Fakultät für Physik

PHYSIK-DEPARTMENT E13

Hochfrequente Zustandsdichte und Phononenlokalisierung in ungeordneten Festkörpern

Constantin Philemon Tomaras

Vollständiger Abdruck der von der Fakultät für Physik

der Technischen Universität München zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften genehmigten Dissertation.

Vorsitzender: Univ.-Prof. Dr. W. Petry

Prüfer der Dissertation:

1. apl. Prof. Dr. W. Schirmacher

2. Univ.-Prof. Dr. J. L. van Hemmen

3. ——————————

Die Dissertation wurde am 05.11.2013 bei der Technischen Universität München eingereicht und durch die Fakultät für Physik am 17.12.2013 angenommen.

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genehmigtes Titelblatt

Localization of sound waves in glasses

Ph.D. Thesis

of

Constantin Tomaras

Contents

1 Introduction

1.1 Preliminary Statements

The present work concludes the theory of Schirmacher et al., which explains the famous "Boson-peak anomaly" of the vibrational density of states of glasses, as an effect related to an elastic medium with weakly fluctuating elastic constants. Although this theory was in quite good agreement with the experimental data, some criticism has been raised, which basically concerned about the high-frequency corrections onto the low frequency approximation of the calculation. The present work answers this question by showing, that these contributions do not alter the previous results, but offer a new possibility to determine the disorder parameter of the theory, directly from the experiment. Therefore a new possibility of proofing the theory is provided, because the disorder parameter, which can now be extracted from the high-frequency density of states, should match the one which is fitted to explain the low frequency properties of the density of vibrational states.

In order to establish the theory, we will provide a short review on what has been done within the last 25 years on the subject, and what has remained unclear. Within the second part we reformulate the theory in the Keldysh formalism, which is the common state of the art method in field theories of disordered solids. Previous approaches always used the old fashioned and questionable replica method instead. Then we investigate the high-frequency density of states within the instanton method, which for theories of disordered electrons always yielded strong localized states. For this we briefly summarize what should be known about the basic structure of the Keldysh path integral, and elaborate the instanton picture for a disordered longitudinal polarized sound wave.

Then we show, how the same instanton correction would look like in the Bosonized theory, following the genuine work of McKane and Stone, which was formulated within the old replica formalism.

After the nature of the high-frequency correction is phenomenological well understood, they are easily generalized onto the vector model (longitudinal and transverse) sound-waves. In the end we will perform numerical calculations to study the nature of the "localization-physics", e. g. if sound waves really become strongly localized (exponential enveloping function), or remain long-range in nature. Although it is an interesting question, these details of the sound-wave function, describing a wave which becomes decelerated through disorder induced non-linear effects, do not alter the frequency-dependence of the density of states, whose generic frequency dependence seems now very well understood.

1.2 Previous approaches onto the density of vibrational states in glasses

Until today there is no commonly accepted definition of the glassy state Biroli (50, 10, 11, 17, 42). From the structural standpoint one can distinguish between network glasses, which are covalently bonded and those, which have more spherically symmetric bonding forces like liquid rare gases (hold together with forces which are well described by a Lennard-Jones Potential) or liquid metals (91, 22).

Glasses are formed by cooling a liquid in a way that the low-temperature ground state, which is always a crystal, is avoided. This can be achieved by sufficiently rapid cooling or by choosing a chemical composition, which strongly suppresses crystalline nucleation.

Macroscopically liquids as well as glasses are homogeneous and isotropic on a macroscopic scale. On the atomic scale the nearest-neighbor statistics, which can be extracted by neutron or X-ray diffraction shows short-range order, which is revealed by characteristic oscillations of the structure factors, which describe the diffraction rings.

Crystals, due to their lattice symmetry show the well-known Bragg peaks in the diffraction pictures.

A breakthrough in the theoretical understanding of the liquid-glass transformation was the mode-coupling theory of Bengtzelius et al., reviewed in (29, 28). In this theory, based on the Mori-Zwanzig projection technique, the correlation function of fluctuating forces in the generalized Langevin equation equation was assumed to factorize into pairs of density propagators. This leads to a feedback, which describes the structural arrest. As precursor of this dynamical transition scaling scenarions were predicted, which lead anomalously slow relaxation. These predictions were verified in many experiments. However, the mode-coupling theory predicts a sharp discontinuous glass transition T_c, which is not observed. Instead, below T_c the diffusive and viscous motion becomes activated, indicating the forming of an energetically ragged configuration landscape. (17). This leads to spatially inhomogenous relaxation processes (dynamical heterogeneity (10, 11). From the quoted reviews it becomes clear, that the important glass transition regime between T_c and the glass-blower temperature T_g (at which he can no more change the shape of the glass) is until today not understood.

It is, however, clear, that the glassy state is distinguished from the liquid state by a finite shear stiffness. The shear modulus of glasses is somewhat smaller than that of the corresponding crystals but of the same order of magnitude.

Within the glassy state there is a strong separation of time scales between the relaxational processes, which still exist (with very long relaxation times), and oscillatory motions, which we quite generally name vibrations. Like any solid material glasses support sound waves with wavelengts ranging from the extension of the sample to the nanometer regime. In the latter regime, however, which corresponds to the frequency range near $\nu = \omega/2\pi$ around 1 THz, the wave picture obviously breaks down. One observes in this regime an enhancement of the vibrational density of states over Debye's $g(\omega) \propto \omega^2$ law, which is based on the wave picture. This anomaly is historically called "boson peak", because it was first observed in Raman scattering, the intensity of which is proportional to a Bose function. This comes from the fluctuation-dissipation theorem. Because the temperature dependence of the intensity was only given by the Bose factor

this meant that the observed anomaly must be a harmonic phenomenon.

The detailed origin of the boson-peak anomaly, which can be detected not only in Raman (71), but also in inelastic neutron (13) and X-ray scattering (72), has been a subject of very intense discussion in the scientific community, studying the high-frequency vibrational dynamics with the mentioned experimental methods but also by simulations (42). Attempts to relate the boson peak to a localization transition (3, 23, 31) failed because it was shown later by simulations (24) and by field-theoretic calculations (37), based on the nonlinear sigma model, that the localization transition in glasses takes place at frequencies near the upper band edge, i.e. near the Debye frequency, much higher than the boson-peak frequency.

A successful explanation of the vibrational excitations of glasses around the boson-frequency emerges from the work of Schirmacher and coworkers.

In 1989, Schirmacher and Wagener (69) model of point masses distributed randomly in three-dimensional space, interacting trough random force constants, which depend on the distance between the points and acquire therefore their randomness. They solved this model with the help of an effective-medium approximation. This was an early version of later theoretical work with spatially varying force constants and elastic constants.

Several years later Schirmacher, Diezmann and Ganter (64) obtained quantitative results on the density of states, studying just the same approach within the coherent potential approximation, which can be understood as a generalized non-crossing approximation. They obtained a disorder-induced boson peak both from the mean-field calculation and a numerical diagonalization of the same random Hamiltonian. This proved that the CPA is not a bad approximation. The eigenvalue statistics obtained by the diagonalization showed again, that the boson peak and the localization transition are quite separate.

If one writes down the diagrammatic series for the Green's function via expansion of the resolvent, averages this over a general external distribution of force constants via a cumulant expansion, and retains only a set of so called rainbow diagrams, after resummation one obtains the CPA self consistency equation for the Green's function. A

general review has been provided by Yonezawa (89). The non-crossing approximation basically collects all diagrams which propagate within the same direction as the Green's function (retarded or advanced). However the missing diagrams which mix retarded and advanced channels, contain the localization phenomenon, either classical localization, or for electrons a special kind of quantum interference known as the weak localization effect. The Green's function calculated by SDG in CPA approximation also showed up the Boson peak anomaly, and was a tremendous success in explaining the high-frequency vibrational spectra of glasses.

However to model a glass via the underlying lattice is unphysical, and was criticized frequently. Therefore a continuum field theoretic approach has been adopted by Schirmacher, Maurer and Poehlmann (65), to get rid of the underlying unphysical lattice.

One just writes down the path-integral representation of the sound-wave Green's function and averages it, over some externally distribution capable of describing the glass, by means of the replica trick. For technical reasons a Gaussian distribution has been proposed, which refers to a very well defined average of the squared sound-velocity $\langle c^2 \rangle$, and the disorder is introduced by a fluctuating band of velocity-squares $\gamma = \langle \delta c^2 \delta c^2 \rangle$ around this mean-value. Within this continuum theory the CPA boils down, to what is known in the literature as the Self Consistent Born Approximation, which also does not take into account time-reversed scattering, and hence localization. However this is sufficient, as one is only interested in low frequency properties where no localization takes place, as low frequency and hence long wavelength sound waves will tunnel through any kind of barrier.

As the disorder parameter sets up the landscape of possible potentials, it also is the parameter which divides low frequencies, e. g. propagating sound waves, from high frequencies, e. g. trapped within the fluctuating sound wave landscape. The continuum approach also exhibited the enhancement on the vibrational density of states with respect to the Debye value, which can be understood in such an approach as marking the transition from nearly unperturbed, to random matrix eigenstates, which both are on the low frequency side.

In addition, they also discussed the effect of a potentially possible anharmonic interac-

tion introducing an additional Mode-Grüneisen parameter dependent non-linear term into the theory.

This theory was generalized onto the vector theory using Lame's formulation of elasticity theory in 2006. The advantage of using this approach is, that Lame's approach is formulated with respect to the constants measuring the energy of infinitesimal shear and bulk deformations. In a glass, the shear-modulus μ is much smaller then the bulk-deformation λ, and hence this is the quantity which should have become random (63).

In 2008 this approach has been investigated in presence of elasto-optical couplings, which gave just a tremendous agreement with the spectra one obtains in the Raman-scattering experiments (71). Until now this is the most successful theory of explaining the static structure factor at the THz-scale of glasses, beside the mode-coupling-approach.

However, something has been missing, as explained by Tomaras in 2010 (80).

Deriving Lame's elasticity theory from first principles, it allows for the inclusion of anharmonic terms which reside not on an additional parameter.

As explained by Landau in the old days, these terms do not contribute to the sound-propagation at any frequency scale, because their phase space is suppressed due to simultaneous energy and momentum conservation, as well as a linear dispersion at the vertex. However, Tomaras showed, that the spectral function in presence of disorder is lacking of momentum conservation and hence these terms have to be taken seriously. Recalculating the Brillouin line-width according to the anharmonic scattering in presence of disorder, yields to the same frequency dependence which for a crystalline solid has been calculated by Akhiezer (2) long time ago using the Boltzmann equation, but with an Mode-Grüneisen parameter.

In contrast, the disorder-dependent theory allows for a finite scattering time, due to anharmonic terms without any additional parameters, and the prefactor of the Brillouin line-width is just the temperature times the variance of the shear modulus. To summarize, the frequency dependent sound-damping line-width in glasses, is at low frequencies around several GHz proportional to ω^2, due to disorder enhanced unconventional anharmonic scattering, and undergoes a crossover to a ω^4 behavior, which is the usual Rayleigh law, as depicted in Figure 1.1 .

At very large frequencies around $1\mathrm{Thz}$ the sound damping line width exhibits a strong shoulder. As this line width also enters in the calculation of the density of states, it is this shoulder which is responsible for the enhancement of the density of states, the so called Boson-peak anomaly.

Beside the tremendous success of Schirmachers theories, to explain the vibrational properties of glasses in terms of weakly fluctuation harmonic force constants, something has been missing within all those investigations, and left some uncertainties onto the results already obtained. Clearly until the present work it is not known how these results are affected by localization corrections. There is some experimental evidence, that these corrections matter and are useful, as we explain within the next section.

1.3 Motivation of going beyond the non-crossing approximation

As already presented in the last section, the vibrational properties of glasses differ strongly from those of regular solids.

This low-frequency enhancement of the density of states with respect to the Debye ω^2-law, the so called "Boson-Peak" yielded to an enormous number of experimental investigations, simulations as well as theoretical efforts (34, 73, 88, 74, 78, 16, 61, 79, 57, 30, 49, 48, 51, 32, 93, 33, 56, 41, 25, 45, 46, 40) and has been discussed vividly since today.

Most theoretical works are simulations of the vibrational spectrum of disordered materials. Beside our own work, already reviewed in the last chapter, there is only a small number of field-theoretical approaches on to the vibrational properties of disordered systems, namely John et al. (36, 38, 35), Burin et al. (14, 58) and Gurarie and Altland (32). The first two approaches are mainly due to localization and not refer to the spectrum of propagating waves in disordered solids.

