{pmatrix} = S_t l_0 n_t^{-1/2} = n_t^{-1/2} \begin{pmatrix} \mathrm{i}(\cosh(rt) - \sinh(rt)) \\ \cosh(rt) + (1 - \frac{\sigma^2}{r})\sinh(rt) \end{pmatrix}.$$

Inserting the ansatz

$$\varphi_0(x,t) = \pi^{-1/4} c_t \cdot q_t^{-1/2} e^{\frac{\mathrm{i}}{2\varepsilon} b_t x^2}$$

with $b_t = p_t q_t^{-1}$ into (11.6) yields

$$\begin{aligned} \frac{\dot{c}_t}{c_t} &= \tfrac{1}{2}(\dot{q}_t q_t^{-1} - \mathrm{i}\sigma^2 b_t) + r \\ \dot{b}_t &= -\mathrm{i}\sigma^2 b_t^2 - 2r b_t. \end{aligned}$$

One can directly show that the second equation holds true for

$$b_t = \mathrm{i}\frac{\cosh(rt) - \sinh(rt)}{\cosh(rt) + (1 - \frac{\sigma^2}{r})\sinh(rt)}.$$

For the first equation we first look at the evolution of the Lagrangian frame $Z_t =$

$S_t Z_0 N_t^{-1/2}$,

$$\dot{Z}_t = \Omega H Z_t - \tfrac{1}{2} Z_t N_t^{-1/2} \dot{N}_t N_t^{-1/2} = \Omega H Z_t + \tfrac{1}{2} Z_t Z_t^* \mathrm{Im}(H) Z_t$$

where we used that $\dot{N}_t = -Z_0^* S_t^* \mathrm{Im}(H) S_t Z_0$, see Proposition 9.2. Hence, for our Hamiltonian we find

$$\dot{q}_t q_t^{-1} = \left(\mathrm{i}\sigma^2 p_t + r q_t + \tfrac{1}{2}\sigma^2 q_t p_t^* p_t\right) q_t^{-1} = \mathrm{i}\sigma^2 b_t + r + \tfrac{1}{2}\sigma^2 |p_t|^2$$

since we consider the one-dimensional setting. This implies

$$\frac{\dot{c}_t}{c_t} = \tfrac{3}{2} r + \frac{1}{4}\sigma^2 n_t^{-1} (\cosh(rt) - \sinh(rt))^2 = \tfrac{3}{2} r - \frac{1}{4}\frac{\dot{n}_t}{n_t}$$

and thus $c_t = n_t^{-1/4} \cdot e^{\frac{3}{2} rt}$, what displays again the splitting into the dissipation factor $e^{\gamma t} = e^{\frac{3}{2} rt}$ and our usual damping factor $e^{\beta_t} = n_t^{-1/4}$.

Evolved excited states

For the recursion matrix for the Black-Scholes-Model shows a particularly nice behaviour. Similarly to the normalisation we deduce

$$l_0^* \mathrm{Im}(H) \bar{l}_0 = -\sigma^2, \qquad l_0^* \overline{H} \Omega H \bar{l}_0 = -2\mathrm{i} r \sigma^2.$$

Using moreover that $l_0^* \Omega \bar{l}_0 = 0$, we find

$$\tfrac{1}{2\mathrm{i}} l_0^* S_t^* \Omega S_t \bar{l}_0 = \tfrac{\sigma^2}{r} n_t^{-1} \sinh(rt) \left(\cosh(rt) - \sinh(rt)\right) = n_t - 1$$

and $M_t = \frac{1}{2\mathrm{i}} n_t^{-1} l_0^* S_t^* \Omega S_t \bar{l}_0 = 1 - n_t^{-1}$. If we regard once again q_t and n_t we notice that both are real for all times $t \geq 0$. A real matrix Q always corresponds to a factorisation in Hermite polynomials, see Theorem 4.2. Here, this means that our polynomials stay Hermite polynomials over time, what also follows from

$$\widetilde{M}_t = M_t + n_t^{-1/2} q_t^{-1} \overline{q}_t \overline{n}_t^{-1/2} = 1 - n_t^{-1} + n_t^{-1} = 1.$$

Figure 25 illustrates the evolution of the coherent state $\varphi_0(l_0)$ and the excited state $\varphi_2(l_0)$ for a interest rate of $r = 0.75$ and a standard deviation $\sigma = 1$. One can nicely see that in contrast to the evolution for the Brownian motion in Figure 24 the excited state preserves its form, both states are growing due to c_t.

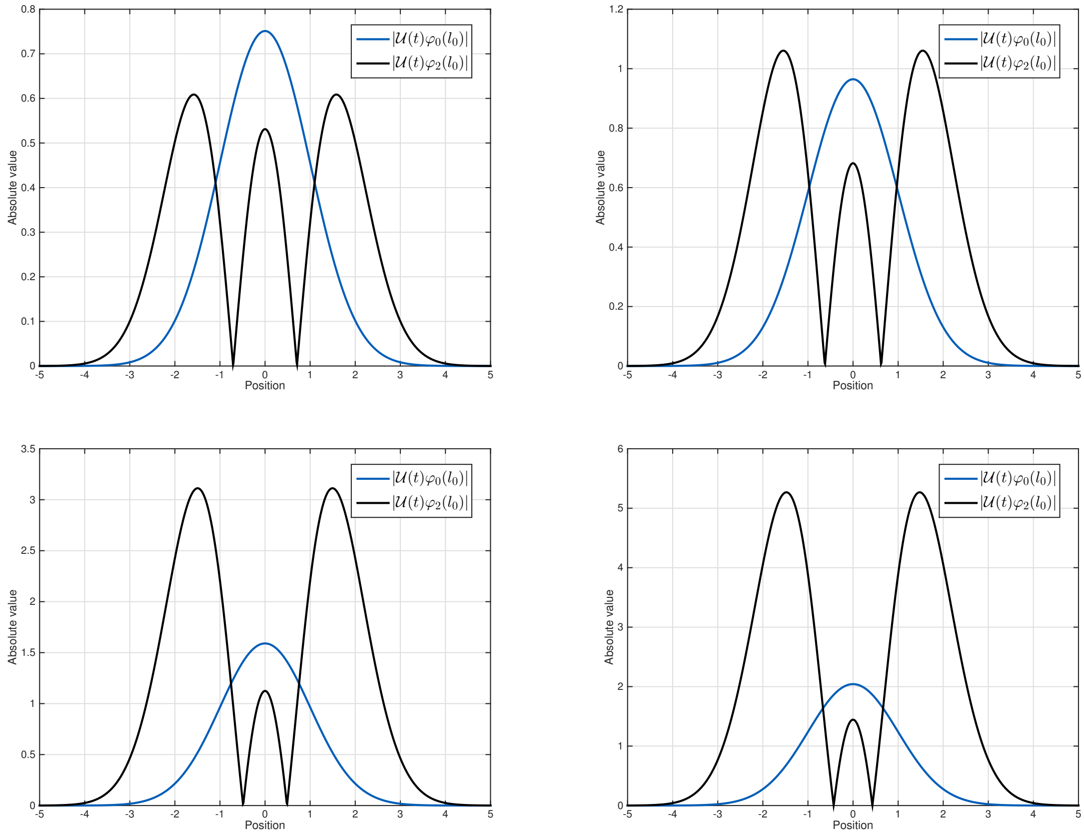

Figure 25.: Contour plots of the absolute values of $\widehat{\mathcal{U}}(t)\varphi_0(l_0)$ and $\widehat{\mathcal{U}}(t)\varphi_2(l_0)$ at time $t = 0$ (upper left), $t = 0.25$ (upper right), $t = 0.75$ (lower left) and $t = 1$ (lower right) for $r = 0.75$ and $\sigma = 1$.

A. Weyl calculus

In this thesis several proofs are based on calculations with Weyl-quantised operators. These steps are, however, more technical and already well summarised in the literature, see for example [Zwo11, §4] or [Fol89, §2.1]. In order to avoid confusion caused by different notations and to make this work self-contained, we restate the fundamentals of Weyl calculus in this appendix.

We start with recalling the definition of a Weyl-quantised operator with semiclassical scaling $\varepsilon > 0$, see Equation (4.1).

Definition A.1 — Weyl operator. Let $a \in \mathcal{S}(\mathbb{R}^{2n})$. We define the operator $\hat{a} = \mathrm{op}_\varepsilon[a]$ acting on $\mathcal{S}(\mathbb{R}^n)$ via

$$(\mathrm{op}_\varepsilon[a]\psi)(x) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} a(\xi, \tfrac{1}{2}(x+y)) e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)} \psi(y)\, dy d\xi, \quad \forall \psi \in \mathcal{S}(\mathbb{R}^n)$$

and call a the symbol of $\hat{a}$.

A formal approach to obtain this definition starts with the Fourier transform $\mathcal{F}^\varepsilon a$ of $a \in \mathcal{S}(\mathbb{R}^{2n})$,

$$(\mathcal{F}^\varepsilon a)(w) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} a(z) e^{-\frac{\mathrm{i}}{\varepsilon} w^T z}\, dz, \quad w \in \mathbb{R}^{2n}.$$

We consider the vector-valued operators $\hat{q}$ and $\hat{p}$ with

$$(\hat{q}_j \varphi)(x) = x_j \varphi_x \quad \text{and} \quad (\hat{p}_j \varphi)(x) = -\mathrm{i}\varepsilon \partial_{x_j} \varphi(x) \quad \text{for} \quad j = 1, \dots, n$$

acting on distributions or functions, respectively. One then associates an operator $a(\hat{p}, \hat{q})$ to $a(p,q)$ such that the symbols $\hat{q}_j$ and $\hat{p}_j$ correspond to the coordinates of a, i.e. we reverse the idea shortly described at the beginning of Section 3.1. In Weyl's original work [Wey27] he considered exponential functions and identified $a(z) = e^{\frac{\mathrm{i}}{\varepsilon} w^T z}$, $w \in \mathbb{R}^{2n}$, with the operator

$$\hat{a} = a(\hat{z}) = e^{\frac{\mathrm{i}}{\varepsilon} w^T \hat{z}} \quad \text{where} \quad \hat{z} = \begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix},$$

see also [Fol89, §2.1]. The action of this operator can be explicitly determined, see for example [Zwo11, Theorem 4.7].

Lemma A.1 Let $w = (p, q) \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $\psi \in \mathcal{S}(\mathbb{R}^n)$. Then,

$$e^{\frac{\mathrm{i}}{\varepsilon} w^T \hat{z}} \psi(x) = e^{\frac{\mathrm{i}}{\varepsilon} q^T (x + p/2)} \psi(x + p), \qquad x \in \mathbb{R}^n.$$

Proof. We consider the partial differential equation

$$-\mathrm{i}\varepsilon\, \partial_t \psi(x,t) = (w^T \hat{z}) \psi(x,t), \quad \psi(x,0) = \psi_0(x).$$

On the one hand, the formal solution to this equation reads $\psi(x,t) = e^{\frac{\mathrm{i}}{\varepsilon}tw^T\hat{z}}\psi_0(x)$. On the other hand, one can verify by a direct calculation that

$$\psi(x,t) = e^{\frac{\mathrm{i}}{\varepsilon}tq^Tx+\frac{\mathrm{i}}{2\varepsilon}t^2p^Tq}\psi_0(x+tp)$$

is the unique solution of this PDE. Thus, evaluating at $t = 1$ yields the result. ■

The formula we deduced for $e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}$ looks quite similar to the Heisenberg-Weyl operator introduced in (4.10). Indeed, it holds

$$T(z) = e^{-\frac{\mathrm{i}}{\varepsilon}z^T\Omega\hat{z}}$$

for $z \in \mathbb{R}^{2n}$.

Moreover, with the determination of the operator of an exponential function, we are now able to associate an operator $\hat{a}$ with every Schwartz function $a \in \mathcal{S}(\mathbb{R}^{2n})$ via

$$\hat{a} = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}}(\mathcal{F}^\varepsilon a)(w)e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,dw. \tag{A.1}$$

We will show in the following that this operator is equivalent to the Weyl-quantisation we stated in the beginning. First of all, we note that operators of this type are known to map Schwartz functions onto tempered distributions, i.e. $\hat{a} : \mathcal{S}(\mathbb{R}^n) \mapsto \mathcal{S}*(\mathbb{R}^n)$, see for example [Fol89, Theorem 1.30]. Then, we aim to write $\hat{a}$ as integral operator, i.e. in the form

$$\hat{a}\varphi(x) = \int_{\mathbb{R}^n} K_a(x,y)\varphi(y)\,dy$$

where $K_a \in \mathcal{D}'(\mathbb{R}^{2n})$ denotes the emphkernel of $\hat{a}$. This representation, that is also more convenient for applications, exists due to the Schwartz kernel theorem, see [Hör83, Theorem 5.2.1].