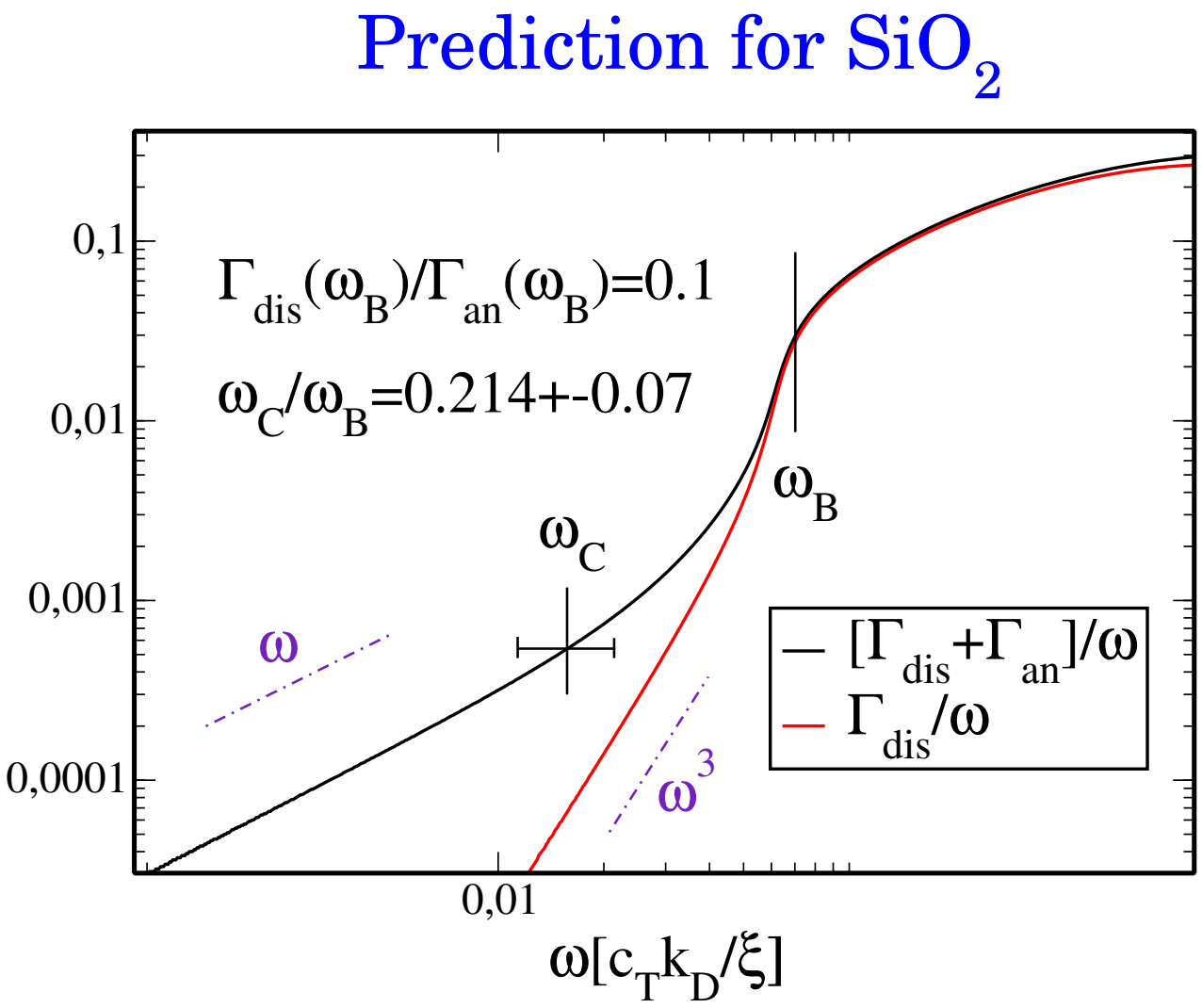

Abbildung 1.1: Inclusion of anharmonic terms allowed by elasticity theory without additional parameter yields Akhiezer-like sound damping in glasses. With the parameters of SiO_2, crossover between dominant anharmonic and dominant disorder induced scattering, should take place at $\omega_C \approx 0.2\omega_B$. This is far away from the frequency range where Akhiezers original theory applies. ω_B is the Boson peak frequency, the frequency at which the enhancement effect of the density of states due to disorder appears. Figure 1.2 shows the related density of states.

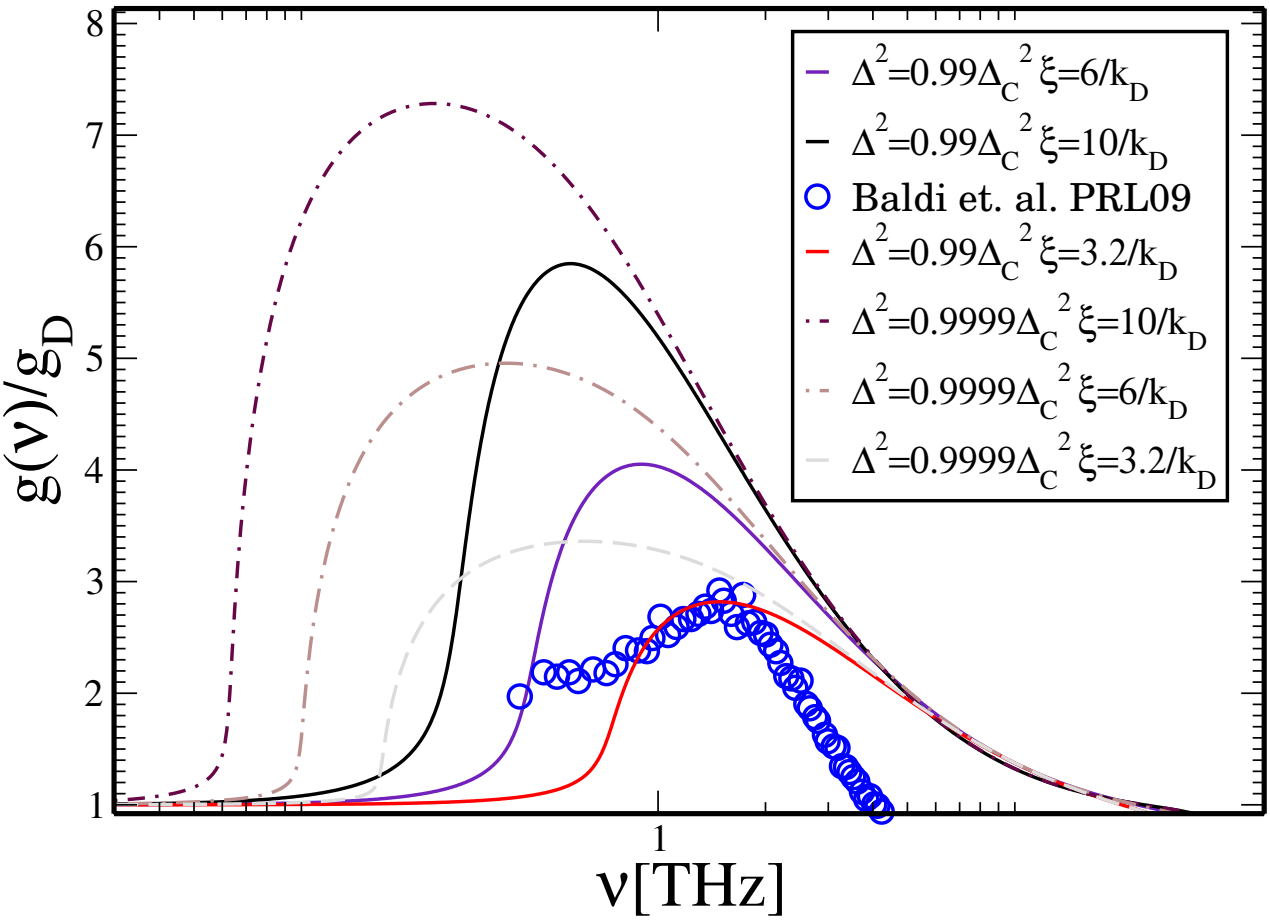

Abbildung 1.2: Evaluation of the density of states normalized to the Debye frequency in case of fluctuating shear modulus, within the SCBA approximation. Δ is the variance of the statistical distributed shear modulus of the otherwise harmonic sound wave theory, normalized onto some value Δ_c. A correlation length ξ of non-local fluctuations has been chosen. The theory is compared with the measurement of Baldi et al. on viscous Silica. The theory describes the position and height of the enhancement effect quite well. Low frequency deviations are likely to be identified with anharmonic behavior, see e.g. (68). At high frequencies the experimental data drop to zero faster than the theory, which is likely to be an exponential drop off. This is related to the fact, that the SCBA neglects the localization contributions to the density of states, which yields to this exponential tail at high frequencies. We will work out a theory of this Lifshitz tail within the present work.

The work of Gurarie and Altland is about wave-propagation in random media, and is discussed from a very general point of view. They criticize our field theoretic approaches, because it does not include the so called weak localization correction. In the quantum mechanical problem of electron-propagation in a random potential, this refers to a divergent $\langle\phi\phi\rangle$ phase correlation due to coherent back scattering.

For quantum mechanics there is an other localization mechanism, the so called strong localization which refers to a short range density $\langle\bar{\phi}\phi\rangle$. This localization happens due to statistical variations of the potential capable of trapping the quantum mechanical particle. For electrons, both mechanism lead to localization at large energies.

Within our recent works, we do not believe that the Boson-peak anomaly is related to any localization mechanism. The reason is, that the Boson-peak is related to a static renormalization of the sound velocity through the self-consistent Born approximation, while all localization corrections vanish in the low frequency limit.

However it is known, that strong localization yields to the appearance of exponential tails of the density of states, in disordered metals and semi-conductors (75). Such tails are called "Urbach tails" (81) or "Lifshitz tails" (47, 77, 26), and are mainly encountered within the gap of the electronic energy-spectrum of disordered semi-conductors(89).

Recent experiments showed exponential tails, to be present at the upper band-edge of the vibrational spectrum of glasses, both with in-elastic Neutron scattering and inelastic Nucleon-Mößbauer scattering (16, 84, 61).

Within the present work we elaborate a field theoretic explanation of this exponential tail of the density of states.

It turns out that the exponential tail of the density of vibrational states stems from the "localization" of sound waves in fluctuations of the random sound velocity,

which is the same physics which yields to strong localization of the electronic density modes $\langle\bar{\phi}\phi\rangle$. We will discuss localization both, from the elementary one-particle theory, as well as within the Bosonized framework known as the non-linear sigma model (44, 7).

As already mentioned the work of the previous two decades explained the Boson-peak anomaly in terms of sound waves with spatially dependent fluctuating sound velocities, or elasticity constants (69, 66, 64, 71). These models have been solved with the

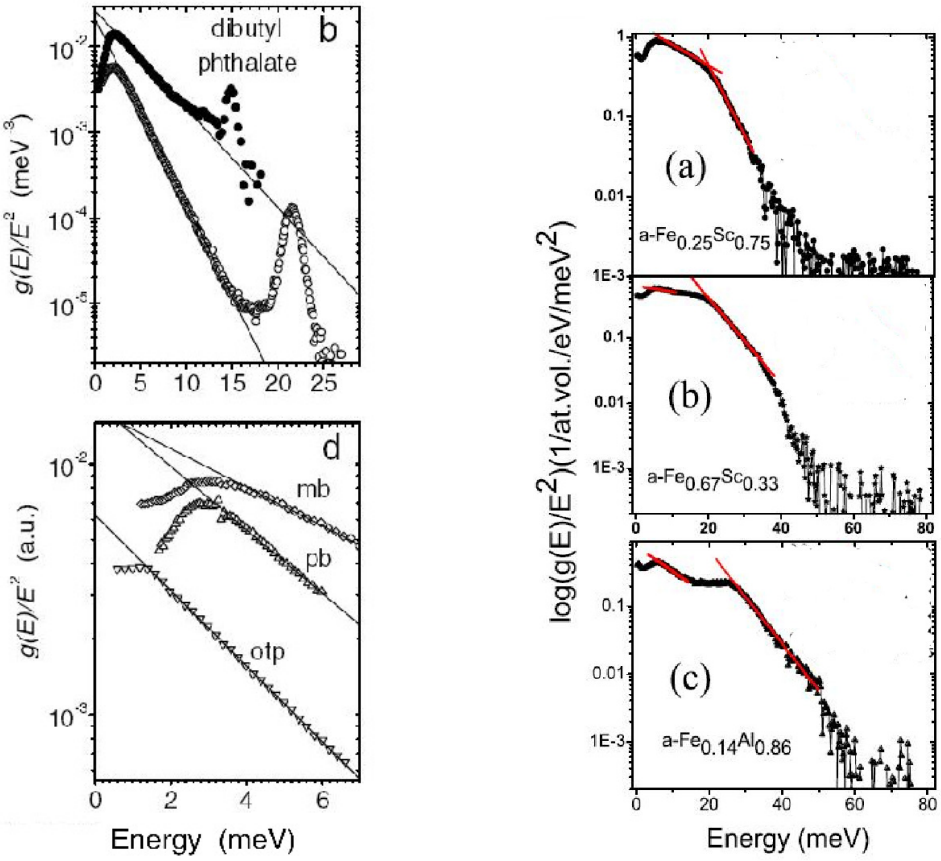

Figure 1.3: Left: reduced density of states $g(E = \hbar\omega)/E^2$ of Dibutylphtalat, obtained from inelastic Neutron-scattering (full symbols) and with nuclear inelastic scattering at Mösbauer-^{57}Fe-isotopes within the same material (open symbols) (16). The different decayrates are not yet full understood.
Right: reduced density of states of Myoglobin (mb), Poly-Butadien (pb) and Ortho-Terphenyl (otp), obtained from inelastic Neutronscattering (16) reduced density of states $g(E = \hbar\omega)/E^2$ of (a) amorphouos $Fe_{0.25}Sc_{0.75}$, (b) amorphouos $Fe_{0.67}Sc_{0.33}$, (c) amorphouos $Fe_{0.14}Al_{0.86}$, obtained from inelastic Neutronscattering (61)

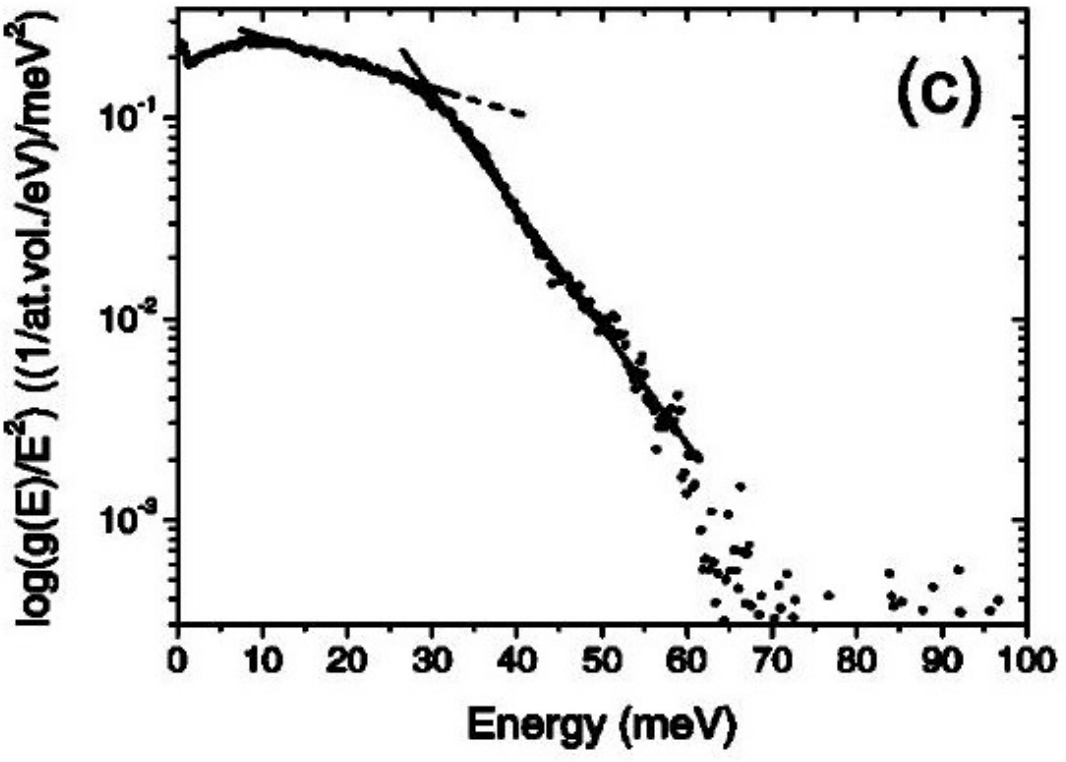

Figure 1.4: reduced density of states $g(E = \hbar\omega)/E^2$ of amorphous $FeSi_2$, obtained from inelastic nucleon scattering (84)

help of ad-hoc molecular field dynamics (effective-medium-approximation, coherent-potential-approximation) as well as with field theoretic methods (self consistent Born-Approximation).

The last theory is a saddle-point approximation of the effective field theory, which comes from the statistical average of the functional integral representation of the vacuum Green's function. With the help of these mean-field solution, it was possible to explain a vast number of quantitative agreements with the experimental measured vibrational spectra. With the help of this mean field theory it was also possible to explain the Raman spectra (71) as well as thermal properties, likewise the specific heat or thermal conductivity of a glass (63). The important aspect of this theory was the explanation of the Boson-peak anomaly which marks the transition from nearly unperturbed propagating waves to random matrix eigenstates. For random matrix eigenstates the wave-number $\mathbf{k}$ has no importance.

Within a generalization of this approach onto large frequencies we will explain the large frequency exponential tails of the above experiments in analogy with the electronic

calculation (75).

As we explained above, these tails are just well known in disordered metals and semiconductors, but have just been recently discovered at the upper band edge of the vibrational spectra of glasses (16, 84, 61). Within the present work we will show that the same theory just happens to have large frequency localization corrections, yielding to the so called Lifshitz tails in glasses. This correction stems from the localization of sound-waves within fluctuations of the sound-velocity, capable of decelerating the phonons. The decay-rate of the exponential tail is just the disorder parameter describing the mean-square deviation from the averaged squared sound velocity.

A consistent explanation of the upper edge of the vibrational spectrum is of extreme importance for the comparison with experimental data, as the discussion has so far concentrated around the low frequency Boson-peak anomaly. The effect of the localization transition which happens at the upper frequency edge was so far unknown.

1.4 The Anderson transition

Just to clarify from which point we enter the discussion of localization in phononic systems, it helps to do some brief review on the present day calculations of weakly disordered electrons without interactions.

In order to explain the vibrational spectra of glasses at low frequencies, Schirmacher et al. always worked within close correspondence to these calculations.

Indeed we will also do so within the present work. The instanton approximation, which we will discuss for the sound-wave problem within the Keldysh framework, has been carried out for electrons within the replica theory by Cardy (15). We will apply this method onto the phononic problem, however using the Keldysh technique which is slightly different. Then we show how the same correction can be rediscovered within the Bosonized version of the theory, using the Keldysh language. This refers to the method developed by McKane and Stone for the Anderson-transition within the replica language.

The transition described by Anderson 1958 appeared initially as the quantum version of the percolation transition in a classical Lorentz model: The electrons get trapped

within the potential hills. At higher energies Mott then showed that there appears a mobility edge (53, 54) which separates localized from delocalized states. Mott and Twose proved furthermore that in one dimension only localized states can exist (55). 1979 the paper of Abrahams, Anderson, Licciardello and Thouless (1) appeared, in which they showed that in addition to the percolative aspect a quantum interference effect is important: The destructive interference of closed scattering paths, traversed in different directions leads to strict localization also in two dimensions. The percolative aspect is characterized only by the density fluctuations, for the interference effect the phase fluctuations (Cooperons) are responsible. The one-parameter scaling theory of Abrahams *et al.* (1) is equivalent to the scaling theory of Wegner (85, 86). He noticed from the symmetry properties of the localization problem an analogy to the nonlinear sigma model of planar magnets or nematic liquids.

1978 Götze published a mode-coupling theory for the Anderson transition in the Mori-Zwanzig formalism, which contained only the density and not the phase fluctuations. (27). After the appearance of the paper of Abrahams *et al.* (1) Vollhardt and Wölfle (82, 83). published a field-theoretically derived mode-coupling theory, which included the interference effect, and, correspondingly predicted localization in one- and two-dimensional systems and a transition in three dimensions. It contains the scaling scenario of Abrahams *et al.*. A generalization of the Mori-Zwanzig mode-coupling theory for the Anderson transition by Götze and co-workers (6), which included the interference effect, appeared afterwards.

The theory of Vollhardt and Wölfle appears as very reliable in describing the Anderson transition. It can be transcribed to give a self-consistent theory for the ac conductivity, in which the unrenormalized conductivity obtained from a one-particle theory appears as input. Further simplified, a mathematical analogy to the determination of a localized state within a potential (18). Using this theory, combined with the coherent-potential approximation, very accurate phase diagrams - as compared to simulations - for the electronic (19, 19, 92, 76) and phononic (12, 70) localization problem could be calculated.

In two articles, which appeared independently, McKane and Stone (52) and Schäfer

and Wegner (62) showed that Wegner's generalized nonlinear sigma model could be derived step by step from the functional integral representation of the Green's function. In order to average over the quenched disorder the replica method was used (20), which is one of the three methods to perform such an average. The second is the super-symmetry method (21), the third is the use of the Keldysh-Schwinger contour (39). After the averaging a non-local ϕ^4-type field theory appears with a nonlinear kinetic term and a mass term, the coupling parameter is given by the variance of the random potential. The action of this theory can be expressed in terms of matrix fields by a Bosonization procedure (Hubbard-Stratonovich transformation (7)) or by the ghost-field method of Fadeev and Popov (8). If the variance is small with respect to the Fermi energy, the matrix field can be determined by a saddle-point approximation (self-consistent Born approximation). This is followed by a gradient expansion of the action around the saddle point to quadratic order, retaining only mass-less fluctuations, which correspond to the angle fluctuations in the normal sigma model. The generalized nonlinear sigma model is established to constrain the matrix fields to leave the disorder-induced mass term invariant. One distinguishes — as in the Wigner-Dyson classifications of random matrices — between the orthogonal, the unitary and the symplectic symmetry class. In addition to these symmetries additional classes of topological symmetry exist, which characterize systems with stable defects, for example a boundary between a metal and a superconductor (4).

By means of the perturbative renormalization group on one-loop order the phenomenological one-parameter scaling theory of Abrahams *et al.* is derived. The transition involves a fixed point of order $\epsilon = d - 2$, showing that the conductivity vanishes under renormalization group flow in two dimensions.

2 Localization within the Keldysh-framework

2.1 Brief summary of the Keldysh formalism

Many excellent reviews about the Keldysh method exist in the literature. For condensed matter path integrals one should read the Kameneev review (39), an older approach using time-ordered field operator expansion for quantum transport has been provided by Rammer and Smith (60), and if one is interested on the use of the method in high-energy physics i highly recommend the lecture of Berges (9). We also mention the Doi-Peliti lecture of Cardy, which is a similar field theory for classical diffusion reaction systems.

In the following we work out the Keldysh formalism within the semi-classical representation, because the above literature focuses on the Keldysh approach to interacting particles within the secondly quantized Heisenberg-picture, which is not used within the present work.

In quantum statistical mechanics one is usually interested in calculating time-dependent observables from

$$o(t) = \mathrm{Tr}\left[\hat{o}e^{-i\hat{H}t}\hat{\rho}e^{i\hat{H}t}\right] \tag{2.1}$$

, where the density matrix carries information about the initial state of the system. In an equilibrium system it commutes with the Hamiltonian $\hat{H}$ and no dynamics appear.

This is the usual Schrödinger picture, and not the Heisenberg picture, which includes adiabatic switching off the interaction.

In the path-integral approach onto the Keldysh formalism one introduces coherent states which are inserted left and right to the density matrix (labeled by $\pm$), together with the usual time-slicing procedure.

$$o(t) = \int \mathcal{D}[\phi_+, \phi_-] \langle\phi|o|\phi_+(t = \delta n)\rangle ... |\phi_+(\delta)\rangle \langle\phi_+(\delta)|e^{-i\hat{H}\delta}|\phi_+(0)\rangle$$
$$\times \langle\phi_+(0)|\hat{\rho}|\phi_-(0)\rangle \langle\phi_-(0)|e^{i\hat{H}\delta}|\phi_-(\delta)\rangle ... \langle\phi_-(t = n\delta)|\phi\rangle \tag{2.2}$$

Note that the quantity $\langle\phi_+|e^{-iHt}|\phi_+\rangle$ is just the usual vacuum propagator which is different from the path integral average

$$\int \mathcal{D}[\phi_+, \phi_-]\phi_+(t)\phi(t')_+ e^{iS} \tag{2.3}$$

due to the fact, that the forward and the backward fields ϕ_+, ϕ_- are connected through the density-matrix factor $\langle\phi_+(0)|\hat{\rho}|\phi_-(0)\rangle$ and the evaluation of the trace at non-measurable time points.

The evaluation of the trace yields the factor

$$\int d\phi \langle\phi|\phi_+(T)\rangle \langle\phi_-(T)|\phi\rangle = \delta(\phi_+(T) - \phi_-(T)) \tag{2.4}$$

which constrains the path integral to those configurations where ϕ_+ equals ϕ_- at the boundary.

From the mathematical point of view one would ask why these two infinitesimal factors cannot simply be ignored. This is well known: one does not change a function (in the present example the Lagrange function which is integrated with respect to time) which makes sense only after integration, when changing it at a countable set of points. It is interesting, because it tells you something about the limits of the time-slicing procedure.

Obviously the continuum limit for time-degrees of freedom is not unique, it depends on the initial state. If it is unique, it is representing a physical system, whose properties are independent of the initial state, which certainly would be the vacuum.

However, on the other hand it just reminds you to evaluate the path integral by finding the regularization you are interested in.

For initial density matrices which can be expressed in terms of an exponential of field operators, you are just left with a replicated vacuum theory in presence of external sources. For example if you are interested in a Gaussian theory with a thermal initial state the action would look like

$$S = i\int_0^T dt \begin{pmatrix} \phi_+(t) & \phi_-(t) \end{pmatrix} \begin{pmatrix} G^{-1}(t) & 0 \\ 0 & -G^{-1}(t) \end{pmatrix} \begin{pmatrix} \phi_+(t) \\ \phi_-(t) \end{pmatrix} \tag{2.5}$$

$$-\beta\phi_+(0)\phi_-(0) - i\delta(\phi_+(T) - \phi_-(T)) \tag{2.6}$$

For an infinite time contour, this can at least be evaluated formally by means of Gaussian functional integration

$$\langle\phi_\pm\phi_\pm\rangle = \int d\delta i \begin{pmatrix} G^{-1}(t,t') & \frac{\beta}{2}\delta_{t0}\delta_{t'0} \\ -\frac{\beta}{2}\delta_{t0}\delta_{t'0} & -G^{-1}(t,t') \end{pmatrix}^{-1} e^{i\delta\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} G^{-1}(t,t') & \frac{\beta}{2}\delta_{t0}\delta_{t'0} \\ -\frac{\beta}{2}\delta_{t0}\delta_{t'0} & -G^{-1}(t,t') \end{pmatrix}^{-1}\begin{pmatrix} 1 \\ 1 \end{pmatrix}}\delta+\ln Z \tag{2.7}$$

Berges et al. (9) used to work within this $\pm$ representation. The difficulty within this representation is the evaluation of the partition function $\ln Z$ which should not contribute to the dynamics.