Lemma A.2 Let $f \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$ and define the operator $\hat{f}$ as Bochner integral

$$\hat{f} = \int_{\mathbb{R}^{2n}} f(w)e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,dw.$$

Then, the kernel of $\hat{f}$ is given by

$$K_f(x,y) = (2\pi\varepsilon)^{n/2}((\mathcal{F}_2^\varepsilon)^{-1}f)(y-x,\tfrac{1}{2}(y+x))$$

for $x, y \in \mathbb{R}^n$ where $\mathcal{F}_2^\varepsilon$ denotes the Fourier transform in the second component.

Proof. The same result can be found in [Fol89, Eq. (1.29)]. With the previous lemma we find for all $\psi \in \mathcal{S}(\mathbb{R}^n)$

$$(\hat{f}\psi)(x) = \int_{\mathbb{R}^{2n}} f(p,q)e^{\frac{\mathrm{i}}{\varepsilon}q^T(x+p/2)}\psi(x+p)\,dpdq = \int_{\mathbb{R}^{2n}} f(y-x,q)e^{\frac{\mathrm{i}}{2\varepsilon}q^T(y+x)}\psi(y)\,dydq,$$

where we substituted $y = x + p$. Thus, by definition

$$K_f(x,y) = \int_{\mathbb{R}^n} f(y-x,q)e^{\frac{\mathrm{i}}{2\varepsilon}q^T(y+x)}\,dq = (2\pi\varepsilon)^{n/2}((\mathcal{F}_2^\varepsilon)^{-1}f)(y-x,\tfrac{1}{2}(y+x)).$$

■

Applying this result to our definition (A.1) we find for the kernel of $\hat{a}$,

$$K_a(x,y) = (2\pi\varepsilon)^{-n/2}(\mathcal{F}_1^\varepsilon a)(y-x,\tfrac{1}{2}(y+x)) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^n} a(\xi,\tfrac{1}{2}(y+x))e^{-\frac{\mathrm{i}}{\varepsilon}\xi^T(y-x)}\,d\xi,$$

what is consistent with the Weyl-quantisation we stated in the beginning. Thus, the Weyl-quantisation can be equivalently expressed in terms of the Fourier transform of a and we will make use of this in the following computations.

We proceed with stating some important properties of the Weyl-quantisation we make use of in this thesis. To start with we formalise our observation for the kernel of $\hat{a}$, see also [Gos10, Proposition 205].

Proposition A.1 — Kernel and symbol. Let $a \in \mathcal{S}(\mathbb{R}^n)$ and $\hat{a} = \mathrm{op}_\varepsilon[a]$. The kernel of $\hat{a}$ and the symbol a are related via

$$K_a(x,y) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^n} a(\xi,\tfrac{1}{2}(x+y))e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)}\,d\xi$$

and

$$a(\xi,x) = \int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}\xi^T y}K_a(x+\tfrac{y}{2},x-\tfrac{y}{2})\,dy.$$

So far, we focused on Weyl-operators associated with Schwartz-functions and interpreted $\hat{a}$ as a map from $\mathcal{S}(\mathbb{R}^n)$ to its dual space $\mathcal{S}^*(\mathbb{R}^n)$. However, for this symbol class, we can study $\hat{a}$ in the more favourable function space $L^2(\mathbb{R}^n)$ due to the next theorem, see also [Zwo11, Theorem 4.21].

Theorem A.1 — L^2-boundedness. If the symbol a belongs to $\mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$, then

$$\mathrm{op}_\varepsilon[a] : L^2(\mathbb{R}^n) \mapsto L^2(\mathbb{R}^n)$$

is linear operator bounded independently of ε.

Proof. The proof is basically a reformulation of Schur's lemma, see [Shu87, Lemma 9.1]. Since $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$, we can follow from the previous proposition that there exist constants C_1 and C_2 such that

$$C_1 = \sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}|K_a(x,y)|\,dy < \infty, \qquad C_2 = \sup_{y\in\mathbb{R}^n}\int_{\mathbb{R}^n}|K_a(x,y)|\,dx < \infty.$$

Let $\varphi \in L^2(\mathbb{R}^n)$. Then,

$$\begin{aligned}\|\hat{a}\varphi\|^2 &= \int_{\mathbb{R}^{3n}} K_a(x,y)\overline{K_a(x,\xi)}\varphi(y)\overline{\varphi(\xi)}\,d(x,y,\xi)\\ &\le \int_{\mathbb{R}^{3n}} |K_a(x,y)||K_a(x,\xi)||\varphi(y)||\varphi(\xi)|\,d(x,y,\xi)\\ &\le \tfrac{1}{2}\int_{\mathbb{R}^{3n}} |K_a(x,y)||K_a(x,\xi)|(|\varphi(y)|^2+|\varphi(\xi)|^2)\,d(x,y,\xi)\end{aligned}$$

For the first integral, we estimate

$$\begin{aligned}\int_{\mathbb{R}^{3n}} |K_a(x,y)||K_a(x,\xi)||\varphi(y)|^2\,d(x,y,\xi) &\le C_1\int_{\mathbb{R}^{2n}} |K_a(x,y)||\varphi(y)|^2\,d(x,y)\\ &\le C_1C_2\int_{\mathbb{R}^n}|\varphi(y)|^2\,dy = C_1C_2\|\varphi\|^2\end{aligned}$$

and with a similar computation for the second integral $\|\hat{a}\varphi\|^2 \le C_1C_2\|\varphi\|^2$. ■

Nevertheless, in this thesis we in particular studied the quadratic operators, i.e. operators with a quadratic symbol $a(z) = \frac{1}{2}z^T Hz$ with $H \in C^{2n\times 2n}$. Clearly, quadratic forms are not Schwartz functions and we utilise the following definition from [Zwo11, §4.4] to extend the class of admissible symbols.

Definition A.2 — Order function. Let $\langle z\rangle := (1+|z|^2)^{1/2}$ for $z \in \mathbb{R}^{2n}$. A measurable function $m : \mathbb{R}^{2n} \mapsto (0;\infty)$ is called an *order function* if there exist constants c and k such that

$$m(w) \le c\langle z-w\rangle^k m(z)$$

for all $w, z \in \mathbb{R}^{2n}$. Given an order function m, we define the corresponding class of symbols as

$$S(m) = \{a \in C^\infty(\mathbb{R}^n)\,;\, \forall\alpha \in \mathbb{N}^n\, \exists c_\alpha > 0 : |\partial_z^\alpha a| \le c_\alpha m\}$$

and for $0 \le \delta \le \frac{1}{2}$

$$S_\delta(m) = \{a \in C^\infty(\mathbb{R}^n)\,;\, \forall\alpha \in \mathbb{N}^n\, \exists c_\alpha > 0 : |\partial_z^\alpha a| \le c_\alpha \varepsilon^{-\delta|\alpha|} m\}.$$

Common examples for order functions are $m(z) = 1$ or $m(z) = \langle z\rangle^k$ for $k \in \mathbb{N}$. In particular, we find that $a \in S(\langle z\rangle^k)$ if

$$|\partial_z^\alpha a(z)| \le c_\alpha\langle z\rangle^k, \qquad \forall\alpha \in \mathbb{N}^n.$$

and thus a polynomial of degree k in z is an element of $S(\langle z\rangle^k)$. This inequality is moreover equivalent to the assumption in [Fol89, Theorem 2.21].

Theorem A.2 — Quantisation of general symbols. Let m be an order function, $\delta \in [0;\frac{1}{2}]$ and $a \in S_\delta(m)$. Then,

$$\mathrm{op}_\varepsilon[a] : \mathcal{S}(\mathbb{R}^n) \mapsto \mathcal{S}(\mathbb{R}^n)$$

is a continuous linear transform.

Proof. In the literature there can be several proofs found for this theorem, for example

[Rob83, Theorem II-36] for a proof a based on a partition of unity or [Zwo11, Theorem 4.16] for a proof using partial integration. We briefly sketch the outline in [Hör94, Theorem 18.1.6] and first observe that for $a \in S(m)$, we restrict ourselves to the case $\delta = 0$ here, and $\varphi \in \mathcal{S}(\mathbb{R}^n)$ with $z = (\xi, y)$

$$
\begin{aligned}
|\mathrm{op}_\varepsilon[a]\varphi(x)| &= |(2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} a(\xi, \frac{1}{2}(x+y)) e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x-y)}\, d\xi\, \varphi(y)\, dy| \\
&\le \int_{\mathbb{R}^n} \sup_{\xi \in \mathbb{R}^n} |a(\xi, y)||\varphi(y)|\, dy \le \sup_{z \in \mathbb{R}^{2n}} |a(z)| \langle z \rangle^{-1} \int_{\mathbb{R}^n} \langle z \rangle |\varphi(y)|\, dy
\end{aligned}
$$

is bounded. Moreover, for $j = 1, \dots, n$

$$
\begin{aligned}
x_j \mathrm{op}_\varepsilon[a]\varphi &= \hat{q}_j \mathrm{op}_\varepsilon[a]\varphi = \mathrm{op}_\varepsilon[q_j \# a]\varphi = \left(\mathrm{op}_\varepsilon[q_j a(p,q)] + \tfrac{\mathrm{i}\varepsilon}{2} \mathrm{op}_\varepsilon[\partial_{p_j} a(p,q)]\right) \varphi, \\
\partial_{x_j} \mathrm{op}_\varepsilon[a]\varphi &= \tfrac{\mathrm{i}}{\varepsilon} \hat{p}_j \mathrm{op}_\varepsilon[a]\varphi = \mathrm{op}_\varepsilon[\tfrac{\mathrm{i}}{\varepsilon} p_j \# a]\varphi = \left(\tfrac{\mathrm{i}}{\varepsilon} \mathrm{op}_\varepsilon[p_j a(p,q)] + \tfrac{1}{2} \mathrm{op}_\varepsilon[\partial_{q_j} a(p,q)]\right) \varphi.
\end{aligned}
$$

Since $p_j a(p,q), q_j a(p,q), \partial_{p_j} a(p,q), \partial_{q_j} a(p,q) \in S(m)$ for $a \in S(m)$, the above estimate is valid and $x_j \cdot \mathrm{op}_\varepsilon[a]\varphi(x)$ and $\partial_{x_j} \mathrm{op}_\varepsilon[a]\varphi(x)$ are bounded for all $j = 1, \dots, n$. Thus, an iterative application shows $\mathrm{op}_\varepsilon[a]\varphi(x) \in \mathcal{S}(\mathbb{R}^n)$. If one wants to evade the Moyal product we formally only introduce in the following, one can obtain the above equations also with Definition A.1 and partial integration. ∎

In the following we will refer to all admissible functions $a \in S_\delta(m)$ for some order function m as symbols. Since we consider linear operator $\hat{a}$ defined on a dense subset of the Hilbert space $L^2(\mathbb{R}^n)$, we may also investigate their Hermitian adjoints.

We define the formal adjoint of an operator $\hat{a} : \mathcal{S}(\mathbb{R}^n) \mapsto \mathcal{S}(\mathbb{R}^n)$ by the identity

$$
\langle \hat{a}\varphi, \psi \rangle = \langle \varphi, \hat{a}^* \psi \rangle
$$

for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$, see [Gos10, §10.2.1].

Proposition A.2 — Adjoint. The adjoint $\hat{a}^*$ of a Weyl-operator $\hat{a}$ is the Weyl-operator with symbol $a^* = \overline{a}$, i.e.

$$
\hat{a}^* = \mathrm{op}_\varepsilon[\overline{a}]
$$

for all symbols a. In particular, $\hat{a}$ is self-adjoint if and only if a is a real function.

Proof. For this result we also refer to [Gos10, Proposition 212]. Let a be a symbol and $\hat{a} = \mathrm{op}_\varepsilon[a]$. With the Wigner relation (3.18) we find for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$,

$$
\langle \varphi, \hat{a}^* \psi \rangle = \int_{\mathbb{R}^n} \mathcal{W}^\varepsilon(\varphi, \psi)(z) a^*(z)\, dz
$$

and

$$
\langle \hat{a}\varphi, \psi \rangle = \overline{\langle \psi, \hat{a}\varphi \rangle} = \int_{\mathbb{R}^n} \overline{\mathcal{W}^\varepsilon(\psi, \varphi)(z) a(z)}\, dz = \int_{\mathbb{R}^n} \mathcal{W}^\varepsilon(\varphi, \psi)(z) \overline{a}(z)\, dz.
$$

∎

The last aim of this chapter is to give precise formulas for linear and quadratic symbols. To do so we first need to investigate the composition of two Weyl-operators $\mathrm{op}_\varepsilon[a]$ and $\mathrm{op}_\varepsilon[b]$. We again use the Fourier form of the Weyl-transform and start with the composition two exponential operators.