Keldysh was the first to discover that because of the structure of the integration contour

$$S = S_{dyn} + S_{in} \tag{2.8}$$

$$S_{dyn} = S[\phi_+] - S[\phi_-] \tag{2.9}$$

$$S_{in} = f(\phi_+(0), \phi_-(0)) \tag{2.10}$$

a rotation in symmetric and anti-symmetric fields

$$\phi_{cl} = \frac{\phi_+ + \phi_-}{\sqrt{2}} \tag{2.11}$$

$$\phi_q = \frac{\phi_+ - \phi_-}{\sqrt{2}} \tag{2.12}$$

greatly simplifies the structure of the theory. The reason is as follows. As $\langle e^{iS} \rangle = 1$ per definition, the averaged dynamical part of the action has to vanish $\langle S_{dyn} \rangle = 0$. The classical component is up to additive constants directly related to the observable. If the dynamical action contains a purely classical term, and the related observable is non-zero, also the dynamical action would be non-zero $\langle S_{dyn} \rangle \neq 0$. The rotation (2.11,2.12) just removes such contributions from the dynamical action. Therefore the dynamical part of the action can not contain a pure classical configuration. Note that this is not true for the part of the action associated with the initial condition.

Here

$$\langle e^{S_{in}} \rangle = \mathrm{Tr}\rho = \int d\phi_{cl} d\phi_q \delta(\phi_q) \rho(\phi_{cl} + \phi_q, \phi_{cl} - \phi_q) = 1 \tag{2.13}$$

but in general the density matrix cannot be suggested to be an unnormalized exponential.

Therefore $\rho(\phi_{cl} + \phi_q, \phi_{cl} - \phi_q)$ depends on the classical field and the integral cancels a normalization factor.

The normalization (2.13) allows for the expansion of the initial condition:

$$\int d\phi_{cl}(0)\rho(\phi_{cl}(0),\phi_q(0))|_{\phi_q=0} = 1 \tag{2.14}$$

$$\mathrm{Tr}\left[\hat{\phi}^n\hat{\rho}\right] = \int d\phi_{cl}\phi_{cl}^n\rho(\phi_{cl}(0),\phi_q(0))|_{\phi_q=0} = \langle\phi^n\rangle \tag{2.15}$$

According to the linked cluster theorem (87)

$$\ln\int d\phi_{cl}e^{i\phi_q\phi_{cl}}\rho(\phi_{cl},\phi_{cl}) = i\langle\phi\rangle\phi_q - \frac{1}{2}(\langle\phi^2\rangle - \langle\phi\rangle^2){\phi_q}^2 + ... \tag{2.16}$$

.

However, this does not fix any initial correlation involving a power of the quantum component.

For this one has to look one step back onto the early time evolution

$$\rho(\delta,\delta) = \int d\phi_+(0)d\phi_-(0)|\phi_+(\delta)\rangle\langle\phi_+(\delta)|e^{-iH\delta}|\phi_+(0)\rangle \tag{2.17}$$
$$\times\langle\phi_+(0)|\rho|\phi_-(0)\rangle\langle\phi_-(0)|e^{iH\delta}|\phi_-(\delta)\rangle\langle\phi_-(0)|$$

$$= \int d\phi_{cl}(0)d\phi_q(0)e^{i\phi_{cl}(\delta)G_r^{-1}(\delta,0)\phi_q(0)+i\phi_{cl}(0)G_r^{-1}(\delta,0)\phi_q(\delta)} \tag{2.18}$$
$$\times\rho(\phi_{cl}(0),\phi_q(0))e^{i(\phi_{cl}(0))G_a^{-1}(0,\delta)(\phi_q(\delta))+i\phi_{cl}(\delta)G_a^{-1}(0,\delta)\phi_q(0)}$$

.

Trough this work ϕ is related to a classical variable, likewise position or displacement. Beside the labeling, the classical part of the density matrix contains already the full quantum mechanical information. Obviously the configuration $\langle\phi_{cl}\rangle = \phi, \langle\phi_q\rangle = 0$ is a possible classical result of a measurement. Quantum mechanics drops in at non-trivial two-point functions $\langle\phi_{cl}^2\rangle \neq \phi^2$.

Therefore one can use the parametrization (2.16) and set the Keldysh-component to zero in the beginning.

Then one can evaluate the integral over the initial classical component via cumulant expansion

$$\rho(\delta,\delta) =$$
$$= \delta(\phi_{cl}(\delta)G_r^{-1}(\delta,0) + G_a^{-1}\phi_{cl}(\delta)) \int d\phi_{cl}(0) e^{i\phi_{cl}(0)G_r^{-1}(\delta,0)\phi_q(\delta)} \rho(\phi_{cl}(0),\phi_q(0)=0) e^{i\phi_{cl}(0)G_a^{-1}(0,\delta)\phi_q(\delta)}$$
$$= \delta(\phi_{cl}(\delta)G_r^{-1}(\delta,0) + G_a^{-1}\phi_{cl}(\delta)) e^{i\langle\phi\rangle G_r^{-1}(\delta,0)\phi_q(\delta) - \frac{1}{2}\phi_q(\delta)G_r^{-1}(\delta,0)(\langle\phi^2\rangle - \langle\phi\rangle^2)G_a^{-1}(0,\delta)\phi_q(\delta) + \ldots} \quad (2.19)$$

Hence, if one characterizes an initial density matrix via correlations of a classical variable, the evolution carried out within an infinitesimal time step requires the classical field to satisfy the classical equation of motion, while the non trivial quantum correlations translate into various initial correlations of the quantum component.

The classical phase-space factor $\delta(\phi_{cl}(\delta)G_r^{-1}(\delta,0)+G_a^{-1}\phi_{cl}(\delta))$ may be dropped, because one may insert the solution $(G_r(\delta,0) + G_a(0,\delta))\,\phi(0)$ yielding an infinite normalization constant only at the first time step, which cannot generate dynamics. This has to happen. For a pure classical configuration $\phi_{cl}, \phi_q = 0$, the dynamical action would be zero. The integral over $e^{iS_{dyn}[\phi_{cl},0]}$ hence is a integral over unity and will diverge. As always working with path integrals, one has to single out those zero modes. In the continuum limit the sum $G_r(t,t) + G_a(t,t)$ cancels, leaving just an initial $\delta(0)$.

So for any non-classical, e.g. statistical initial condition, the Keldysh matrix is tri-diagonal,

$$S = i \int \begin{pmatrix} \phi_{cl} & \phi_q \end{pmatrix} \begin{pmatrix} 0 & G_r^{-1} \\ G_a^{-1} & G_k^{-1}(\phi_q) \end{pmatrix} \begin{pmatrix} \phi_{cl} \\ \phi_q \end{pmatrix} \quad (2.20)$$

which can now be easily evaluated, by inversion of the tridiagonal matrix.

This is the common way of regulating the Keldysh path integral. However it does not follow immediately.

For the case of writing down an operator expansion of the density-matrix likewise in the previous example the initial condition already contains both, classical and quantum fields.

Applying the rotation (2.112.12) in quadratic (Bosonic) theory, one finds the dynamical

action to be

$$S = i \int_0^T dt \begin{pmatrix} \phi_{cl} & \phi_q \end{pmatrix} \begin{pmatrix} G_K^{-1} & G^{-1} \\ G^{-1} & -G_K^{-1} \end{pmatrix} \begin{pmatrix} \phi_{cl} \\ \phi_q \end{pmatrix} \tag{2.21}$$

with $G_K^{-1}(t,t') = \frac{i\beta}{2}\delta(t)\delta(t')$. The linear constraint, which we don't write into the action from now, can be enforced by evaluating the path integral over such configuration where the quantum component vanishes at the boundary $\phi_q(T) = 0$. Also the higher moments of ϕ_q have to vanish. Therefore this term can be guessed to belong to the dynamical part of the action.

Integrating out the initial classical field yields a tridiagonal matrix, where the off-diagonal components and the quantum-quantum component of the action, got an infinitesimal regularization.

Now the Green's function can be easily inverted by means of inversion of the tridiagonal matrix with out further normalization factors

$$\langle \phi_{cl/q} \phi_{cl/q} \rangle = \begin{pmatrix} G \circ G_K \circ G & G \\ G & 0 \end{pmatrix} \tag{2.22}$$

To summarize, one can ignore about the classical-classical part of the initial density matrix, because it is a pure normalization which does not contribute to dynamics.

The best way to get rid of it is to perform an infinitesimal evolution step.

Then again the quadratic system is described by a tridiagonal matrix

$$S = i \int_{-\infty}^{\infty} dt \begin{pmatrix} \phi_{cl} & \phi_q \end{pmatrix} \begin{pmatrix} 0 & G^{-1} + i\epsilon \\ G^{-1} - i\epsilon & G_K^{-1} \end{pmatrix} \begin{pmatrix} \phi_{cl} \\ \phi_q \end{pmatrix} \tag{2.23}$$

which is readily inverted. We inserted convergence factors which do not alter the value of the integral as $\phi_q \phi_{cl} i\epsilon - i\epsilon \phi_{cl} \phi_q = 0$.

The reason is, that G^{-1} has zero values and can in general not be inverted. Without the ϵ term, one would have to exclude those zeros from the integral, and integrate over the

fluctuations, which would also be a possibility.

The ϵ term allows for direct inversion, where $(G^{-1}\pm i\epsilon)^{-1} = G_{r/a}$ is the usual retarded/advanced Green's function, according to the usual response formalism. Through the construction of fixing the initial Keldysh component via infinitesimal evolution of correlations of the classical expectation value, this convergence factor also appears within the Keldysh component.

For Gaussian initial correlations, ${G^{-1}}_K(t,t') = -\int\int {G^{-1}}_r(t,t_1)\langle\phi_k(t_1)\phi_k(t_2)\rangle^{-1}{G^{-1}}_a(t_2,t')$.

This is, because we at least now, that the full action is tri-diagonal, and hence inversion of the G^{-1} matrix yields $\langle\phi_k(t)\phi_k(t')\rangle = -G_r \circ G_K^{-1} \circ G_a$.

In addition we extended the time-integration from $-\infty$ to ∞: first after the evaluation of the observable, time-evolution can be trivially extended to ∞ by means of

$$\mathrm{Tr}[\hat{o}e^{-i\hat{H}T}\hat{\rho}e^{i\hat{H}T}] = \mathrm{Tr}[e^{iH(t-T)}e^{-iH(t-T)}\hat{o}e^{-i\hat{H}T}\hat{\rho}e^{i\hat{H}T}] \tag{2.24}$$

, yielding a new constraint at $t = \infty$.

However, as we already knew, that this deformation only contributes a factor of 1 we could also keep the old constraint.

Second, the additional unity from $-\infty$ to 0 can be inserted by means of

$$\rho(\phi_+(0),\phi_-(0)) = \langle\phi_+(0)|\hat{\rho}|\phi_-(0)\rangle = \langle\phi_+(0)|e^{-iH\delta}e^{iH\delta}\hat{\rho}e^{-iH\delta}e^{iH\delta}|\phi_-(0)\rangle \tag{2.25}$$

$$= \langle\phi_+(0)|e^{-iH\delta}|\phi_+(-\delta)\rangle\langle\phi_+(-\delta)|e^{iH\delta}\hat{\rho}e^{-iH\delta}|\phi_-(-\delta)\rangle\langle\phi_-(-\delta)|e^{iH\delta}|\phi_-(0)\rangle \tag{2.26}$$

$$= \langle\phi_+(0)|e^{-iH\delta}|\phi_+(-\delta)\rangle\langle\phi_+(0)|e^{-iH\delta}e^{iH\delta}\hat{\rho}e^{-iH\delta}e^{iH\delta}|\phi_-(0)\rangle\langle\phi_-(-\delta)|e^{iH\delta}|\phi_-(0)\rangle \tag{2.27}$$

$$= \langle\phi_+(0)|\hat{\rho}|\phi_-(0)\rangle\langle\phi_+(0)|e^{-iH\delta}|\phi_+(-\delta)\rangle\langle\phi_-(-\delta)|e^{iH\delta}|\phi_-(0)\rangle \tag{2.28}$$

.

It is then also known, that if G_K satisfies $G_K = G_R \circ G_K^{-1} \circ G_A$ it can be parametrized as $G_K = G_R \circ F - F \circ G_A$, where the Wigner-transformed of F would be called the Wigner distribution function, which satisfies the equation of motion $[-G_r^{-1}, F] = 0$. An

elementary example is provided within Appendix II.

Hence, one does not need to care much about the parametrization of the initial state. Of course one can use (2.2) in general with an arbitrary complicated state, and use Doi-Peliti-like schemes to derive exact equations of motions for the specific state. However, from the symmetry of the Keldysh action one at least knows how to include initial n-particle correlation functions directly into the dynamical part of the action, and therefore can get rid of the partition function Z, which for example was a difficulty in theory of disordered solids, where this quantity was disorder dependent.

The big advantage for the dynamical approach is hence, to replace the regularization (2.19) with one which allows for an easier evaluation (2.23) of the integral.

For theories of disordered solids there is also a second advantage. The perturbation expansion of the propagator on a single branch $\phi_+\phi_+$ would need a special normalization-factor, the so called vacuum diagrams, which include the quantity which is disorder dependent.

In a vacuum or finite temperature approach one had therefore to average the logarithm of the partition function which needs to be expanded by means of the replica trick. This always yielded problems with the analytic continuation of some replica indices, in order the evaluate some diagrams.

In contrast the Keldysh partition function always evaluates to unity in absence of sources, and in the perturbation series vacuum diagrams cancel each other, because it is an expansion with respect to the difference of the action on the forward and backward branch $S_{dyn} = S[\phi_+] - S[\phi_-]$.

Also interacting theories can be treated efficiently with the Keldysh method.