Lemma A.3 Let $w, l \in \mathbb{R}^{2n}$. Then,

$$e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}e^{\frac{\mathrm{i}}{\varepsilon}l^T\hat{z}} = e^{-\frac{\mathrm{i}}{2\varepsilon}w^T\Omega l}e^{\frac{\mathrm{i}}{\varepsilon}(w+l)^T\hat{z}}.$$

Proof. We denote $w = (p, q)$, $l = (p', q')$ and choose an arbitrary $\psi \in \mathcal{S}(\mathbb{R}^n)$. Then, we have by Lemma A.1 $e^{\frac{\mathrm{i}}{\varepsilon}(w+l)^T\hat{z}}\psi(x) = e^{\frac{\mathrm{i}}{\varepsilon}(q+q')^T(x+\frac{p+p'}{2})}\psi(x + (p + p'))$ and

$$\begin{aligned}
e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}e^{\frac{\mathrm{i}}{\varepsilon}l^T\hat{z}}\psi(x) &= e^{\frac{\mathrm{i}}{\varepsilon}q^T(x+\frac{p}{2})}e^{\frac{\mathrm{i}}{\varepsilon}q'^T(x+p+\frac{p'}{2})}\psi(x + p' + p)\\
&= e^{\frac{\mathrm{i}}{\varepsilon}q^T(x+\frac{p+p'}{2})-\frac{\mathrm{i}}{2\varepsilon}q^Tp'}e^{\frac{\mathrm{i}}{\varepsilon}q'^T(x+\frac{p+p'}{2})+\frac{\mathrm{i}}{2\varepsilon}q'^Tp}\psi(x + p' + p)\\
&= e^{\frac{\mathrm{i}}{2\varepsilon}(p^Tq'-q^Tp')}e^{\frac{\mathrm{i}}{\varepsilon}(w+l)^T\hat{z}}\psi(x).
\end{aligned}$$

■

The above lemma can also be found as part of [Zwo11, Theorem 4.7]. With the composition of the exponential operators we are now able to deduce the composition of arbitrary Weyl-operators via the Fourier representation, see also [Zwo11, Theorem 4.11].

Theorem A.3 — Composition of Weyl-operators. Let a, b be two suitable symbols. Then, $\mathrm{op}_\varepsilon[a]\mathrm{op}_\varepsilon[b] = \mathrm{op}_\varepsilon[a\#b]$ where

$$(a\#b)(z) = e^{\frac{\mathrm{i}\varepsilon}{2}\nabla_z^T\Omega\nabla_{z'}}(a(z)b(z')) \mid_{z=z'}, \quad z \in \mathbb{R}^{2n}.$$

We call $\#$ the *Moyal product* of a and b.

Proof. We first note that

$$\begin{aligned}
\mathrm{op}_\varepsilon[a]\mathrm{op}_\varepsilon[b] &= (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{4n}}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}e^{\frac{\mathrm{i}}{\varepsilon}l^T\hat{z}}\,dwdl\\
&= (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{4n}}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)e^{-\frac{\mathrm{i}}{2\varepsilon}w^T\Omega l}e^{\frac{\mathrm{i}}{\varepsilon}(w+l)^T\hat{z}}\,dwdl\\
&= (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{4n}}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(u-w)e^{-\frac{\mathrm{i}}{2\varepsilon}w^T\Omega u}e^{\frac{\mathrm{i}}{\varepsilon}u^T\hat{z}}\,dwdu,
\end{aligned}$$

i.e. $\mathrm{op}_\varepsilon[a]\mathrm{op}_\varepsilon[b] = \mathrm{op}_\varepsilon[c]$, where $(\mathcal{F}^\varepsilon c)(u) = (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{2n}}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(u-w)e^{-\frac{\mathrm{i}}{2\varepsilon}w^T\Omega u}\,dw$ for $u \in \mathbb{R}^{2n}$ and it remains to show that this is equivalent to the Moyal product $a\#b$. With the inverse Fourier transform, we have

$$a(z) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}}(\mathcal{F}^\varepsilon a)(w)e^{\frac{\mathrm{i}}{\varepsilon}w^Tz}\,dw \quad \text{and} \quad b(z') = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}}(\mathcal{F}^\varepsilon b)(l)e^{\frac{\mathrm{i}}{\varepsilon}l^Tz'}\,dl$$

and thus

$$a(z)b(z') = (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{4n}}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)e^{\frac{\mathrm{i}}{\varepsilon}(w^Tz+l^Tz')}\,dwdl.$$

Moreover, for the action of the operator $e^{\frac{i\varepsilon}{2}\nabla_z^T\Omega\nabla_{z'}}$ we cite [Zwo11, Theorem 4.8],

$$e^{-\frac{i\varepsilon}{2}\nabla_x^T Q\nabla_x}\psi(x) = (2\pi\varepsilon)^{-n/2}|\det(Q)|^{-1/2}e^{\frac{i\pi}{4}\mathrm{sgn}(Q)}\int_{\mathbb{R}^n} e^{-\frac{i}{2\varepsilon}y^TQ^{-1}y}\psi(x+y)\,dy$$

for all $\psi \in \mathcal{S}^{\mathbb{R}^n}$. Thus, by taking the dimensions times four and $Q = \frac{1}{2}\begin{pmatrix} 0 & -\Omega \\ \Omega & 0 \end{pmatrix}$ we find

$$\begin{aligned}
e^{\frac{i\varepsilon}{2}\nabla_z^T\Omega\nabla_{z'}}e^{\frac{i}{\varepsilon}(w^Tz+l^Tz')} &= (2\pi\varepsilon)^{-2n}e^{\frac{i}{\varepsilon}(w^Tz+l^Tz')}\int_{\mathbb{R}^{4n}} e^{\frac{2i}{\varepsilon}z_1^T\Omega z_2}e^{\frac{i}{\varepsilon}(w^Tz_1+l^Tz_2)}\,dz_1dz_2 \\
&= (2\pi\varepsilon)^{-2n}e^{\frac{i}{\varepsilon}(w^Tz+l^Tz')}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} e^{\frac{i}{\varepsilon}z_1^T(w+2\Omega z_2)}\,dz_1\; e^{\frac{i}{\varepsilon}l^Tz_2}\,dz_2 \\
&= (2\pi\varepsilon)^{-2n}e^{\frac{i}{\varepsilon}(w^Tz+l^Tz')}\int_{\mathbb{R}^{2n}} \delta_{\{2z_2=\Omega w\}}e^{\frac{i}{\varepsilon}l^Tz_2}\,dz_2 \\
&= e^{\frac{i}{\varepsilon}(w^Tz+l^Tz')}e^{-\frac{i}{2\varepsilon}w^T\Omega l}.
\end{aligned}$$

All in all,

$$e^{\frac{i\varepsilon}{2}\nabla_z^T\Omega\nabla_{z'}}(a(z)b(z'))\,|_{z=z'} = (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{4n}} e^{\frac{i}{\varepsilon}(w+l)^Tz}e^{-\frac{i}{2\varepsilon}w^T\Omega l}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)\,dwdl$$

and the Fourier transform of this expression is given by

$$\begin{aligned}
(\mathcal{F}^\varepsilon a\# b)(u) &= (2\pi\varepsilon)^{-3n}\int_{\mathbb{R}^{6n}} e^{-\frac{i}{\varepsilon}u^Tz}e^{\frac{i}{\varepsilon}(w+l)^Tz}e^{-\frac{i}{2\varepsilon}w^T\Omega l}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)\,dwdldz \\
&= (2\pi\varepsilon)^{-3n}\int_{\mathbb{R}^{4n}}\int_{\mathbb{R}^{2n}} e^{-\frac{i}{\varepsilon}z^T(w+l-u)}\,dz\; e^{-\frac{i}{2\varepsilon}w^T\Omega l}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)\,dwdl \\
&= (2\pi\varepsilon)^{-2n}\int_{\mathbb{R}^{4n}} \delta_{\{u=w+l\}}e^{-\frac{i}{2\varepsilon}w^T\Omega l}(\mathcal{F}^\varepsilon a)(w)(\mathcal{F}^\varepsilon b)(l)\,dwdl
\end{aligned}$$

what finishes the proof. ■

Corollary A.1 — Semiclassical expansion. Let a, b be two suitable symbols. Then,

$$(a\# b)(z) = \sum_{k=0}^{N} \tfrac{1}{k!}\left(\tfrac{i\varepsilon}{2}\right)^k\left(\nabla_z^T\Omega\nabla_{z'}\right)^k(a(z)b(z'))\,|_{z=z'} + (\varepsilon^{N+1}), \quad z \in \mathbb{R}^{2n}.$$

In particular, we find that if a or b are at most quadratic in z, we find

$$a\# b = ab + \tfrac{i\varepsilon}{2}\nabla a^T\Omega\nabla b - \tfrac{\varepsilon^2}{8}\mathrm{tr}(D^2a\Omega D^2b\Omega^T)$$

where D^2 denotes the Hessian matrix of a resp. b.

We refer for the proof of the well-definedness of the semiclassical expansion to [Zwo11, Theorem 4.12]. The formula for the quadratic symbols follows as direct application of this expansion. We can furthermore introduce here as well the *Poisson bracket*

$$\{a, b\} = \nabla a^T\Omega\nabla b$$

and it follows that for quadratic symbols a or b it holds

$$[\mathrm{op}_\varepsilon[a], \mathrm{op}_\varepsilon[b]] = \mathrm{i}\varepsilon\, \mathrm{op}_\varepsilon[\{a, b\}]. \tag{A.2}$$

The expansion furthermore yields a very short proof for the Weyl-operator of a quadratic function.

Lemma A.4 — Linear and quadratic symbols. Let $z = (p, q) \in \mathbb{R}^{2n}$, $a(z) = \alpha^T z$, $\alpha \in \mathbb{C}^{2n}$ be a linear function in z and $b(z) = \frac{1}{2} z^T H z$ with

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \in \mathbb{C}^{2n \times 2n}$$

quadratic. The Weyl-quantisations of a and b are then given by

$$\mathrm{op}_\varepsilon[a] = \alpha^T \hat{z}, \quad \text{and} \quad \mathrm{op}_\varepsilon[b] = \tfrac{1}{2} \hat{z}^T H \hat{z} - \tfrac{\mathrm{i}\varepsilon}{2} \mathrm{tr}(H_{12} - H_{21}). \tag{A.3}$$

Proof. The equation for the linear function follows directly from the Definition A.1 of the Weyl-operator. For the quadratic function, we first note that

$$\mathrm{op}_\varepsilon[z^T H z] = \mathrm{op}_\varepsilon[z]^T \mathrm{op}_\varepsilon[Hz] - \tfrac{\mathrm{i}\varepsilon}{2} \sum_{j=1}^{2n} (\nabla z_j)^T \Omega \nabla (Hz)_j = \hat{z}^T H \hat{z} - \tfrac{\mathrm{i}\varepsilon}{2} \sum_{j=1}^{2n} e_j^T \Omega H_j$$

where H_j denotes the j-th column of H. For the sum we can also write

$$\sum_{j=1}^{2n} e_j^T \Omega H_j = \sum_{j=1}^{n} H_{j,n+j} - \sum_{j=n+1}^{2n} H_{j,j-n} = \mathrm{tr}(H_{12}) - \mathrm{tr}(H_{21}).$$

■

B. Metaplectic group

Metaplectic operators play a fundamental role in the construction of generalised squeezed states in Section 7.3 and the time evolution under quadratic Hamiltonians. As a consequence we insert here a summary of the definitions and main results for metaplectic operators given in [Gos10]. We start with a more detailed study of symplectic matrices. Recall that $\mathrm{Sp}(n, \mathbb{R})$ denotes the set of all real, symplectic $2n \times 2n$- matrices, i.e. $S \in \mathrm{Sp}(n, \mathbb{R})$ satisfies

$$S^T \Omega S = \Omega, \qquad \Omega = \begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}.$$

In this chapter we will always assume that a symplectic matrix S is given in the block form

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathbb{R}^{2n \times 2n}. \tag{B.1}$$

Lemma B.1 A matrix $S \in \mathbb{R}^{2n \times 2n}$ of form (B.1) is symplectic if and only if

$$A^T C = C^T A, \quad B^T D = D^T B, \quad A^T D - C^T B = \mathrm{Id}.$$

Proof. This result follows from a direct calculation, we have

$$S^T \Omega S = \begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix} \begin{pmatrix} -C & -D \\ A & B \end{pmatrix} = \begin{pmatrix} C^T A - A^T C & C^T B - A^T D \\ D^T A - B^T C & D^T B - B^T D \end{pmatrix}.$$

■

For the construction of the metaplectic group it suffices to observe free symplectic matrices that generate $\mathrm{Sp}(n, \mathbb{R})$ as we will show later on.

Definition B.1 — Free symplectic matrix. We call a matrix $S \in \mathbb{R}^{2n \times 2n}$ in the form (B.1) a *free* symplectic matrix, if $\det(C) \neq 0$, see [Gos10, Definition 47].

The condition $\det(C) \neq 0$ can be interpreted in terms of linear system

$$\begin{pmatrix} p \\ q \end{pmatrix} = S \begin{pmatrix} p' \\ q' \end{pmatrix}. \tag{B.2}$$

If S is a free symplectic matrix, then we find for a given pair $(q, q') \in \mathbb{R}^n \oplus \mathbb{R}^n$ a unique solution $(p, p') \in \mathbb{R}^n \oplus \mathbb{R}^n$.

Lemma B.2 — Generating function. Let S as in (B.1) be a free symplectic matrix. Then, Equation (B.2) holds true if and only if

$$p = \partial_q \sigma(q, q') \quad \text{and} \quad p' = -\partial_{q'} \sigma(q, q') \tag{B.3}$$

where $\sigma : \mathbb{R}^n \oplus \mathbb{R}^n \mapsto \mathbb{R}$ denotes the quadratic form

$$\sigma(q, q') = \tfrac{1}{2} q^T A C^{-1} q - q'^T C^{-1} q + \tfrac{1}{2} q'^T C^{-1} D q'. \tag{B.4}$$

We call σ the *generating function* of S. Conversely, if

$$\sigma(q, q') = \tfrac{1}{2} q^T K q - q'^T L q + \tfrac{1}{2} q'^T M q'$$

with $K, L, M \in \mathbb{R}^{n \times n}$ and $\det(L) \neq 0$, the matrix

$$S_\sigma = \begin{pmatrix} KL^{-1} & KL^{-1}M - L^T \\ L^{-1} & L^{-1}M \end{pmatrix}$$

is a free symplectic matrix generated by σ.

Proof. This result can also be found as [Gos10, Proposition 50]. Equality (B.2) can be rewritten as

$$\begin{aligned} p &= Ap' + Bq', \\ q &= Cp' + Dq', \end{aligned}$$

and since C is invertible,

$$\begin{aligned} p &= -AC^{-1}Dq' + AC^{-1}q + Bq', \\ p' &= -C^{-1}Dq' + C^{-1}q. \end{aligned}$$

It remains to show that $AC^{-1}D - B = C^{-T}$. From Lemma B.1, we know that if S is symplectic, it holds $C^T A = A^T C$ and $A^T D - C^T B = \mathrm{Id}$. Thus,

$$AC^{-1}D - B = C^{-T} A^T D - B = C^{-T}(\mathrm{Id} + C^T B) - B = C^{-T}$$

and (B.3) defines the unique solution of (B.2). For the conversion we compare the generating functions and observe

$$C = L^{-1}, \quad C^{-1}D = M, \quad AC^{-1} = K \quad \text{and} \quad B = AC^{-1}D - C^{-T}.$$

■

If we already anticipate the notion of metaplectic operators we used in Section 7.3, for example in Proposition 7.5 and 7.6, we can stress that a metaplectic operator $\hat{S}$ is often accompanied by its inverse $\hat{S}^{-1}$. The existence and form of this inverse is based on following conclusion, see [Gos10, Corollary 52].

Corollary B.1 Let $S \in \mathrm{Sp}(n,\mathbb{R})$ be a free symplectic matrix with generating function σ. Then, S^{-1} is also a free symplectic matrix and generated by

$$\sigma^*(q,q') = -\sigma(q',q). \tag{B.5}$$

Proof. Since S is symplectic, S is invertible with

$$S^{-1} = \Omega^T S^T \Omega = \begin{pmatrix} 0 & \mathrm{Id} \\ -\mathrm{Id} & 0 \end{pmatrix} \begin{pmatrix} C^T & -A^T \\ D^T & -B^T \end{pmatrix} = \begin{pmatrix} D^T & -B^T \\ -C^T & A^T \end{pmatrix}.$$

Moreover, $\det(-C^T) = (-1)^n \det(C) \neq 0$ and with (B.4),

$$\begin{aligned} \sigma^*(q,q') &= \tfrac{1}{2} q^T D^T (-C^T)^{-1} q - q'^T (-C^T)^{-1} q + \tfrac{1}{2} q'^T (-C^T)^{-1} A^T q' \\ &= -\left(\tfrac{1}{2} q^T C^{-1} D q - q^T C^{-1} q' + \tfrac{1}{2} q'^T A C^{-1} q'\right) = -\sigma(q',q). \end{aligned}$$

■

We have to add here that our definition of a free symplectic matrix is a particular one. In general one considers a Lagrangian subspace $L \subset \mathbb{C}^{2n}$ and a symplectic matrix $S \in \mathrm{Sp}(n,\mathbb{R})$. Clearly,

$$SL := \{S\ell\,;\, \ell \in L\}$$

is again a Lagrangian subspace since S is symplectic and we call S *free w.r.t.* L if

$$L \cap SL = \{0\},$$

see [Gos06, Definition 2.33]. Our definition is equivalent to general definition with $L_0 = \{(p,0) \in \mathbb{R}^{2n}\,;\, p \in \mathbb{R}^n\}$. We can also describe the action of $\mathrm{Sp}(n,\mathbb{R})$ onto Lagrangian subspaces in more detail.

Lemma B.3 Let $L_1, L_1', L_2, L_2' \subset \mathbb{R}^n \oplus \mathbb{R}^n$ be Lagrangian subspaces satisfying

$$L_1 \cap L_1' = L_2 \cap L_2' = \{0\}.$$

Then, there exists a unique symplectic matrix $S \in \mathrm{Sp}(n,\mathbb{R})$ such that $L_2 = SL_1$ and $L_2' = SL_1'$.

Proof. This result can also be found as [Gos06, Theorem 1.26]. Let

$$\begin{aligned} L_1 &= \mathrm{span}\{e_1,\ldots,e_n\}, \quad & L_1' &= \mathrm{span}\{f_1,\ldots,f_n\} \\ L_2 &= \mathrm{span}\{e_1',\ldots,e_n'\}, \quad & L_2' &= \mathrm{span}\{f_1',\ldots,f_n'\}. \end{aligned}$$

Then, the sets $\mathrm{span}\{e_1,\ldots,e_n,f_1,\ldots f_n\}$ and $\mathrm{span}\{e_1',\ldots,e_n',f_1',\ldots f_n'\}$ form two symplectic basis of $\mathbb{R}^{2n}$, see Theorem 2.1 and there exists a unique symplectic mapping

$$\Phi_S : \mathbb{R}^{2n} \mapsto \mathbb{R}^{2n},\ z \to Sz$$

such that $\Phi_S(e_j) = e_j'$, $\Phi_S(f_j) = f_j'$ for all $j = 1,\ldots,n$ and $S \in \mathrm{Sp}(n,\mathbb{R})$. ■

Next, our goal is to establish generators for $\mathrm{Sp}(n,\mathbb{R})$. The main observation for this is the following factorisation result, see [Gos10, Theorem 60].

Theorem B.1 For every symplectic matrix $S \in \mathrm{Sp}(n,\mathbb{R})$ there exist to free symplectic matrices S_σ and $S_{\sigma'}$ with generating functions σ resp. σ' such that

$$S = S_\sigma S_{\sigma'}.$$

Proof. Let $L, L' \subset \mathbb{R}^n \oplus \mathbb{R}^n$ be two arbitrary Lagrangian subspaces satisfying

$$L_0 \cap L' = L' \cap SL_0 = \{0\}.$$

Then, due to the previous lemma there exists a symplectic matrix $S_1 \in \mathrm{Sp}(n,\mathbb{R})$ such that $L' = S_1 L_0$ and $SL_0 = S_1 L'$. Moreover, we can construct a $S_2' \in \mathrm{Sp}(n,\mathbb{R})$ such that $L' = S_2' L_0$ and thus

$$SL_0 = S_1 S_2' L_0$$

and since the product of symplectic matrices is again symplectic, there exists a symplectic matrix S'' with $L_0 = S'' L_0$. All in all we set $S_2 = S_2' S''$ and find $S = S_1 S_2$ with

$$S_1 L_0 \cap L_0 = L' \cap L_0 = \{0\}, \quad \text{and} \quad S_2 L_0 \cap L_0 = S_2' L_0 \cap L_0 = L' \cap L_0 = \{0\}$$

and S_1 and S_2 are free symplectic matrices. ∎

Thus, we can write every symplectic matrix as product of two free symplectic matrices and we will now consider three particular matrices that generate all free symplectic matrices: Let $P = P^T \in \mathbb{R}^{n\times n}$ and $L \in \mathbb{R}^{n\times n}$ be invertible and denote

$$V_P = \begin{pmatrix} \mathrm{Id} & P \\ 0 & \mathrm{Id} \end{pmatrix}, \quad U_P = \begin{pmatrix} P & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}, \quad W_L = \begin{pmatrix} L^T & 0 \\ 0 & L^{-1} \end{pmatrix}.$$

One can easily check that all three matrices are symplectic.

Proposition B.1 Every free symplectic matrix S of the form (B.1) can be factorised as

$$S = U_{AC^{-1}} W_{C^T} V_{C^{-1}D}$$

or, equivalently,

$$S = V_{AC^{-1}} \Omega W_{C^T} V_{C^{-1}D}$$

Proof. This statement is a reformulation of [Gos10, Proposition 62]. Using that $B = AC^{-1}D - C^{-T}$ if S is symplectic, one can directly verify that

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} AC^{-1} & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^{-T} \end{pmatrix} \begin{pmatrix} \mathrm{Id} & C^{-1}D \\ 0 & \mathrm{Id} \end{pmatrix}.$$

Moreover it holds, $U_P = V_P \Omega$ for all symmetric matrices $P \in \mathbb{R}^{n\times n}$. The symmetry of AC^{-1} and $C^{-1}D$ was already discussed in the proof of Lemma B.2 and C is invertible by definition, thus all requirements are fulfilled. ∎

The previous proposition and Theorem B.1 imply the following result that can also be found as [Gos10, Corollary 63].

Corollary B.2 — Generators of the symplectic group. Each of the sets

$$\{V_P, W_L, \Omega\,;\; P = P^T, \det(L) \neq 0\} \quad \text{and} \quad \{U_P, W_L\,;\; P = P^T, \det(L) \neq 0\}$$

generates the set $\mathrm{Sp}(n, \mathbb{R})$.

This statement finishes the repetition of symplectic matrices and we proceed with assigning to any free symplectic matrix S an operator $\hat{S}$ determined by its generating function, see [Gos10, Eq. (7.3)].

Definition B.2 — Quadratic Fourier transform. Let $S \in \mathrm{Sp}(n, \mathbb{R})$ be a free symplectic matrix of the form (B.1) and σ the corresponding generating function. We define

$$(\hat{S}_\sigma \psi)(x) = (2\pi\varepsilon)^{-n/2} \det(C)^{-1/2} \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\sigma(x,x')} \psi(x')\, dx' \tag{B.6}$$

for all $\psi \in \mathcal{S}(\mathbb{R}^n)$.

An illustrative example is the standard Fourier transform $\mathcal{F}^\varepsilon$: We have

$$\sigma(x, x') = -x^T x',$$

i.e. $K = M = 0$ and $L = \mathrm{Id}$. Hence, the corresponding symplectic matrix is Ω, $\mathcal{F}^\varepsilon = \hat{\Omega}$. For general operators the following statement holds true, see [Gos10, Proposition].

Proposition B.2 The operator $\hat{S}_\sigma$ given in (B.6) is a unitary operator that maps $L^2(\mathbb{R}^n)$ onto itself and its inverse is given by

$$\hat{S}_\sigma^{-1} = \hat{S}_{\sigma^*}$$

with σ^* as in (B.5).