First of all the dynamical term for the two-particle interaction would be

$$V = n_+ n_+ - n_- n_- = n_{cl} n_q + n_q n_{cl} \tag{2.29}$$

$$n_{cl} = \phi_{cl}\phi_{cl} + \phi_q \phi_q \tag{2.30}$$

$$n_q = 2\phi_q \phi_{cl} \tag{2.31}$$

The term to describe an initial 2 particle distribution would hence be

$$\int\int n_q(x,t)S^{-1}(x,t,y,t')n_q(y,t') = \int\int \phi_{cl}(x,t)\phi_q(x,t)S^{-1}(x,t,y,t')\phi_{cl}(y,t)\phi_q(y,t) \quad (2.32)$$

, because it is the only one which can not be generated from a Hamiltonian quantum evolution and does also not affect the normalization of the path integral.

We will later see, that averaging a quadratic theory will yield to a term of similar structure, however with an additional factor i. It is hence fair to say, that time evolution within disordered potential is at least technical similar with time evolution in presence of non-trivial two particle initial correlations.

Like in vacuum or finite temperature field theory, one may show that the 1-particle propagator satisfies Dyson's equation

$$\begin{pmatrix} 0 & G_r^{-1} - \Sigma_r \\ G_a^{-1} - \Sigma_a & -\Sigma_K \end{pmatrix} \begin{pmatrix} G_K & G_a \\ G_r & 0 \end{pmatrix} = \delta(t-t') \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (2.33)$$

where the Self-energy Σ is believed to share the spectral structure of the 1-particle Green's function, and calculated from the usual truncation rules.

After Wigner-transformation and additional Gradient expansion this happens to be the Boltzmann-equation.

Also the Bethe-Salpeter equation for the 2 particle Green's function can be generalized

$$\begin{pmatrix} 0 & D^{-1} - \Pi_r \\ D^{-1} - \Pi_a & -\Pi_K \end{pmatrix} \begin{pmatrix} S_K & S \\ S & 0 \end{pmatrix} = \delta(t-t') \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (2.34)$$

where D is the free irreducible density propagator, and π the self-energy part of the irreducible 4-point function with respect to the free propagator D.

Equations of this type follow from an expansion of the action in terms of the density modes. Frequently equations of this type are examined to discuss many-body localiza-

tion.

However for the previous approach, the two-point function is of greater importance, as for vibrational excitations in glasses, the experimental observable which is frequently investigated is the dynamical structure factor $S(\mathbf{x}, \mathbf{x}', t, t') = \langle \rho_{cl}(\mathbf{x}t)\rho_{cl}(\mathbf{x}'t') \rangle$. For sound-waves, the density is (up to a constant) just the divergence of the displacement-field $\rho = \nabla \circ \vec{u} + \rho_0$, and hence it is sufficient to study the dynamics of the two-point function.

2.2 Sound wave action

Throughout this work we are interested in the dynamics of the displacement field $\mathbf{u}(\mathbf{x}, t)$ describing the deformation of an elastic continuum at position $\mathbf{x}$ and time t. We want to rework the theory of localization, e. g. the instanton formalism of Cardy, and the usual non-linear sigma model for this kind of waves.

For sake of simplicity we will start out with a single kind of sound-waves, e. g. longitudinal phonons $\nabla \times \hat{\mathbf{u}}(\mathbf{x}) = 0$. If $\hat{\mathbf{u}}(\mathbf{x})$ is a real valued displacement operator, the energy operator of the sound waves would be

$$\hat{H} = \frac{1}{2} \int d^d x \left(c^2 \nabla \circ \hat{\mathbf{u}}(\mathbf{x}) \nabla \circ \hat{\mathbf{u}}(\mathbf{x}) + \hat{\pi}(\mathbf{x}) \circ \hat{\pi}(\mathbf{x}) \right) \tag{2.35}$$

, where $\hat{\Pi}(\mathbf{x})$ would be the canonical momentum operator $\hat{\pi} = (\pi_x, \pi_y, \pi_z)$. (The density of the elastic medium has been set to 1).

The time-slicing procedure would be insertion of eigen-states of $\hat{u}(\mathbf{x})$ right to the evolution operator, and eigenstates of $\hat{\Pi}(\mathbf{x})$ left to the evolution operator.

The fundamental axiom of quantum mechanics states $\langle \pi(\mathbf{x}) | u(\mathbf{x}) \rangle = e^{i\Pi(\mathbf{x}) \circ \mathbf{u}(\mathbf{x})}$, where we also set $\hbar = 1$.

So

$$\langle \Pi | e^{-i\hat{H}\delta} | u \rangle = \exp\left[i \int d^d x \Pi \circ \mathbf{u} - \frac{i}{2} \int d^d x \left(c^2 \nabla \circ u(\mathbf{x})^2 + |\pi(\mathbf{x})|^2 \right) \delta \right] \tag{2.36}$$

.

After time-slicing and continuum limit one gets the action

$$S = \int dt d^d x \left[\Pi \circ \partial_t \mathbf{u} - \frac{c^2 \nabla \circ \mathbf{u}(\mathbf{x},t)^2 + |\pi(\mathbf{x},t)|^2}{2} \right] \tag{2.37}$$

on each branch.

In the Keldysh description the momentum-field can readily be integrated out leaving an action in terms of the real valued displacement field

$$S = \frac{1}{2} \int dt d^d x \mathbf{u}(\mathbf{x},t) \circ (-\partial_t^2 + c^2 \Delta) \mathbf{u}(\mathbf{x},t) \tag{2.38}$$

on each branch.

Initial correlations of the momentum-field can be ignored, because it is a pure regularization. Keeping those terms rigorously would just translate into a modified initial correlation of the displacement field. This is the great advantage of the Keldysh-description for dynamical purpose. Initial correlations (regularization) can be replaced (ignored) with some which make the evaluation of the path integral more feasible.

We elaborate this regularization further for the case of a thermal initial state in the one-dimensional example

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} = \frac{\exp\left[-\frac{\beta}{2} \int dx \left(\partial_x \hat{u}(x)^2 + \hat{\pi}(x)^2 \right) \right]}{Z} \tag{2.39}$$

This may be included by adding a Matsubara branch at $t = 0$, integrating the action within imaginary time direction. Then the Keldysh-component would have been set au-

tomatically to $G_K^{-1} = \frac{1}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)$, which is the outcome of the Matsubara summation, as performed in (87).

However, we can also try to include this directly onto the the Keldysh contour

$$\rho(u_+(0), u_-(0)) = \int d\pi_+(0)\langle u_+(0)|\pi_+(0)\rangle\langle\pi_+(0)|\frac{\exp\left[-\frac{\beta}{2}\int d^dx\,(\partial_x\hat{u}(x)^2 + \hat{\pi}(x)^2)\right]}{Z}|u_-(0)\rangle \tag{2.40}$$

$$= \int d\pi_+(0)\frac{\exp\left[-i\delta\partial_t u_+(0)\pi_+(0) - \frac{\beta}{2}\left(\partial_x u_-\partial_x u_- + \pi_+\pi_+\right)\right]}{Z} \tag{2.41}$$

$$= \frac{\exp\left[-\frac{\delta^2}{2\beta}\partial_t u_+\partial_t u_+ - \frac{\beta}{2}\partial_x u_-\partial_x u_- + const.\right]}{Z} \tag{2.42}$$

.

The temperature factor is related with the small time-step. Hence one sets $\beta = \delta\beta'$ yielding

$$\frac{\exp\left[-\frac{\delta}{2}\left(\beta'^{-1}\partial_t u_+\partial_t u_+ + \beta'\partial_x u_-\partial_x u_-\right) + const.\right]}{Z} \tag{2.43}$$

.

Clearly (2.43) is a linear evolution factor. With this one can calculate the limit

$\lim_{\delta\to 0}\langle u_{cl}(\delta)u_{cl}(0)\rangle$, which determines the initial Keldysh component through tridiagonal inversion.

Setting $\delta = \beta$, would immediately restore the Boltzmann factor with the initial classical sound wave energy.

Again, the initial normalization can be killed integrating out the classical displacement fields and the full momentum field (the β'-factor is included into the derivatives for the moment)

$$\int du_{cl}(0)\frac{\exp\left[-\frac{\delta}{2}\left\{\left((\partial_t u_{cl})+(\partial_x u_{cl})^2\right)+\left((\partial_t u_q)^2+(\partial_x u_q)\right)\right\}-\delta\left(\partial_t u_{cl}\partial_t u_q-\partial_x u_{cl}\partial_x u_q\right)\right]}{Z'} \tag{2.44}$$

$$= \int du_{cl}(0)\frac{\exp\left[-\frac{\delta}{2}\begin{pmatrix} u_{cl} & u_q\end{pmatrix}\begin{pmatrix}\partial_t^l\partial_t^r+\partial_x^l\partial_x^r & -\partial_t^l\partial_t^r+\partial_x^l\partial_x^r\\ -\partial_t^l\partial_t^r+\partial_x^l\partial_x^r & \left(\partial_t^l\partial_t^r+\partial_x^l\partial_x^r\right)\end{pmatrix}\begin{pmatrix}u_{cl}\\ u_q\end{pmatrix}\right]}{Z'} \tag{2.45}$$

$$= \exp\left[\frac{\delta}{2}\int d^dx u_q\frac{(-\partial_t^l\partial_t^r+\partial_x^l\partial_x^r)^2-\left(\partial_t^l\partial_t^r+\partial_x^l\partial_x^r\right)^2}{\left(\partial_t^l\partial_t^r+\partial_x^l\partial_x^r\right)}u_q\right] \tag{2.46}$$

$$= \exp\left[\frac{\delta}{2}\int d^dk d\omega d\omega' u_q(\omega,k)\frac{(-\omega\omega'+k^2)^2-(\omega\omega'+k^2)^2}{(\omega\omega'+k^2)}u_q(\omega',k)\right] \tag{2.47}$$

$$= \exp\left[-\frac{\delta}{2}\int d^dk d\omega d\omega' u_q(\omega,k)\frac{\omega\omega' k^2}{(\omega\omega'+k^2)}u_q(\omega',k)\right] \tag{2.48}$$

One has to think about the allowed frequencies.

For the non-interacting sound wave system, the Keldysh partition function is a product of wave number dependent exponentials. The initial factor is Gaussian distributed with the quantum field, initially the quantum component has zero expectation value.

Hence for the classical frequency $\omega(k) = ck$ the action is zero, and no quantum evolution is carried out, $u_q = 0$ automatically.

For non-classical frequencies $u_q(t/\hbar) = 0$, due to the evaluation of the trace at the boundary, hence $\omega_n(k) = ck(1 + \frac{n\pi}{\delta})$.

Hence quantum mechanics drops out in the limit of large times or large temperatures.

Evaluating the the Keldysh partition function yields

$$\sum_{nm}\langle u_{cl}(\omega_n,k)u_{cl}(\omega_m,k\rangle = \frac{\beta}{2}\sum_{nm}\frac{1}{\omega_n^2-k^2+i\epsilon}\frac{\omega_n\omega_m k^2}{(\omega_n\omega_m+k^2)}\frac{1}{\omega_m^2-k^2-i\epsilon} \tag{2.49}$$

$$= \frac{1}{2}\sum_n\frac{\beta k^2}{(\omega_n^2+\beta^2k^2)} = \frac{1}{2}\delta^2 k\coth(\beta k) \tag{2.50}$$

In order to have a finite classical correlation function, the small δ factor has to be identified with the regularization factor ϵ of the dynamical Green's function

$$S_{dyn} = S[u_+] - S[u_-] \tag{2.51}$$

$$= \frac{1}{2}\int_{-\infty}^{\infty} dt d^d x \begin{pmatrix} u_{cl} & u_q \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 + c^2\Delta + i\epsilon \\ -\partial_t^2 + c^2\Delta - i\epsilon & \epsilon^2 \int d\omega\omega \coth(\frac{\beta\hbar\omega}{2}) e^{i\omega t} \end{pmatrix} \begin{pmatrix} u_{cl} \\ u_q \end{pmatrix} \tag{2.52}$$

and hence

$$\langle u_{cl}(\omega,k) u_{cl}(\omega,k)\rangle = \frac{1}{2}\frac{\epsilon^2 k \coth(\frac{\beta\hbar\omega}{2})}{(\omega - ck)^2 + \epsilon^2} = \begin{cases} \frac{\omega}{2}\coth(\frac{\beta\hbar\omega}{2}) & \omega = ck \\ 0 & \omega \neq ck \end{cases} \tag{2.53}$$

.

Note that the appearance of the frequency-factor in front of the hyperbolic cotangent is due to the use of the semi-classical expansion. In the secondly quantized picture, this factor is canceled by the normalization of phonon creation and annihilation operators $a^+ \propto \frac{1}{\sqrt{\omega}}$, and hence the normalization of the phonon coherent states.
In general this is a very difficult method to determine the initial thermal state.

Within the Keldysh prescription this can be omitted, by introducing an generic e. g. anharmonic interaction and calculate the self-energy correction to linear order for arbitrary states.

Then the equilibrium density matrix is determined from the requirement that these corrections have to vanish, which for Bosons yields to the Bose-factor with undetermined β factor.

In any case, an arbitrary state can be introduced using the tridiagonal inversion procedure.

2.3 Keldysh action

For scalar sound waves the dynamical action is hence given by

$$S_{dyn} = S[u_+] - S[u_-] \tag{2.54}$$

$$= \frac{1}{2}\int dtdt'd^dx \begin{pmatrix} \mathbf{u}_{cl} & \mathbf{u}_q \end{pmatrix} \circ \begin{pmatrix} 0 & -\partial_t^2 - c^2\overleftarrow{\nabla}\nabla \circ -i\epsilon \\ -\partial_t^2 - c^2\overleftarrow{\nabla}\nabla \circ +i\epsilon & G_k^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{cl} \\ \mathbf{u}_q \end{pmatrix} \tag{2.55}$$

where the Keldysh component G_K^{-1} accounts for the initial 2-point function. $\overleftarrow{\nabla}$ is the left acting gradient operator $\mathbf{u} \circ \overleftarrow{\nabla} = \nabla \circ \mathbf{u}$.