We call the subgroup of all unitary operators $\mathcal{U}(L^2(\mathbb{R}^n))$ generated by the quadratic Fourier transforms the *metaplectic group* $\mathrm{Mp}(n, \mathbb{R})$. Elements of $\mathrm{Mp}(n, \mathbb{R})$ are denoted as *metaplectic operators*, see [Gos10, Definition 109]. Similarly to the symplectic matrices we will now show that all metaplectic operators are generated by the Fourier transforms

$$\hat{V}_P \psi(x) = e^{\frac{\mathrm{i}}{2\varepsilon} x^T P x} \psi(x) \quad \text{and} \quad \hat{W}_L \psi(x) = \det(L)^{1/2} \psi(Lx)$$

for $\psi \in L^2(\mathbb{R}^n)$ and $\hat{\Omega}$. The next statement also provides an explanation for the previous proposition: $\hat{V}_P$, $\hat{W}_L$ and $\hat{\Omega}$ are unitary operators and hence also their consecutive application is unitary.

Proposition B.3 Let $\sigma(q, q') = \frac{1}{2} q^T K q - q'^T L q + \frac{1}{2} q'^T M q'$ where K and M are symmetric and L an invertible $n \times n$-matrix. Then,

$$\hat{S}_\sigma = \hat{V}_K \hat{W}_L \hat{\Omega} \hat{V}_M.$$

Proof. This result equals the first part of [Gos10, Proposition 108]. By definition,

$$\begin{aligned}
\hat{S}_\sigma \psi(x) &= (2\pi\varepsilon)^{-n/2} \det(L)^{1/4} \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}(\frac{1}{2}x^T Kx - x'^T Lx + \frac{1}{2}x'^T Mx')} \psi(x')\, dx' \\
&= (2\pi\varepsilon)^{-n/2} \det(L)^{1/4} \int_{\mathbb{R}^n} \hat{V}_K e^{-\frac{\mathrm{i}}{\varepsilon}x'^T Lx} \hat{V}_M \psi(x')\, dx' \\
&= \hat{V}_K \hat{W}_L (2\pi\varepsilon)^{-n/2} \int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}x'^T x} \hat{V}_M \psi(x')\, dx' \\
&= \hat{V}_K \hat{W}_L \hat{\Omega} \hat{V}_M \psi(x).
\end{aligned}$$

■

Analogously to the symplectic matrices we next show that every metaplectic operator can be written as two quadratic Fourier transforms and thus the metaplectic group $\mathrm{Mp}(n, \mathbb{R})$ is generated by the operators $\hat{V}_P$, $\hat{W}_L$ and $\hat{\Omega}$.

Theorem B.2 Every $\hat{S} \in \mathrm{Mp}(n, \mathbb{R})$ can be written as

$$\hat{S} = \hat{S}_\sigma \hat{S}_{\sigma'},$$

where $\hat{S}_\sigma$ and $\hat{S}_{\sigma'}$ are two quadratic Fourier transforms.

Proof. We overleap the proof of this result as it invokes the projection from $\mathrm{Mp}(n, \mathbb{R})$ to $\mathrm{Sp}(n, \mathbb{R})$ we will establish in the following and refer to [Gos97]. ■

We stress here that both, the factorisation of the symplectic matrices and the metaplectic operators are both not unique.

Corollary B.3 — Generators of the metaplectic group. The metaplectic group is generated by the operators $\hat{V}_P$, $\hat{W}_L$ and $\hat{\Omega}$.

So far, we assigned an operator to every symplectic matrix $S \in \mathrm{Sp}(n, \mathbb{R})$. The next logical question is if we can reversely also find a corresponding symplectic matrix for every metaplectic operator.

Theorem B.3 — The projection π^{Mp}. The mapping $\hat{S}_\sigma \to S_\sigma$ which associates to the quadratic Fourier transform (B.6) the free symplectic matrix generated by σ extends to a surjective group homomorphism

$$\pi^{\mathrm{Mp}} : \mathrm{Mp}(n, \mathbb{R}) \mapsto \mathrm{Sp}(n, \mathbb{R})$$

with $\mathrm{kern}(\pi^{\mathrm{Mp}}) = \{-\mathrm{id}, \mathrm{id}\}$. Hence π^{Mp} is a twofold covering of the symplectic group.

Proof. The proof of this result is very extensive and we therefor refer for a detailed formulation to [Gos10, §7.3]. The main idea of the proof is to explicitly construct the projection from the lowering operator

$$\hat{A}(l) = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} l^T \Omega \hat{z},$$

where $l \in \mathbb{C}^{2n}$. Since $\mathcal{F}^\varepsilon = \hat{\Omega}$, we can utilise Lemma 4.5 and directly obtain

$$\hat{\Omega}\hat{A}(l)\hat{\Omega}^{-1} = \hat{A}(\Omega l).$$

Analogously one can show that $\hat{W}_L \hat{A}(l) \hat{W}_L^{-1} = \hat{A}(W_L l)$ and $\hat{V}_P \hat{A}(l) \hat{V}_P^{-1} = \hat{A}(V_P l)$. Since $\hat{V}_{-P}$, $\hat{W}_L$ and $\hat{\Omega}$ generate the metaplectic group it follows that for all $\hat{S} \in \mathrm{Mp}(n, \mathbb{R})$ there exists a matrix $S \in \mathbb{R}^{2n \times 2n}$ such that

$$\hat{S}\hat{A}(l)\hat{S}^{-1} = \hat{A}(Sl) = \mathrm{op}_\varepsilon[A(\ell) \circ S^{-1}].$$

We denote by $\Phi_{\hat{S}}(\hat{A}(\ell))$ the mapping $\hat{A}(\ell) \to \mathrm{op}_\varepsilon[A(\ell) \circ S^{-1}]$. The projection π^{Mp} can then be written as

$$\pi^{\mathrm{Mp}}(\hat{S}) = \hat{A}^{-1}(\ell)\Phi_{\hat{S}}(\hat{A}(\ell))\hat{A}(\ell),$$

see also [Gos10, Definition 121], and it remains to show that S is symplectic. With Lemma 4.1 we find for all $l, l' \in \mathbb{C}^{2n}$,

$$\tfrac{1}{2\mathrm{i}} l^T S^T \Omega S l' = \left[\hat{A}(Sl), \hat{A}(Sl')\right] = \left[\hat{S}\hat{A}(l)\hat{S}^{-1}, \hat{S}\hat{A}(l')\hat{S}^{-1}\right] = \hat{S}\left[\hat{A}(l), \hat{A}(l')\right]\hat{S}^{-1} = \tfrac{1}{2\mathrm{i}} l^T \Omega l'$$

and thus $S^T \Omega S = \Omega$. ■

By the above proof quadratic Fourier transforms are indeed mapped to the corresponding free symplectic matrices and since π^{Mp} is a homomorphism, we find

$$\pi^{\mathrm{Mp}}(S_\sigma S_{\sigma'}) = \pi^{\mathrm{Mp}}(S_\sigma)\pi^{\mathrm{Mp}}(S_{\sigma'}).$$

From these two observation we can deduce the next corollary, see also [Gos10, Proposition 122].

Corollary B.4 The projection π^{Mp} satisfies

$$\pi^{\mathrm{Mp}}(\hat{\Omega}) = \Omega, \qquad \pi^{\mathrm{Mp}}(\hat{V}_P) = V_P, \qquad \pi^{\mathrm{Mp}}(\hat{W}_L) = W_L.$$

Proof. Since Ω is a free symplectic matrix, we directly conclude $\pi^{\mathrm{Mp}}(\hat{\Omega}) = \Omega$. We note that for $\psi \in \mathcal{S}(\mathbb{R}^n)$,

$$\hat{V}_P\hat{\Omega}\psi(x) = (2\pi\varepsilon)^{-n/2} \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{2\varepsilon} x^T P x - \frac{\mathrm{i}}{\varepsilon} x'^T x} \psi(x')\, dx' = \hat{S}_\sigma \psi(x)$$

where the free symplectic matrix S_σ is due to Lemma B.2 given by

$$S_\sigma = \begin{pmatrix} P & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}.$$

So, we find for the projection

$$\pi^{\mathrm{Mp}}(\hat{V}_P) = \pi^{\mathrm{Mp}}(\hat{V}_P\hat{\Omega}\hat{\Omega}^{-1}) = \pi^{\mathrm{Mp}}(\hat{S}_\sigma)\pi^{\mathrm{Mp}}(\hat{\Omega}^{-1}) = S_\sigma\Omega^{-1} = V_P$$

Analogously,

$$\hat{\Omega}\hat{W}_L\psi(x) = (2\pi\varepsilon)^{-n/2}\det(L)^{-1/2}\int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}x'^T L^{-T}x}\psi(x')\,dx' = \hat{S}_{\sigma'}\psi(x)$$

with $S_{\sigma'} = \begin{pmatrix} 0 & -L^{-1} \\ L^T & 0 \end{pmatrix}$ and

$$\pi^{\mathrm{Mp}}(\hat{W}_L) = \pi^{\mathrm{Mp}}(\hat{\Omega}^{-1})\pi^{\mathrm{Mp}}(\hat{\Omega}\hat{W}_L) = \Omega^{-1}S_{\sigma'} = W_L.$$

■

So, we related symplectic matrices and metaplectic operators via a quadratic form σ and showed that the symplectic group $\mathrm{Sp}(n,\mathbb{R})$ can be generated from the matrices V_P, W_L and Ω where P is symmetric and L invertible, while the metaplectic group $\mathrm{Mp}(n,\mathbb{R})$ is generated from the corresponding operators $\hat{V}_P, \hat{W}_L$ and $\hat{\Omega}$. We now use this basic constructions to proof the properties of metaplectic operators needed in this thesis. In Section 7.3 we required the relation between metaplectic and Weyl-operators, see [Gos10, Theorem 215].

Theorem B.4 — Metaplectic covariance of Weyl-operators. Let $S \in \mathrm{Sp}(n,\mathbb{R})$, $\hat{S} \in \mathrm{Mp}(n,\mathbb{R})$ such that $\pi^{\mathrm{Mp}}(\hat{S}) = S$. Then, we have for every Weyl-operator $\hat{a}$ with symbol a

$$\mathrm{op}_\varepsilon[a \circ S] = \mathrm{op}_\varepsilon[a(Sz)] = \hat{S}^{-1}\hat{a}\hat{S}.$$

Proof. With the definition of the Weyl-operator via the Fourier transform (A.1) we find

$$\begin{aligned}\mathrm{op}_\varepsilon[a\circ S] &= (2\pi\varepsilon)^{-n}\int \mathcal{F}^\varepsilon(a\circ S)(w)e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,dw = (2\pi\varepsilon)^{-n}\int \mathcal{F}^\varepsilon(a)(S^{-T}w)e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,dw \\ &= (2\pi\varepsilon)^{-n}\int \mathcal{F}^\varepsilon(a)(w)e^{\frac{\mathrm{i}}{\varepsilon}w^TS\hat{z}}\,dw\end{aligned}$$

and it suffices to show that $e^{\frac{\mathrm{i}}{\varepsilon}w^TS\hat{z}} = \hat{S}^{-1}e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\hat{S}$. Since $\hat{V}_{-P}$, $\hat{W}_L$ and $\hat{\Omega}$ generate $\mathrm{Mp}(n,\mathbb{R})$ and every symplectic matrix S can be factorised into V_{-P}, W_L and Ω, we only need to show the identity for these three matrices. Let $w = (p,q) \in \mathbb{R}^n \oplus \mathbb{R}^n$ and $\psi \in \mathcal{S}(\mathbb{R}^n)$. We then have

$$\begin{aligned}\left(\hat{V}_{-P}\,e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,\hat{V}_P\right)\psi(x) &= e^{-\frac{\mathrm{i}}{2\varepsilon}x^TPx}e^{\frac{\mathrm{i}}{\varepsilon}q^T(x+p/2)}e^{\frac{\mathrm{i}}{2\varepsilon}(x+p)^TP(x+p)}\psi(x+p) \\ &= e^{\frac{\mathrm{i}}{\varepsilon}(Pq+q)^T(x+p/2)}\psi(x+p) = e^{\frac{\mathrm{i}}{\varepsilon}w^TV_P\hat{z}}, \\ \left(\hat{W}_{L^{-1}}\,e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,\hat{W}_L\right)\psi(x) &= e^{\frac{\mathrm{i}}{\varepsilon}q^T(L^{-1}x+p/2)}\psi(x+Lp) \\ &= e^{\frac{\mathrm{i}}{\varepsilon}(L^{-T}q)^T(x+Lp/2)}\psi(x+Lp) = e^{\frac{\mathrm{i}}{\varepsilon}w^TW_L\hat{z}},\end{aligned}$$

and

$$\left(\hat{\Omega}^{-1}\, e^{\frac{\mathrm{i}}{\varepsilon}w^T\hat{z}}\,\hat{\Omega}\right)\psi(x) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}x^T\xi}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}q^T(\xi+p/2)}e^{-\frac{\mathrm{i}}{\varepsilon}(\xi+p)^Tx'}\psi(x')\,dx'd\xi$$
$$= (2\pi\varepsilon)^{-n}e^{\frac{\mathrm{i}}{2\varepsilon}p^Tq}\int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}p^Tx'}\psi(x')\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\xi^T(x+q-x')}\,d\xi dx'$$
$$= (2\pi\varepsilon)^{-n}e^{\frac{\mathrm{i}}{2\varepsilon}p^Tq}\int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}p^Tx'}\psi(x')\delta(x+q-x')\,dx'$$
$$= e^{-\frac{\mathrm{i}}{\varepsilon}p^T(x+q/2)}\psi(x+q) = e^{\frac{\mathrm{i}}{\varepsilon}w^T\Omega\hat{z}}.$$

■

Due to the Wigner-Weyl correspondence we first stated in (3.18), we can infer from the previous theorem the following statement about the relation of metaplectic operators and the Wigner transform, see also [Gos10, Corollary 217].