If one wants to add for example an initial energy-correlation function, which is a special kind of 4-point function, one would have to add the term

$$\int\int \mathbf{u}_q^i(\mathbf{x},t)\mathbf{u}_{cl}^j(\mathbf{x},t)\Phi_{ij}^{lm}(\mathbf{x},t;\mathbf{y}t')\mathbf{u}_q^l(\mathbf{y}t')\mathbf{u}_{cl}^m(\mathbf{y}t') \tag{2.56}$$

, because it is the only one which allows for a conservation of the Keldysh partition function (equals 1), but cannot be generated by a 4-point part of the Hamiltonian.

The same term would be generated, by attaching the elastic medium to some kind of external heat bath (90). Here Φ would be called the spectral function of the heat bath.

Now to the disorder.

It is very well established, that the vibrational degrees of freedom of a glass, can be phenomenological described by a set of randomly distributed systems with spatial dependent force constants.

It needs not necessarily be Gaussian, however modeling a glass, it should be spatially independent on average.

So we introduce an arbitrary statistical weight $P[c^2(\mathbf{x})]$ with

$$\sum P[c^2(\mathbf{x})]c^2(\mathbf{x}) = c^2 \tag{2.57}$$

, and arbitrary higher correlation functions. If its Gaussian then only the second irreducible correlation function

$$\sum P[c^2(\mathbf{x})]\left(c^2(\mathbf{x})-c^2\right)\left(c^2(\mathbf{y})-c^2\right)=K(\mathbf{x},\mathbf{y}) \tag{2.58}$$

is different from zero.

Therefore, one has to calculate observable quantities from (2.55), with arbitrary $c^2(\mathbf{x})$, and average them over all configurations. This limit is believed to be exchangeable, average the diagrammatic series for a certain observable first, and then try to re sum. In the Keldysh-prescription this can be done immediately.

In vacuum or thermal field theory the path integral always contains a possible infinite phase factor $e^{i\varphi}$ which is included in the normalization of the partition function, depending on the Hamiltonian and hence the statistical fluctuating quantity, which needs to be taken into account.

In Keldysh theory, this factor will be always canceled by the same on the backward branch $e^{-i\varphi}$, and no disorder dependent normalization occurs.

Therefore the statistical average over the Keldysh partition function can be done immediately via cumulant expansion (59, 87)

$$\sum P[c^2(\mathbf{x})]e^{ic^2(\mathbf{x})(\nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q)} \tag{2.59}$$
$$=e^{ic^2\int u_{cl}\Delta u_q-\frac{1}{2}\int\int K^{-1}_{(2)}(\mathbf{x},\mathbf{y})(\nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q)(\nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q)+\frac{1}{3}\int\int\int K^{-1}_{(3)}(\mathbf{x},\mathbf{y},\mathbf{z})(\nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q)(\nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q)(\nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q)+\ldots}$$

where K_n^{-1} is the inverse n-sound velocity correlation function.

Therefore a theory of disordered phonons is a free theory, subjected to the disorder induced interaction

$$S_{dis}[u_{cl},u_q]=\sum_{n=2}^{\infty}K^{-1}_{(n)}\prod_{i=1}^{n}\int d^d\mathbf{x}_i dt_i(\nabla_{\mathbf{x}_i}\circ\mathbf{u}_{cl}(\mathbf{x}_i,t_i)\nabla_{\mathbf{x}_i}\circ\mathbf{u}_q(\mathbf{x}_i,t_i)) \tag{2.60}$$

. For weakly correlated disorder, this series can always be truncated at $n=2$, which

however has the problem of allowing for imaginary sound velocities, which is believed to be unphysical. Recent investigations showed, that there is no difference between a Gaussian and a truncated Gaussian distribution, as long as the fluctuation of the sound velocity is not to large (43).

To second order the theory is structural similar with the theory of phonons which couple to a heath bad, the dissipative quantum tunneling problem (90). However, due to the extra factor of i the real and imaginary part of the spectral function would have been interchanged, and there is no time correlation.

2.4 Instanton approach onto localization

Up to Gaussian order in the disorder term the path integral one has to solve is

$$\int \mathcal{D}[u_q, u_{cl}] e^{iS} \tag{2.61}$$

$$iS = \frac{i}{2}\int dt dt' d^d x \begin{pmatrix} \mathbf{u}_{cl} & \mathbf{u}_q \end{pmatrix} \circ \begin{pmatrix} 0 & -\partial_t^2 + c^2\Delta + i\epsilon \\ -\partial_t^2 + c^2\Delta - i\epsilon & G_k^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{cl} \\ \mathbf{u}_q \end{pmatrix}$$
$$-\frac{\gamma}{2}\int dt dt' d^d x \left(\nabla \circ \mathbf{u}_q \nabla \circ \mathbf{u}_{cl}\right)_{t,x} \left(\nabla \circ \mathbf{u}_q \nabla \circ \mathbf{u}_{cl}\right)_{t',x} \tag{2.62}$$

where we introduced the so called disorder parameter

$$K(\mathbf{x} - \mathbf{y}) = \frac{\gamma}{2}\delta(\mathbf{x} - \mathbf{y}) \tag{2.63}$$

, describing the range of the local fluctuations of the squared sound velocity.

A saddle-point approximation of an ordinary integral over an exponential assumes that the exponential can be written into the form

$$e^{iNf(x)} \tag{2.64}$$

with N a large number. Then the exponential factor is strong oscillating and the integral is dominated by the stationary-points of $f(x)$, while corrections can be shown to be of the order $1/N$. However this is not true for the expression (2.62). The disorder part is of the form

$$e^{-\frac{\gamma}{2}f(x)} \tag{2.65}$$

, a factor which is dominated by the minima of $f(x)$ as long as γ is a large number.

In order to identify some expansion parameter think of the following. Scattering within a static potential cannot change the energy/frequency of a sound wave. The same holds for the weighted average over individual static potentials. Hence locally $\partial_x u \propto \omega$ holds. The disorder part of the action hence scales according to

$$e^{-\frac{\omega^{4-d}}{2\gamma}(\partial\tilde{u})^4} \tag{2.66}$$

, where γ has moved to the denominator due to the scaling transformation $u = \gamma^{-\frac{1}{2}}\tilde{u}$. Hence in 3 dimension a simple saddle-point works for frequencies large with respect to the disorder parameter.

Clearly if ω falls below the disorder-parameter no simple saddle-point applies. This would be a strong coupling theory.

On the other hand if the frequency of the sound wave is large, it is scattered between large fluctuations of the sound velocities, there will be regions of large fluctuations of sound velocities substantially lower then the statistical average.

For such configurations the exponential would be like

$$e^{\frac{-\omega^4+i\omega^2}{2\gamma}} \tag{2.67}$$

, which tells you a simple saddle-point will in general work for frequencies large with respect to the disorder parameter.

Minimizing the action with respect to the fields u_q, u_{cl} at finite time-contour yields

$$i\left(-\partial_t^2 + c^2\Delta\right)\mathbf{u}_{cl} = \gamma\nabla\left[\left(\int_0^T dt'\nabla\circ\mathbf{u}_q(t')\nabla\circ\mathbf{u}_{cl}(t')\right)\nabla\circ\mathbf{u}_{cl}(t)\right] \tag{2.68}$$

$$i\left(-\partial_t^2 + c^2\Delta\right)\mathbf{u}_q = \gamma\nabla\left[\left(\int_0^T dt'\nabla\circ\mathbf{u}_q(t')\nabla\circ\mathbf{u}_{cl}(t')\right)\nabla\circ\mathbf{u}_q(t)\right] \tag{2.69}$$

.

First of all, if one seeks for a solution with $\mathbf{u}_q = 0$, the above equations just reduce to the ordinary classical wave equation

$$\left(-\partial_t^2 + c^2\Delta\right)\mathbf{u}_{cl} = 0 \tag{2.70}$$

.

This is no accident as another global prefactor is $\frac{1}{\hbar}$ which we set to 1, hence the high frequency expansion also incorporates a semi-classical expansion, which for a non-interacting set of harmonic oscillators is known to be exact.

Note that for configurations of zero quantum component, the evolution on the forward branch equals the evolution on the backward branch $\mathbf{u}_+(xt) = \mathbf{u}_-(yt)$.

For observable quantities this equation must always be satisfied as

$$u_+(t) = \mathrm{Tr}\left[\hat{\mathbf{u}}\hat{\rho}(t)\right] = \mathrm{Tr}\left[\hat{\rho}(t)\hat{\mathbf{u}}\right] = \mathbf{u}_-(t) \tag{2.71}$$

$$\langle u\rangle = \frac{1}{2}(\mathbf{u}_+ + \mathbf{u}_-) = \frac{1}{\sqrt{2}}\mathbf{u}_{cl} \tag{2.72}$$

$$0 = \frac{1}{2}(\mathbf{u}_+ - \mathbf{u}_-) = \frac{1}{\sqrt{2}}\mathbf{u}_q \tag{2.73}$$

.

So the classical field always corresponds to observables (up to additive vacuum constants). For an observable quantity, the expectation value of the quantum-component has to vanish.

So what does a non-zero $\mathbf{u}_q$ mean? First of all, one has to remember that the saddle-

point solution is different from the exact expectation value of the field. If $\mathbf{u}_q$ is different from zero it is guaranteed that the exact expectation value $\langle \mathbf{u}_q \rangle = \mathbf{u}_q + O(1/\omega)$ will be reset to zero by the higher corrections.

To explore the meaning of the quantum component one has to remember about the time slicing procedure. Here $\mathbf{u}_+(t)$ is always one time-step ahead of $\mathbf{u}_-(t)$. So within time slicing the correct equation would be

$$\mathbf{u}_+(t-\delta) = \mathrm{Tr}\left[\hat{\mathbf{u}}\hat{\rho}(t)\right] = \mathrm{Tr}\left[\hat{\rho}(t)\hat{\mathbf{u}}\right] = \mathbf{u}_-(t) \tag{2.74}$$

which reduces to (2.71) in the continuum limit.

Therefore it is clear that the anti-symmetric combination $\mathbf{u}_+(t) - \mathbf{u}_-(t)$ should be interpreted as $\mathbf{u}_+(t+\delta) - \mathbf{u}_-(t)$ whose expectation value is proportional to the time derivative of the displacement field times an infinite small regularization factor, which can be canceled f.e. by Gaussian functional integration.

Hence non-zero quantum components within a saddle-point approximation contribute to correlation functions, which in the present theory comes from a finite action, and only have to vanish at the single instant at boundary $\mathbf{u}_q(T) = 0$.

One can read of a possible saddle-point solution setting $\mathbf{u}_{cl} = \mathbf{u} = i\mathbf{u}_q/\Theta(t)$ (quantum component has been chosen in order to satisfy a causal evolution equation) yielding a single equation for the real valued displacement field:

$$\left(-\partial_t^2 + (c^2 - 3\gamma \int_{-\infty}^{t} dt' (\nabla \circ \mathbf{u}(x,t'))^2)\Delta\right)\mathbf{u}(x,t) = 0 \tag{2.75}$$

This is a classical theory of localization. If there is a region where a finite imaginary strain condensates, this yields to a region whose sound velocity is substantially lower than the average of the material.

The most interesting thing is the factor of 3 in front of the disorder parameter in equation (2.75). On the level of the action the the force constant is

$$c^2(x) = (c^2 - \gamma(\nabla \circ \mathbf{u})^2) \tag{2.76}$$

, which differs from the sound-velocity by the additional additive term $2\gamma(\nabla \circ \mathbf{u})^2\Delta\mathbf{u}$. This term describes the amplitude shift of a phonon moving in the spatial varying force-constant landscape.

According to classical wave mechanics, wave propagation from the region with lowered sound velocity, into the region with the average higher sound velocity will be suppressed, yielding a positive ratio $\Delta(\mathbf{u})_i \propto (\mathbf{u})_i^n$.

Equation (2.75) is believed (15) to be safely replaced with the frequency diagonal

$$\left(\omega^2 + \left(c^2 - 3\gamma\nabla \circ \mathbf{u}(\omega, x)\nabla \circ \mathbf{u}(\omega, x)\right)\Delta\right)\mathbf{u}(\omega, x) = 0 \tag{2.77}$$

yielding

$$\Delta\mathbf{u}(\omega, x) = -\frac{\omega^2}{(c^2 - 3\gamma\nabla \circ \mathbf{u}(\omega, x)\nabla \circ \mathbf{u}(\omega, x))}\mathbf{u}(\omega, x) \tag{2.78}$$

Localization happens if $\frac{\Delta(\mathbf{u})_i}{(\mathbf{u})_i} > 0$, which is equivalent with $(c^2 - 3\gamma\nabla \circ \mathbf{u}(\omega, x)\nabla \circ \mathbf{u}(\omega, x)) < 0$. The corresponding force-constants are $(c^2 - \gamma\nabla \circ \mathbf{u}(\omega, x)\nabla \circ \mathbf{u}(\omega, x))$, which can be positive anyway.

In words: Localization happens if the local variation of the force-constant falls below the critical value $\frac{2}{3}c^2$, where c^2 would be the average force constant in absence of the non-linear memory-effect.

In the latter we show, that equation (2.75) necessarily yields to such local critical behavior.