Corollary B.5 — Metaplectic covariance of Wigner transforms. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$ and $\hat{S} \in \mathrm{Mp}(n,\mathbb{R})$ with $S = \pi^{\mathrm{Mp}}(\hat{S}) \in \mathrm{Sp}(n,\mathbb{R})$. We have

$$\mathcal{W}^\varepsilon(\hat{S}\varphi, \hat{S}\psi)(z) = \mathcal{W}^\varepsilon(\varphi,\psi)(S^{-1}z)$$

for $z \in \mathbb{R}^n \oplus \mathbb{R}^n$.

Proof. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$. We find for all symbols $a \in \mathcal{S}(\mathbb{R}^n \oplus \mathbb{R}^n)$,

$$\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\hat{S}\varphi,\hat{S}\psi)(z)a(z)\,dz = \langle \hat{S}\varphi, \hat{a}\hat{S}\psi\rangle = \langle \varphi, \hat{S}^{-1}\hat{a}\hat{S}\psi\rangle = \langle \varphi, \mathrm{op}_\varepsilon[a\circ S]\psi\rangle$$
$$= \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi,\psi)(z)a(Sz)\,dz = \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi,\psi)(S^{-1}z)a(z)\,dz.$$

■

In Chapter 7 we used metaplectic operators to generate squeezed states from the multi-dimensional Hermite functions

$$\varphi_0(x) = (\pi\varepsilon)^{-n/4}e^{-\frac{1}{2\varepsilon}|x|^2}, \qquad \varphi_k(x) = \prod_{j=1}^n h_{k_j}(x_j)\varphi_0(x)$$

for $k \in \mathbb{N}^n$ and $x \in \mathbb{R}^n$. For the coherent state φ_0 we are able to give an explicit formula for the squeezing in terms of the block matrices A, B, C, D, see also [Gos10, Proposition 252].

Proposition B.4 — Metaplectic operators and squeezed states. Let $\hat{S} \in \mathrm{Mp}(n,\mathbb{R})$ with $S = \pi^{\mathrm{Mp}}(\hat{S}) \in \mathrm{Sp}(n,\mathbb{R})$ of the form (B.1). We find

$$\hat{S}\varphi_0(x) = e^{\mathrm{i}\gamma}(\pi\varepsilon)^{-n/4}\det(X)^{1/4}e^{-\frac{1}{2\varepsilon}x^T\Gamma x}$$

where $\gamma \in \mathbb{R}$ and $\Gamma = X + \mathrm{i}Y$ with symmetric matrices $X, Y \in \mathbb{R}^{n\times n}$ given by

$$X = (AC^T + BD^T)(CC^T + DD^T)^{-1}, \qquad Y = (CC^T + DD^T)^{-1}.$$

Proof. From Lemma 3.9 we know that $\mathcal{W}^\varepsilon(\varphi_0)(z) = \pi^{-n} e^{-\frac{1}{\varepsilon} z^T z}$ and thus with the previous corollary

$$\mathcal{W}^\varepsilon(\hat{S}\varphi_0)(z) = \mathcal{W}^\varepsilon(\varphi_0)(S^{-1}z) = \pi^{-n} e^{-\frac{1}{\varepsilon} z^T S^{-T} S^{-1} z}.$$

We can calculate this matrix explicitly and obtain

$$S^{-T}S^{-1} = \Omega^T S S^T \Omega = \begin{pmatrix} CC^T + DD^T & -(DB^T + CA^T) \\ -(BD^T + AC^T) & AA^T + BB^T \end{pmatrix}.$$

Comparing this identity with (2.16),

$$\begin{pmatrix} \mathrm{Im}(\Gamma)^{-1} & -\mathrm{Im}(\Gamma)^{-1}\mathrm{Re}(\Gamma) \\ -\mathrm{Re}(\Gamma)\mathrm{Im}(\Gamma)^{-1} & \mathrm{Re}(\Gamma)\mathrm{Im}(\Gamma)^{-1}\mathrm{Re}(\Gamma) + \mathrm{Im}(\Gamma) \end{pmatrix} = \begin{pmatrix} CC^T + DD^T & -DB^T - CA^T \\ -BD^T - AC^T & AA^T + BB^T \end{pmatrix}$$

shows the claim. ■

As a last note we want to mention the relation of metaplectic operators and quadratic Hamiltonians that we investigate in the second part of this thesis. If $\hat{\mathcal{H}} = \frac{1}{2}\hat{z}^T H \hat{z}$ with $H = H^T \in \mathbb{C}^{2n\times 2n}$ is time-independent, then the flow of the Schrödinger equation

$$\mathrm{i}\varepsilon\,\partial_t \psi = \widehat{\mathcal{H}}\psi$$

is the solution of the differential equation $\dot{S}_t = \Omega H S_t$, i.e. $S_t = e^{t\Omega H}$. One can show that this matrix is symplectic, see Lemma 8.12, and we thus find a metaplectic operator $\hat{S}$ with $\pi^{\mathrm{Mp}}(\hat{S}) = S$.

Theorem B.5 — Metaplectic operators and quadratic Hamiltonians. Let $t \to \hat{S}_t$ be the lift to $\mathrm{Mp}(n, \mathbb{R})$ of the flow $t \to S_t = e^{t\Omega H}$. For every $\psi_0 \in \mathcal{S}(\mathbb{R}^n)$, the function ψ defined by $\psi(x,t) = \hat{S}_t\psi_0(x)$ is a solution of the partial differential equation

$$\mathrm{i}\varepsilon\,\partial_t \psi = \widehat{\mathcal{H}}\psi, \qquad \psi(\cdot, 0) = \psi_0(x).$$

Equivalently, the function $t \to \hat{S}_t$ solves the abstract equation

$$\mathrm{i}\varepsilon\,\partial_t \hat{S}_t = \widehat{\mathcal{H}}\hat{S}_t, \qquad \hat{S}_0 = \mathrm{id}.$$

We will study the existence of such evolution operators for the Schrödinger equation in the next chapter where we also in detail investigate non-Hermitian Hamiltonians. The proof of the above theorem follows similarly to the proof of Theorem C.1.

C. One-parameter semigroups

Since the dynamical part of this thesis heavily relies on the time evolution operators $\widehat{\mathcal{U}}(t)$, we investigate in this chapter the theory of one-parameter semigroups in more detail and subsequently provide a proof of Proposition 9.1.

We start with the functional equation Cauchy stated in 1821, see [Cau21, §V]. His aim was to determine continuous functions $T : \mathbb{R} \mapsto \mathbb{R}$ satisfying

$$T(t+s) = T(t)T(s)$$

for all $s, t \in \mathbb{R}$. This identity is significant for the description of dynamical systems. Let $\varphi_0 \in \mathbb{R}$ be the state of a system at time $t = 0$ and define $\varphi(t) := T(t)\varphi_0$. Then, the above equality ensures that

$$\varphi(t+s) = T(t+s)\varphi_0 = T(t)T(s)\varphi_0 = T(t)\varphi_0(s)$$

and hence the state $\varphi(t+s)$ at time $t+s$ is the same as the state at time t starting from $\varphi(s)$, i.e. the time evolution is unique, see [EN00, §I.1.5]. We will now generalise this idea to operators.

Let X be a Banach space with norm $\|\cdot\|_X$ and $\mathcal{L}(X)$ denote the set of all bounded linear operators from X to X. We endow $\mathcal{L}(X)$ with the operator norm $\|\cdot\|_{\mathcal{L}(X)}$ defined by

$$\|T\|_{\mathcal{L}(X)} = \sup \tfrac{\|Tx\|_X}{\|x\|_X},$$

see [RS80, §V.I.1]. For the following definition we refer to [Vra03, Definition 2.1.1].

Definition C.1 — One-parameter semigroup. A family $\{T(t)\,;\, t \geq 0\}$ in $\mathcal{L}(X)$ is a *one-parameter semigroup*, or simply *semigroup*, if

$$\begin{aligned} T(0) &= \mathrm{id}, \\ T(t+s) &= T(t)T(s) \qquad \text{for all } t, s \geq 0, \end{aligned} \tag{C.1}$$

where id denotes the identity operator, $\mathrm{id}\, x = x$ for all $x \in X$.

With the uniform and the strong operator topology on $\mathcal{L}(X)$, see again [RS80, §V.I.1], we can furthermore specify certain semigroups. We call a semigroup $\{T(t)\,;\, t \geq 0\}$ *uniformly continuous* if

$$\lim_{t \downarrow 0} T(t) = \mathrm{id}$$

and *strongly continuous* if

$$\lim_{t\downarrow 0} T(t)x = x, \qquad \text{for all } x \in X.$$

In particular, each uniformly continuous semigroup is also a strongly continuous semigroup. Beyond that, we can now also establish the term *contractive* we used without further explanation in Section 9.1.

Proposition C.1 — Contraction semigroup. Let $\{T(t)\,;\, t \geq 0\}$ denote a strongly continuous semigroup on a Banach space X. Then, there exist constants $\gamma \geq 0$ and $c \geq 1$ such that

$$\|T(t)\|_{\mathcal{L}(X)} \leq ce^{\gamma t}$$

for all $t \geq 0$. If $c = 1$ and $\gamma = 0$, we call $\{T(t)\}_{t\geq 0}$ a *contraction semigroup*.

Proof. This statement is adopted from [EN00, Proposition 5.5]. Since $T(t)$ is a bounded linear operator for all $t \geq 0$, there exists a constant $c \geq 1$ such that $\|T(s)\|_{\mathcal{L}(X)} \leq c$ for all $s \in [0;1]$. For any $t \geq 0$ we can write $t = s + m$ for some $m \in \mathbb{N}$ and $s \in [0;1]$. Equation (C.1) then implies

$$\|T(t)\|_{\mathcal{L}(X)} = \|T(s + m \cdot 1)\|_{\mathcal{L}(X)} \leq \|T(s)\|_{\mathcal{L}(X)} \|T(1)\|^m_{\mathcal{L}(X)} \leq c^{m+1}.$$

By denoting $\gamma = \ln(c)$, we can moreover write $c^{m+1} = ce^{m\gamma} \leq ce^{t\gamma}$ what finishes the proof. ■

Returning to Cauchy's original problem, we can easily see that $T(t) = e^{\alpha t}$ for all $\alpha \in \mathbb{R}$ gives a solution and one can additionally show that this is the only continuous solution, see [EN00, Proposition 1.3]. Moreover, the semigroup $\{e^{\alpha t}\,;\, t \geq 0\}$ solves the initial value problem

$$\partial_t T(t) = \alpha T(t) \quad \text{for all } t \geq 0$$

with $T(0) = 1$. In Section 9.1 though, we were starting from the differential equation, namely the Schrödinger equation, and trying to determine a corresponding semigroup. Given the previous initial value problem, we could determine α via

$$\alpha = \partial_t T(t)\ |_{t=0} = \lim_{t\downarrow 0} \tfrac{1}{t}(T(t) - 1).$$

We adapt this idea for general semigroups, see [Vra03, Definition 2.1.2].

Definition C.2 — Infinitesimal generator. The *infinitesimal generator* or *generator* of a semigroup $\{T(t)\,;\, t \geq 0\}$ is an operator $A : D(A) \mapsto X$ with domain

$$D(A) = \{x \in X\,;\, \lim_{t\downarrow 0} \tfrac{1}{t}(T(t)x - x) \text{ exists } \} \subset X$$

defined by $Ax = \lim_{t\downarrow 0} \frac{1}{t}(T(t)x - x)$.

Since the properties of linear operators in general heavily depend on their domain, we will in the following always name operators in the form $(A, D(A))$. The next statement verifies that the generator of a semigroup indeed has the desired characteristics.

Theorem C.1 Let $\{T(t)\}_{t\geq 0}$ be a strongly continuous semigroup with infinitesimal generator $(A, D(A))$. Then, if $x \in D(A)$ we have $T(t)x \in D(A)$ for all $t \geq 0$ and

$$\partial_t T(t)x = AT(t)x = T(t)Ax.$$

The derivative at $t = 0$ denotes only the right derivative, for $t > 0$ the derivative is two-sided.

Proof. This result is quoted from [McB87, Theorem 2.20]. Let $x \in D(A)$. We have to show that the limit

$$\lim_{h\downarrow 0} \tfrac{1}{h}(T(t+h)x - T(t)x) = T(t)\lim_{h\downarrow 0} \tfrac{1}{h}(T(h)x - x)$$

exists. But since $x \in D(A)$, the right hand side converges and due to the continuity of $\{T(t)\}_{t\geq 0}$ it converges to $T(t)Ax$. Hence $T(t)x \in D(A)$ and with $T(t+h) = T(h+t)$ it moreover follows that

$$T(t)Ax = AT(t)x$$

for all $x \in D(A)$. It remains to calculate the derivative. Let $t \geq 0$, then the derivative from the right is a direct consequence of the above computation,

$$\lim_{h\downarrow 0} \tfrac{1}{h}(T(t+h)x - T(t)x) = T(t)Ax = AT(t)x$$

for all $x \in D(A)$. For the derivative from the left side, we find

$$\begin{aligned}\lim_{h\uparrow 0} \tfrac{1}{h}(T(t+h)x - T(t)x) &= \lim_{h\downarrow 0} \tfrac{1}{-h}(T(t-h)x - T(t)x) = \lim_{h\downarrow 0} \tfrac{1}{h}T(t-h)(T(h)x - x)\\ &= \lim_{h\downarrow 0} T(t-h)(\tfrac{T(h)x-x}{h} - Ax) + \lim_{h\downarrow 0} T(t-h)Ax.\end{aligned}$$

The first term tends to zero since $T(t-h)$ is a bounded operator for all $0 \leq h \leq t$, the second term goes to $T(t)Ax$ as $\{T(t)\}_{t\geq 0}$ is strongly continuous. ∎

Our aim in the following is to characterise operators that generate a semigroup. For uniformly continuous semigroups this result is straightforward and well-known, see for example [EN00, Theorem 2.2.1].

Theorem C.2 — Generators of uniformly continuous semigroups. A linear operator $(A, D(A))$ is the generator of a uniformly continuous semigroup if and only if $D(A) = X$ and $A \in \mathcal{L}(X)$.

Proof. We only show that a bounded linear operator A that is defined on X generates a uniformly continuous semigroup and refer for the full proof to the indicated literature.

Since A is bounded, we can define

$$T(t) = \sum_{k=0}^{\infty} \tfrac{t^k}{k!} A^k = e^{tA}$$

for all $t \geq 0$, the convergence of the power series follows similarly as for the matrix exponential. Moreover, from the properties of the exponential sum it follows directly that $\{T(t)\,;\, t \geq 0\}$ defines a one-parameter semigroup. It remains to show that this semigroup is uniformly convergent and generated by A. We have

$$\|T(t) - \mathrm{id}\|_{\mathcal{L}(X)} = \|\sum_{k=1}^{\infty} \tfrac{t^k}{k!} A^k\|_{\mathcal{L}(X)} \leq t \sum_{k=0}^{\infty} \tfrac{t^k}{k!} \|A^{k+1}\|_{\mathcal{L}(X)} = t\|A\|_{\mathcal{L}(X)} e^{t\|A\|_{\mathcal{L}(X)}}$$

and hence $\lim\limits_{t\downarrow 0} \|T(t) - \mathrm{id}\|_{\mathcal{L}(X)} = 0$. Furthermore, with an analogous line of argumentation

$$\|\tfrac{1}{t}(T(t) - \mathrm{id}) - A\|_{\mathcal{L}(X)} = \|\sum_{k=1}^{\infty} \tfrac{t^{k-1}}{k!} A^k - A\|_{\mathcal{L}(X)} = \|\sum_{k=2}^{\infty} \tfrac{t^{k-1}}{k!} A^k\|_{\mathcal{L}(X)} \leq t\|A\|^2_{\mathcal{L}(X)} e^{t\|A\|_{\mathcal{L}(X)}}$$

and $\lim\limits_{t\downarrow 0} \|\tfrac{1}{t}(T(t) - \mathrm{id}) - A\|_{\mathcal{L}(X)} = 0$. ■

Unfortunately, quadratic operators discussed in this thesis are in general unbounded operators and we have to focus on strongly continuous semigroups.

However, we keep in mind that we can write the generator of an uniformly continuous semigroup conveniently as the exponential of the generator. For unbounded operators, we can not guarantee the convergences of the power series. But we recall that one can equivalently define the exponential $e^{\alpha t}$ for $\alpha \in \mathbb{R}$ as

$$e^{t\alpha} = \lim_{k\to\infty} (1 + \tfrac{t\alpha}{k})^k = \lim_{k\to\infty} (1 - \tfrac{t\alpha}{k})^{-k} = \lim_{k\to\infty} \left(\tfrac{k}{t}(\tfrac{k}{t} - \alpha)^{-1}\right)^k,$$

where we used that $e^{t\alpha} = \left(e^{-t\alpha}\right)^{-1}$, see [McB87, §3]. This observation motivates the next definition for linear operators, see [McB87, Definition 3.1].

Definition C.3 — Resolvent. Let $A : D(A) \mapsto X$ be a linear operator on a Banach space X. The *resolvent set* of A is the set of complex numbers

$$\rho(A) = \{\lambda \in \mathbb{C}\,;\, (\lambda\mathrm{id} - A)^{-1} \in \mathcal{L}(X)\}$$

and we call for all $\lambda \in \rho(A)$ the operator $R(\lambda, A) = (\lambda\mathrm{id} - A)^{-1}$ *resolvent* of A at λ. The spectrum of A is the complement of $\rho(A)$, $\sigma(A) = \mathbb{C}\backslash\rho(A)$.

If we compare λ with our original idea, we find $\lambda = \frac{k}{t}$ and thus $\lambda > 0$. Moreover, the limit of $\left(\frac{k}{t}(\frac{k}{t} - \alpha)^{-1}\right)^k$ is bounded, if

$$\tfrac{k}{t}(\tfrac{k}{t} - \alpha)^{-1} < 1.$$

Again, there is an analogue interpretation of this observation on the operator level.

Theorem C.3 — Hille Yosida. A linear operator $(A, D(A))$ generates a strongly continuous contraction semigroup if and only if $(A, D(A))$ is a closed, densely defined operator and for every $\lambda > 0$ one has $\lambda \in \rho(A)$ and

$$\|\lambda R(\lambda, A)\|_{\mathcal{L}(X)} \leq 1.$$

Proof. Let $(A, D(A))$ generate a strongly continuous contraction semigroup $\{T(t)\}_{t\geq 0}$. In order to show that $D(A)$ is dense in X we have to construct for all $x \in X$ a sequence $x_m \in D(A)$ with $x_m \to x$. Following the idea from [Vra03, Theorem 2.4.1] we set for each $x \in X$ and $m \in \mathbb{N}$,

$$x_m := m \int_0^{1/m} T(\tau)x \, d\tau.$$

We first show that this expression converges to x. We have for all $t \geq 0$ and $h > 0$

$$\begin{aligned} \|\tfrac{1}{h} \int_t^{t+h} T(\tau)x \, d\tau - T(t)x\|_X &= \|\tfrac{1}{h} \int_t^{t+h} T(\tau)x - T(t)x \, d\tau\|_X \\ &\leq \tfrac{1}{h} \int_t^{t+h} \|T(\tau)x - T(t)x\|_X \, d\tau \end{aligned}$$

and since $\{T(t)\,;\, t \geq 0\}$ is strongly continuous, $\lim_{h\downarrow 0} \frac{1}{h} \int_t^{t+h} T(\tau)x \, d\tau = T(t)x$. In particular,

$$\lim_{m\to\infty} x_m = T(0)x = x.$$

This implies for the limit

$$\lim_{t\downarrow 0} \tfrac{1}{t}(T(t)x_m - x_m) = m \lim_{t\downarrow 0} \int_0^{1/m} T(t+\tau)x - T(\tau)x \, d\tau$$

and by substituting $s = t + \tau$,

$$m \int_0^{1/m} T(t+\tau)x - T(\tau)x \, d\tau = m \int_t^{1/m+t} T(s)x \, ds - m \int_0^{1/m} T(\tau)x \, d\tau \to T(t)x - x$$

for $m \to \infty$ and the limit exists. Hence, $x_m \in D(A)$ and $D(A)$ is dense in X. To prove that A is closed, assume that $x_m \in D(A)$ with $x_m \to x$ and $Ax_m \to y$ for $x, y \in D(A)$. We have to show that $x \in D(A)$ and $Ax = y$. With Theorem C.1 it holds

$$T(t)x_m - x_m = \int_0^t \partial_t T(\tau)x_m \, d\tau = \int_0^t T(\tau)Ax_m \, d\tau$$

and by taking the limit, we obtain $T(t)x - x = \int_0^t T(\tau)y \, d\tau$. Thus, with the integral representation introduced above,

$$\lim_{t\downarrow 0} \tfrac{1}{t}(T(t)x - x) = \lim_{t\downarrow 0} \tfrac{1}{t} \int_0^t T(\tau)y \, d\tau = y$$

and $x \in D(A)$ with $Ax = y$. The claim for the resolvent follows from the identity

$R(\lambda) = R(\lambda, A)$ for all $\lambda \in \rho(A)$ with $\lambda > 0$, where

$$R(\lambda)x = \int_0^\infty e^{-\lambda t} T(t)x\,dt \qquad \text{for all } x \in X,$$

see for example [Vra03, Theorem 3.1.1]. Then, for $a, b \geq 0$ with $a \leq b$, since $\{T(t)\}_{t\geq 0}$ is contractive,

$$\| \int_a^b e^{-\lambda t} T(t)x\,dt \|_X \leq \int_a^b e^{-\lambda t} \|T(t)x\|_X\,dt \leq \|x\|_X \int_a^b e^{-\lambda t}\,dt = \tfrac{e^{-\lambda a} - e^{-\lambda b}}{\lambda} \|x\|_X,$$

i.e. the integral is bounded and taking the limits $a \to 0$ and $b \to \infty$ shows

$$\|R(\lambda)x\|_X \leq \tfrac{1}{\lambda}\|x\|_X \qquad \text{for all } x \in X.$$

For the conversion, we assume that $A : D(A) \mapsto X$ is a closed linear operator and define for all $\lambda > 0$ the *Yosida approximation* of A,

$$A_\lambda = \lambda A R(\lambda, A).$$

One can show that A_λ is a bounded linear operator on X satisfying $\lim_{\lambda\to\infty} A_\lambda x = Ax$ for all $x \in D(A)$, see [Vra03, Lemma 3.2.1], that generates a uniformly continuous contraction semigroup $\{e^{tA_\lambda}\}_{t\geq 0}$, see [Vra03, Lemma 3.2.2].

Again, by taking the limits

$$\lim_{\lambda\to\infty} e^{tA_\lambda} x = T(t)x$$

one finds a semigroup $\{T(t)\}_{t\geq 0}$ that is strongly continuous, contractive and generated by A, see [Vra03, §3.2]. ■

The condition on the resolvent in the previous theorem, can be rewritten as

$$\|(\lambda \mathrm{id} - A)^{-1} x\|_X \leq \tfrac{1}{\lambda}\|x\|_X$$

for all $x \in X$ and $\lambda > 0$. Determining the inverse of $\lambda\mathrm{id} - A$ might be very challenging, and we therefor introduce the following notion, see [EN00, Definition 3.13].