A phenomenological solution of the real-time integro differential equation (2.75) can be developed as follows: Consider a classical solution to the wave-equation $\mathbf{u}_q = 0$

which is located at position $\mathbf{x_0}$ at $t = 0$

$$\mathbf{u}_{cl} = \mathbf{u}\cos(\omega t - \mathbf{kx}) \tag{2.79}$$

. As it is a classical solution it has the average sound velocity of the material $c = \frac{\omega}{|\mathbf{k}|}$. At short times below the first period $t \ll \frac{2\pi}{\omega}$ the integral in equations (2.682.69) can safely be neglected, because it does only produce time-oscillating corrections which should not contribute to a long time steady state, likewise localized standing waves.

Hence knowing a classical displacement at the position $\mathbf{x_0}$ at $t = 0$ to zeroth order in the disorder parameter γ

$$\mathbf{u}_{cl}^{(1)} = \mathbf{u}\cos(\omega t - \mathbf{k} \circ \mathbf{x}) \tag{2.80}$$

$$i\mathbf{u}_{q}^{(2)} = \mathbf{u}\cos(\omega t - \mathbf{k} \circ \mathbf{x}) \tag{2.81}$$

solves the instanton equation with non-zero quantum component, but only for positions reachable without disorder corrections from the integral hence for $\omega|\mathbf{x} - \mathbf{x_0}| < 2\pi c$.

Now insert this into the equation (2.75) and integrate over the first period.

Within the second period $\frac{2\pi}{\omega} < t < \frac{4\pi}{\omega}$ the sound wave satisfies a wave equation with lowered sound velocity

$$\left(-\partial_t^2 + (c^2 - \frac{3}{2}\gamma k^2 \langle|\mathbf{u}^{(1)}|^2\rangle_{0<t<2\pi/\omega})\Delta\right)\mathbf{u}^{(2)} = 3\gamma\left[\left(\int \nabla \circ \mathbf{u}^{(2)} \nabla \circ \mathbf{u}^{(2)}\right)\Delta\mathbf{u}\right] \tag{2.82}$$

.

Again this can be solved by neglecting the integral first, yielding (2.82) with again lowered sound velocity, within the third period.

In order to have frequency conservation throughout the different time periods, the ever lowered sound velocity has to be compensated by a ever shortened wavelength.

This can be iterated so forth, until the sound velocity reaches the critical value zero, and

also the wavelength has gone to zero; wave propagation has stopped.

One can start of symmetrically with an wave from the opposite site which will stop at the same point. The function which has been produced this way can be guessed to have an Gaussian envelope.

Figure 6.1 just shows an possible outcome of this procedure.

Note that the effective wave number of this function is not k but $\langle k \rangle = \frac{1}{N} \sum_n k^{(n)}$, where n is the index of periods. In terms of the plane-wave propagator the peak will hence be shifted towards larger wave numbers. This approximation of the memory kernel can be thought to become exact in the limit of large frequencies, because the time-difference between $\mathbf{u}^{(n)}$ and $\mathbf{u}^{(n+1)}$ becomes infinitely close. Also for large frequencies the integral becomes,

$$\lim_{T\to 0} \frac{1}{T} \int_0^{T\to 0} dt f(t) \sim \lim_{T\to 0} f(t) \tag{2.83}$$

can safely be replaced with its integrand, yielding just equation (2.77).

Note that the other possible instanton solution $\mathbf{u}'_q = -\mathbf{u}_q$, yields to a raised sound velocity, hence a raised wavelength, which is not capable of localizing sound waves.

Finally some normalization condition has to be chosen, in order to obtain a unique solution to (2.75).

As stated above, any propagating wave-like solution has to property of continuously decreasing the sound velocity within a fixed arrow of propagation. At the critical point x_c

$$(c^2 - 3\gamma \nabla \circ \mathbf{u}(\omega, x_c)^2) = 0 \tag{2.84}$$

, the Laplacian of the wave-function changes its sign, $\Delta \mathbf{u}(\omega, x_c \pm \delta) \lesseqgtr \mathbf{u}$. Hence for a continuous second derivative, the Laplacian at the critical point must vanish:

$\Delta \mathbf{u}(\omega, x_c) = 0$. Reinsertion in eq. (2.75) yields $\mathbf{u}(x_c) = 0$, which tells you that the critical sound-velocity has to be reached at a node point. Depending on the sign of $\nabla \circ \mathbf{u}$,

x_c divides the wave-like oscillating region $\Delta\mathbf{u}(\omega, |x| > |x_c|) = -|c^2(\mathbf{u})|\mathbf{u}$, from the critical region $\Delta\mathbf{u}(\omega, |x| > |x_c|) = |c^2(\mathbf{u})|\mathbf{u}$ where no further oscillations appear. In the critical region, the sound velocity decreases monotonously until the force constant reaches the critical value 0. A further cut-off has to be included in order to render force constants positive. If the theory is represented in terms of plane waves, this means a cut-off wave-number $c^2 - \gamma k_{max}^2 |\mathbf{u}(\mathbf{k}_{max})|^2 = 0$. Such cut-offs have to be provided by the higher order terms in the cumulant expansion of the probability distribution of the force constants.

It is now fair to say, that within this argumentation it is phenomenological understood, that equation (2.75) is capable of localizing sound-waves.

Of course solving a non-linear integro-partial differential equation like (2.75) exactly is quite difficult. We will perform some numerics on this equation in section 3.

At least the frequency diagonal approximation is easily solved by means of the Runge-Kutta algorithm, also performed also within section 3.

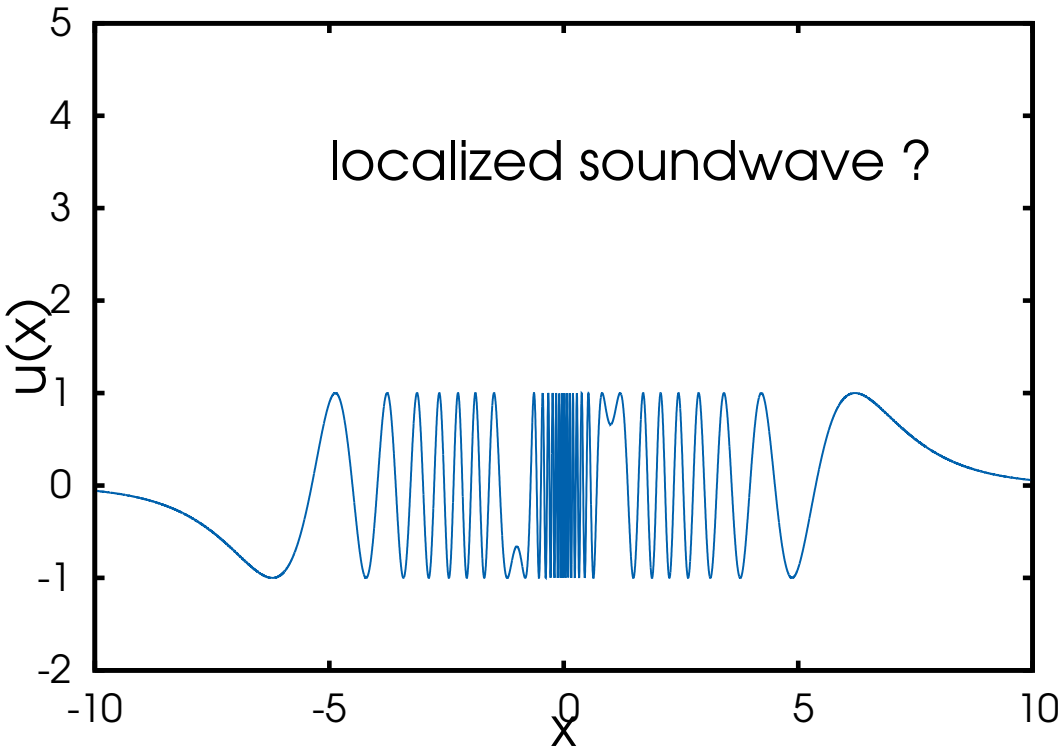

Figure 2.1: A typical state which would be obtained, by iterated forward integration of the instanton equation (2.75)

We discuss the one-dimensional example. Introducing $v = \partial_x u$ yields the system

$$\partial_x v = -\frac{\omega^2}{c^2 - 3\gamma v^2} u$$

$$\partial_x u = v$$

. As depicted in FIgure 2.2, integrating this system numerically with initial velocity $v = 0$ and small amplitude yields to a function of exponential envelope.

This is because the right hand side of

$$2\gamma v^2 \partial_x^2 u = \omega^2 u + (c^2 - \gamma v^2)\partial_x^2 u$$

is positive as long as the sound velocity is decreasing. (For $v = 0$ locally and local wave-like solution the right-hand side is $\frac{\gamma\omega^2}{c^2} u$, yielding a monotonously decreasing enveloping function.)

2.5 Green's function

From the structure of the quadratic theory (2.55) it is clear that the retarded Green's function of the displacement field, which is the inverse of $-\partial_t^2 + c^2(x)\Delta + i\epsilon$ is just the quantum classical correlation function

$$G_r^{ij}(xt, yt') = \langle \mathbf{u}_q^i \mathbf{u}_{cl}^j \rangle = \int \mathcal{D}[u_{cl}, u_q] \mathbf{u}_{cl}^i(xt) \mathbf{u}_q^j(yt') e^{iS} \tag{2.85}$$

.

As always in mean-field theory one expands the action up to quadratic order

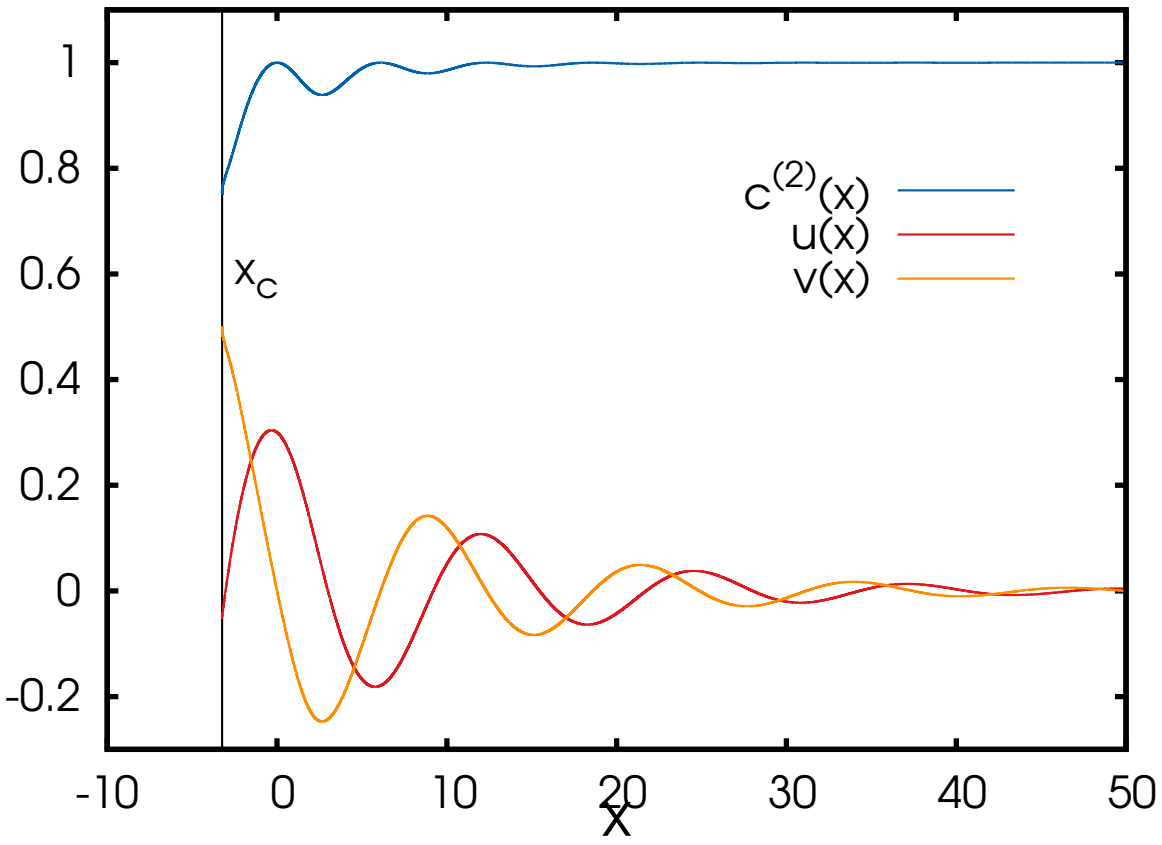

Figure 2.2: Runge-Kutta solution to (2.77) with v(0)=0,u(0)=0.3

$$S = S_0 + S_2 + S_3 + S_4 \tag{2.86}$$

with

$$iS_0 = \frac{1}{2}\int\int \begin{pmatrix} \mathbf{u}^T & \mathbf{u}^T \end{pmatrix} \begin{pmatrix} 0 & G^{-1} + \gamma\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ \\ G^{-1} + \gamma\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ & \gamma\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{u} \end{pmatrix} \tag{2.87}$$

$$iS_2 = \frac{1}{2}\int\int (\delta\mathbf{u}_q\delta\mathbf{u}_{cl}) \begin{pmatrix} 0 & G^{-1} + \gamma\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ \\ G^{-1} + \gamma\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ & (G^{-1})_K \end{pmatrix} \begin{pmatrix} \delta\mathbf{u}_{cl} \\ \delta\mathbf{u}_q \end{pmatrix} \tag{2.88}$$

$$+\frac{\gamma}{2}\int\int \left(\delta\mathbf{u}_{cl}\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ\delta\mathbf{u}_{cl} - \delta\mathbf{u}_q\overleftarrow{\nabla}(\nabla\circ\mathbf{u}\nabla\circ\mathbf{u})\nabla\circ\delta\mathbf{u}_q\right) \tag{2.89}$$

$$iS_3 = -\gamma\int\int (\nabla\circ\delta\mathbf{u}_q\nabla\circ\mathbf{u} - i\nabla\circ\mathbf{u}\nabla\circ\delta\mathbf{u}_{cl})\nabla\circ\delta\mathbf{u}_q\nabla\circ\delta\mathbf{u}_{cl} \tag{2.90}$$

$$iS_4 = -\frac{\gamma}{2}\int\int \nabla\circ\delta\mathbf{u}_q\nabla\circ\delta\mathbf{u}_{cl}\nabla\circ\delta\mathbf{u}_q\nabla\circ\delta\mathbf{u}_{cl} \tag{2.91}$$

The term (2.89) arises due to the normalization logic of the Keldysh integral an can be set to zero (compare with (2.21)). If it is kept rigorously, by inversion of the full 2x2 matrix, it is found to cancel reducible contributions of the quantum component to second order on the level of expectation values.