Definition C.4 — Dissipative operator. A linear operator $(A, D(A))$ on a Banach space X is called *dissipative*, if

$$\|(\lambda \mathrm{id} - A)x\|_X \geq \lambda \|x\|_X \tag{C.2}$$

for all $x \in D(A)$ and $\lambda > 0$.

If we consider operators acting on a Hilbert space H we can identify H with its dual space and rewrite (C.2) in terms of the scalar product.

Lemma C.1 A linear operator $(A, D(A))$ on a Hilbert space H is dissipative if and only if

$$\mathrm{Re}(\langle x, Ax\rangle_{\mathrm{H}}) \leq 0 \tag{C.3}$$

for all $x \in D(A)$.

Proof. This lemma is a reformulation of [EN00, Proposition 3.23]. Let $(A, D(A))$ be a dissipative operator and $\lambda > 0$. For all $x \in D(A)$ and $\lambda > 0$, we have

$$\lambda^2 \|x\|_{\mathrm{H}}^2 \leq \langle \lambda x - Ax, \lambda x - Ax \rangle_{\mathrm{H}} = \lambda^2 \|x\|_{\mathrm{H}}^2 + \|Ax\|_{\mathrm{H}}^2 - 2\lambda \mathrm{Re}(\langle x, Ax \rangle_{\mathrm{H}}),$$
$$\mathrm{Re}(\langle x, Ax \rangle_{\mathrm{H}}) \leq \tfrac{1}{2\lambda} \|Ax\|_{\mathrm{H}}^2.$$

Taking the limit $\lambda \to \infty$ yields $\mathrm{Re}(\langle x, Ax \rangle_{\mathrm{H}}) \leq 0$ for all $x \in D(A)$. Vice versa, assume that (C.3) holds for all $x \in D(A)$ and take $\lambda > 0$. Then, the Cauchy Schwarz inequality implies

$$\|\lambda x\|_{\mathrm{H}} \|\lambda x - Ax\|_{\mathrm{H}} \geq |\langle \lambda x, \lambda x - Ax \rangle_{\mathrm{H}}| \geq \|\lambda x\|_{\mathrm{H}}^2 + \lambda \mathrm{Re}(\langle x, Ax \rangle_{\mathrm{H}}) \geq \lambda^2 \|x\|_{\mathrm{H}}^2.$$

■

Since an lower bound for an operator implies that its inverse exists and is continuous, see [Gol66, Theorem I.3.7], we can rewrite the Hille-Yosida theorem in terms of dissipative operators. This statement originally goes back to [LP61].

Theorem C.4 — Lumer Phillips. Let $(A, D(A))$ be a densely defined closed linear operator on a Banach space X. Then, $(A, D(A))$ generates a strongly continuous contraction semigroup on X if and only if A is dissipative and there exists a $\mu > 0$ such that $\mathrm{range}(\mu \mathrm{id} - A) = X$.

Proof. This result can also be found in [EN00, Theorem II.3.15]. Let $(A, D(A))$ be the generator of a strongly continuous contraction semigroup. Then, by the Hille-Yosida Theorem, $(\lambda \mathrm{id} - A)^{-1}$ is a linear operator for all $\lambda > 0$ and satisfies

$$\|(\lambda \mathrm{id} - A)^{-1} x\|_X \leq \tfrac{1}{\lambda} \|x\|_X$$

for all $x \in D(A)$. In other words, $(\lambda \mathrm{id} - A)$ is a bijective operator on X for all $\lambda > 0$ and it holds

$$\|(\lambda \mathrm{id} - A)x\|_X \geq \lambda \|x\|_X.$$

For the conversion assume that $(A, D(A))$ is a dissipative operator and $\mu \mathrm{id} - A$ surjective for a $\mu > 0$. Then, $\mu \in \rho(A)$ and

$$\|R(\mu, A\|_{\mathcal{L}(X)} \leq \tfrac{1}{\mu}$$

since $(A, D(A))$ is dissipative. The series expansion for the resolvent, see [EN00, Proposition IV.1.3] moreover yields for all $\lambda \in (0, 2\mu)$,

$$R(\lambda, A) = \sum_{k=0}^{\infty} (\mu - \lambda)^k R(\mu, A)^{k+1}.$$

An iterative application of this result shows $(0, \infty) \subset \rho(A)$ and $\|R(\lambda, A\|_{\mathcal{L}(X)} \leq \frac{1}{\lambda}$ for all $\lambda > 0$. The existence of a strongly continuous contraction semigroup then follows by the

Hille-Yosida Theorem C.3. ■

A corollary to this theorem can be given in terms of the adjoint operator A^*. This way is more convenient for us, since we do not have to check the range of an operator, but only its adjoint that can be easily deduced for quadratic operators.

Let X be a Banach space, X^* its dual space and $(A, D(A))$ a linear operator on X. Then, the adjoint A^* of A is defined via

$$(A^*y)(x) = y(Ax)$$

for all $x \in D(A) \subset X$ and $y \in D(A^*) \subset X^*$ see [RS80, §V.I.2]. If we consider a Hilbertspace H, then we can rewrite this as

$$\langle Ax, y\rangle_{\mathrm{H}} = \langle x, A^*y\rangle_{\mathrm{H}}$$

for all $x \in D(A) \subset \mathrm{H}$ and $y \in D(A^*) \subset \mathrm{H}$.

Corollary C.1 Let $(A, D(A))$ be a densely defined closed linear operator on a Banach space X. If both A and its adjoint A^* are dissipative, then $(A, D(A))$ generates a strongly continuous contraction semigroup on X.

Proof. A proof of this result can be found in [EN00, Corollary II.3.17]. ■

We turn now to the quadratic operators investigated in the dynamic part of this thesis. We consider the Hilbert space $L^2(\mathbb{R}^n)$ and

$$-\tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}} = -\tfrac{\mathrm{i}}{2\varepsilon}\hat{z}^T H\hat{z}, \qquad \text{with } H = H^T \in \mathbb{C}^{2n\times 2n}.$$

Since $\hat{z}$ is self-adjoint, we easily find $\widehat{\mathcal{H}}^* = \frac{1}{2}\hat{z}^T\overline{H}\hat{z}$ and $\widehat{\mathcal{H}}$ is self-adjoint if and only if $\mathrm{Im}(H) = 0$. In general, we try to handle a linear, but unbounded, non-selfadjoint operator.

Lemma C.2 The quadratic operator $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ is a closed operator on the dense subset $\mathcal{S}(\mathbb{R}^n)$ of $L^2(\mathbb{R}^n)$ and dissipative if and only if

$$\mathrm{Im}(H) \leq 0.$$

Proof. Consider $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ and its adjoint $\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}^*$ both on the domain $\mathcal{S}(\mathbb{R}^n)$. Then, we stress for the closedness of $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ that

$$\left(-\tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}\right)^{**} = -\tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$$

and the adjoint of a densely defined operator is closed by [Gol66, Theorem II.2.6]. Furthermore with Lemma C.1 $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ is dissipative if and only if

$$\mathrm{Re}(\langle\varphi, -\tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}\varphi\rangle) = \mathrm{Re}\left(\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi)(z)\cdot -\tfrac{\mathrm{i}}{2\varepsilon}z^T Hz\,dz\right) = \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi)(z)\cdot\tfrac{1}{2\varepsilon}z^T\mathrm{Im}\,(H)\,z\,dz$$

is non-positive for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$. We now choose φ to be a Gaussian with phase space centre $z_0 = (p_0, q_0) \in \mathbb{R}^n \oplus \mathbb{R}^n$, i.e.

$$\varphi_0(z_0; x) = (\pi\varepsilon)^{-n/4} e^{\frac{\mathrm{i}}{2\varepsilon}|x-q_0|^2 + \frac{\mathrm{i}}{\varepsilon} p_0^T(x-q_0)},$$

as in Section 6.3. Then, $\mathcal{W}^\varepsilon(\varphi_0(z_0))(z) = (\pi\varepsilon)^{-n} e^{-|z-z_0|^2/\varepsilon}$ is a strictly positive Gaussian centred at z_0 and

$$\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi_0(z_0))(z) \cdot \tfrac{1}{2\varepsilon} z^T \mathrm{Im}\,(H)\, z\, dz = \tfrac{1}{\varepsilon}\, z_0^T \mathrm{Im}(H) z_0 + \mathrm{tr}(\mathrm{Im}(H)).$$

Since H is symmetric it also holds $\mathrm{Im}(H)^T = \mathrm{Im}(H)$ and by the spectral theorem, $\mathrm{Im}(H)$ is diagonalisable with an orthogonal matrix $S \in \mathbb{R}^{2n\times 2n}$. Hence, if $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ is dissipative,

$$\tfrac{1}{\varepsilon}\, z_0^T \mathrm{diag}(\lambda_1, \ldots, \lambda_{2n}) z_0 \leq -\sum_{j=k}^{2n} \lambda_k$$

where $\lambda_1, \ldots, \lambda_{2n}$ denote the eigenvalues of $\mathrm{Im}(H)$. This implies that all eigenvalues are non-positive: Assume that $\lambda_j = \max\{\lambda_k\,;\, k = 1, \ldots, 2n\} > 0$. Then, we obtain for $z_0 = \sqrt{c\varepsilon} \cdot e_j$ with $c > 0$

$$c \cdot \lambda_j \leq -\sum_{k=1}^{2n} \lambda_k < 2n \cdot \lambda_j$$

but this is a contradiction, since we may take $c > 2n$.

For the inversion assume that $\mathrm{Im}(H) \leq 0$. Then, it follows by the mean value theorem that there exists a $c \geq 0$ such that

$$\mathrm{Re}(\langle \varphi, -\tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}\varphi\rangle) = -c \cdot \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi)(z)\, dz \leq 0$$

where we utilise the marginal densities from Lemma 3.7 and $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ is dissipative. ■

Theorem C.5 — Time evolution for quadratic Hamiltonians. The operator $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ with $\widehat{\mathcal{H}} = \frac{1}{2}\hat{z}^T H \hat{z}$ and $H = H^T \in \mathbb{C}^{2n\times 2n}$ generates a strongly continuous contraction semigroup $\{\widehat{\mathcal{U}}(t)\,;\, t \geq 0\}$ that satisfies

$$\mathrm{i}\varepsilon\, \partial_t \widehat{\mathcal{U}}(t) = \widehat{\mathcal{H}}\widehat{\mathcal{U}}(t)$$

for all $t \geq 0$ if $\mathrm{Im}(H) \leq 0$.

Proof. From the previous lemma we know that $-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}$ is a closed, dissipative operator, Moreover, we find equivalently

$$\mathrm{Re}(\langle \varphi, \tfrac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}}^*\varphi\rangle) = \mathrm{Re}\left(\int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi)(z) \cdot \tfrac{\mathrm{i}}{2\varepsilon} z^T \overline{H} z\, dz\right) = \int_{\mathbb{R}^{2n}} \mathcal{W}^\varepsilon(\varphi)(z) \cdot \tfrac{1}{2\varepsilon} z^T \mathrm{Im}\,(H)\, z\, dz$$

and thus also the adjoint $(-\frac{\mathrm{i}}{\varepsilon}\widehat{\mathcal{H}})^*$ is dissipative if $\mathrm{Im}(H) \leq 0$. The claim then follows by Corollary C.1 and Theorem C.1. ■

D. Acknowledgement

First of all I would like to thank my parents without whom I wouldn't have been able to study. I am very grateful for your support and patience.

Then, I would like to especially thank my supervisor Caroline Lasser for always encouraging me to follow my ideas and motivating me whenever I needed it. I could not imagine a better mentor.

I also need to mention Roman Schubert who I visited at the beginning of my PhD in Bristol and who answered all of my questions so patiently. Thanks for showing me that a pub can also be a great place to work!

Moreover, I very appreciate the discussions I had with George Hagedorn and Tomoki Ohsawa on the wave packets and Lagrangian subspaces. You gave me a lot more insight into these topics.

A special thanks goes to my colleagues at TUM who made work, and especially coffee breaks, much more fun. Just to name a few:
Anna, Karin, Katharina, Andi, Max, Schorsch, Benedict, Horst, David, Johannes, Ilja, Giulio, Patrick, Eva - yes, sometimes I wonder too how I ever finished this work.

In particular, I need to emphasis my gratitude for Paul, who just started his PhD, but helped me with so many comments on my thesis and Michi for providing the best, free coffee ever.

Another thanks goes to Alex, Nico and Torsten who accompanied me through my mathematical studies, Alex for being my back up and Torsten for frequently asking me when I will finally finish.

Last but not least, I thank Philipp for his appreciation and assistance through my PhD. You are not only the technical support of my choice, but also my best friend.

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