One should not worry about the finite action S_0 appearing, because it might not be trace conserving. Of course the average of the remaining part of the action with respect to the shifted field must restore the Trace-conservation:

$$\langle S_0 + S_2 + S_3 + S_4 \rangle = 0 \tag{2.92}$$

Now for the evaluation of the Green's function to quadratic order in the fluctuations.

One should remember that the fluctuating fields have the constraints

$$\langle \delta \mathbf{u}_{cl}(\mathbf{x}, T) \rangle = 0 \tag{2.93}$$

$$\langle \delta \mathbf{u}_{q}(\mathbf{x}, T) \rangle = 0 \tag{2.94}$$

which need to be taken into account evaluating the path integral

$$G_r^{ij}(\mathbf{x}T, \mathbf{0}0) = \langle \mathbf{u}_{cl}^i(\mathbf{x}T) \mathbf{u}_q^j(\mathbf{0}0) \rangle \tag{2.95}$$

$$= \int \mathcal{D}[u_{cl}, u_q] e^{iS[u]} e^{i\vec{\delta u} G^{-1}(uu) \vec{\delta u}} \tag{2.96}$$

Obviously for times at the boundary T the quantum component has to vanish.

Hence it can be expanded within a Fourier series $\mathbf{u}(\mathbf{x}t) = \sum_n \mathbf{u}_q^n(\mathbf{x}) \sqrt{\frac{1}{T}} \sin(\frac{n\pi}{T} t)$.

Then the same expansion holds for $\delta \mathbf{u}_q$ and $\delta \mathbf{u}_{cl}$.

So in frequency space (2.85) becomes a product of discrete frequencies

$$G_r^{ij}(\mathbf{x}T) = \int \mathcal{D}[u_{cl}, u_q] \prod_n u_{cl}^i(\mathbf{x}T) u_q^j(\mathbf{0}0) \left[e^{iS[u_n]} e^{i \int d^d\mathbf{x} \delta u_n^{cl}(\mathbf{x}) (\omega_n^2 + (c^2 + \gamma u_n(\mathbf{x}) \Delta u_n(\mathbf{x}))) \delta u_n^q(\mathbf{x})} \right] \tag{2.97}$$

The Fourier-transformation of

$$\int dt e^{i\Omega t} sin(\omega t) \Theta(T - t) = \frac{i}{2} \int_0^T dt (e^{i(\Omega+\omega)t} - e^{-i(\Omega-\omega)t}) = i e^{i\Omega T} \left(\frac{\Omega i \sin(\omega T) - \omega(\cos(\omega T)) + 2\omega}{\Omega^2 - \omega^2} \right)$$

yields a separation into the quantum (short time oscillating functions) and a classical

(independent of time at large times) part. Obviously, continuation of the discrete frequency ω_n to continuous ω is equivalent with the long time limit, which is also the classical limit.

Obviously within the frequency diagonal instanton approximation, the integral becomes a product over the frequency dependent factor

$$1 = \prod_{\omega_n} 1 = \prod_{\omega_n} \int \mathcal{D}[u_{cl}(\omega_n), u_q(\omega_n)] e^{iS[u_i(\omega_n)]} \tag{2.98}$$

and the Fourier mode of the classical Green's function is given by

$$G_r^{ij}(\omega \mathbf{x}) = \int \mathcal{D}[u_{cl}(\omega_n), u_q(\omega_n)] \mathbf{u}_{cl}^i(\mathbf{x}\omega) \mathbf{u}_q^j(\mathbf{0}\omega) e^{iS[u_i(\omega)]} \tag{2.99}$$

.

In a light scattering experiment, the strain $\nabla \circ \mathbf{u}$ is coupled to some external source field $\mathcal{E}(t) = \mathcal{E}_0 e^{i\omega t}$, which adds the term $\int \nabla \circ \mathbf{u}_q(\omega, x) \mathcal{E}_0$ onto the action.

Then the linear strain response to such a perturbation is given by

$$\mathrm{Im}\left[\Delta G_r(\omega, \mathbf{x})\right] \tag{2.100}$$

. Therefore it is clear that $\mathrm{Im} G_r(\omega, \mathbf{x})$ is the local density of vibrational states.

First, the finite instanton action $S_0[u(\omega)]$ contributes an exponential pre-factor $e^{-|S_0(\omega)|}$ to the local density of states. This may be estimated as follows. Using the equation of motion (2.75)

$$iS[\gamma = 0, iu_q = u, u_{cl} = 0] = \int \mathbf{u} \circ (-\partial_t^2 + c^2 \Delta)\mathbf{u} = -\gamma \int \int \nabla \circ \mathbf{u} \nabla \circ \mathbf{u} \nabla \circ \mathbf{u} \nabla \circ \mathbf{u} \tag{2.101}$$

one can get rid of the traveling wave term, yielding

$$iS_0(\omega) = iS[\gamma, iu_q = u, u_{cl} = u] = \int \mathbf{u} \circ (\omega^2 + c^2\Delta)\mathbf{u} + \frac{\gamma}{2}\int \nabla \circ \mathbf{u}\nabla \circ \mathbf{u}\nabla \circ \mathbf{u}\nabla \circ \mathbf{u} \quad (2.102)$$

$$= -\frac{\gamma}{2}\int d^d x \left(\nabla \circ \mathbf{u}(\omega, \mathbf{x})\right)^4 \quad (2.103)$$

. Again we applied the frequency diagonal decoupling of the disorder term.

If instantons are happen to be "traveling" waves within the region of localization (but with a sound velocity modulating its self to zero via a nonlinear effect), a wave-like ansatz

$$u(\omega, \mathbf{x}) = u(\omega\mathbf{x}) \quad (2.104)$$

will be sufficient. Additionally the disorder parameter and frequency can be scaled out of the instanton equation via $u(\omega\mathbf{x}) = \frac{1}{\sqrt{\gamma}\omega}\tilde{u}(\omega\mathbf{x})$.

Again within the frequency diagonal decoupling, the disorder term the integral becomes

$$S_0(\omega) = -\frac{c^4}{2\gamma}\frac{\omega^d}{c^d\rho_0}\int_{\rho^2(\tilde{k})<1} d^d\tilde{k}\rho^2(\tilde{k})\rho^2(-\tilde{k}) \sim -\frac{c^4}{2\gamma}\frac{\omega^d}{c^d\rho_0}A \quad (2.105)$$

. Here we used the wave-number representation of the integral, because it is the most natural way of introducing a cutoff for large deformations yielding negative sound velocities. In addition we restored the density of the elastic medium. By this we established a field theoretic derivation on the Lifshitz argument (47).

Next to the response function.

The Green's function is tri-diagonal and can readily be inverted

$$\langle \delta u_i(\omega,\mathbf{x})\delta u_j(\omega,\mathbf{x})\rangle = e^{-\frac{c^4}{2\gamma}\frac{\omega^d}{c^d\rho_0}A}\begin{pmatrix} 0 & G_r^{ij}(\omega,\mathbf{x}) \\ (G_r^{ij}(\omega,\mathbf{x}))^* & \int_{\mathbf{y}} G_r^{il}\circ(G_k^{-1})_{lm}\circ(G_r^{mj})^+ \end{pmatrix} \tag{2.106}$$

$$G_r^{ij}(\omega,\mathbf{x}) = \delta_{ij}(\omega^2 + i\epsilon + (c^2 - 3\gamma\rho(x)^2)\Delta))^{-1} \tag{2.107}$$

.

Note that this is an advantage in comparison to the replica calculation (15), where one has to think about possible 0 states of the replica matrix.

The dynamical structure factor happens to be

$$S(\omega,\mathbf{x},\mathbf{y}) = \nabla_x \circ \nabla_y G_K(\omega,\mathbf{x},\mathbf{y}) \tag{2.108}$$

which contains, the hyperbolic cotangent of the free Bose system.

This is the weak point of the "normalization-free" paradigm of the Keldysh formalism. If you consider the state of the system in presence of disorder to be a thermal one, the initial correlation of the thermal state has to be calculated within a field theory, whose normalization will become disorder dependent.

On the other hand, as $\nabla \circ \nabla G_{r,a}$ is just the linear response function for an external potential which couples to the density perturbation. Therefore $\langle u_{cl}(\delta)u_{cl}(0)\rangle$, can also be determined from the experiment.

It is accepted through the literature, that localized and extended states can not exist at a common frequency, otherwise the localized states can become extended. If you want so, the order parameter of the classical localization transition is the quantum component $u_q(\omega)$ which has to vanish at the critical frequency $u_q(\omega_c) = 0$. So the density of states can be guessed to be composed of 2 parts:

$$g(\omega^2) = g_{vib}(\omega^2)\Theta(\omega_c^2 - \omega^2) + g_{loc}(\omega^2)\Theta(\omega^2 - \omega_c^2) \tag{2.109}$$

.

Note that $g_{vib}(\omega^2)$ within this approximation is just the density of states of the free system. As these states contribute to transport properties like the thermal conductivity $g_{vib}(\omega^2)$ has to be normalized to satisfy, f. e. the Dulong-Petit law. The same normalization factor should be given to g_{loc}, due to the correspondence $g_{vib} = g_{loc}|_{u=0}$.

Then, if localization happens for frequencies lower than the Debye energy, on which both density of states have been normalized, something has to happen with the propagating part in order to render the transport properties unchanged.

One possibility is the existence of an additional scattering mechanism, which shifts the states of the free system towards higher energies. Clearly corrections achieving this, have been calculated extensively through SCBA and CPA methods, which will produce an anomalous excess in $\frac{g_{vib}^{(corr)}(\omega^2)}{g_{vib}(\omega^2)}$. Hence, the Boson peak frequency is a preliminar of the exact localization threshold ω_c^2.

2.6 Corrections

Of course the perturbation theory of the model is of ϕ^4-type. As the propagator of the theory has the instanton factor $e^{-\frac{c^4\omega^3}{2\gamma c^3\rho_0}A}$ in three dimensions, all diagrams in the "deep localized regime" $1 \ll \frac{c^4\omega^3}{2\gamma c^3\rho_0}A$ are exponentially suppressed.

The fourth order term is well known. The retarded advanced self-energy in Born approximation will be

$$\Sigma_{r,a}^{(Born)}(\omega, q) = -i\gamma q^2 \sum_k G_{a,r}(k,\omega)(k-q)^2 \tag{2.110}$$

and the propagator $G_{(r,a)}$ will be replaced with the full propagator

$$G_{r,a} = e^{-S_0(\omega)}(\omega^2 + (1 - 3\gamma\rho^2(\omega, \mathbf{x}))\Delta + \Sigma_{r,a}(\omega, x))^{-1} \tag{2.111}$$

$$\rho(\omega, \mathbf{x}) = \nabla \circ \mathbf{u}(\omega, \mathbf{x}) \tag{2.112}$$

. We reduce perturbation theory to an elementary stage, by modeling the sound-velocity landscape by a Gaussian distribution $c^2 = 1 - e^{-\frac{(\omega x)^2}{2\sigma^2}}$, which replaces the propagator (2.111), with

$$G_{r,a} = \frac{e^{-S_0(\omega)}}{\omega^2 \pm i\epsilon - c^2(1 - 3\frac{\omega^d}{c^d\rho_0})k^2 + \Sigma_{r,a}(\omega, k)} \tag{2.113}$$

.

In case of low frequencies $3\frac{\omega^d}{c^d\rho_0} \ll 1$ we recover the familiar self consistent born approximation.

This neglects about the so called crossed diagrams

$$\Sigma_{r/a}^{(cross)} = i\gamma^2\Delta(\Delta G_r \circ \Delta G_a \circ \Delta G_r) \tag{2.114}$$

$$\approx i\gamma q^2 \Sigma_{r,a}^{(Born)}(\omega) \int d^d k |\frac{k^2}{(\omega^2 \pm i\epsilon - c^2(1 - 3\frac{\omega^d}{c^d\rho_0})k^2)}|^2 \tag{2.115}$$

, which for quantum mechanical waves scattered in a random potential yields to the weak localization effect. Due to the absence of the k - powers which come from the correlation of the elastic energy, the electronic crossed self-energy is infrared divergent below two dimensions $\Sigma^{(cross)} \propto \frac{1}{E}$. One has to treat these IR-divergences by means of the perturbative renormalization group, which yields a Thouless like scaling scenario (1), proving that for quantum mechanics all states are localized below $d = 2$.

In contrast, the corresponding diagrams of the elastic mediums are finite within the infrared sector, and possible UV-divergences are safely regulated by introducing a lattice, which for phonons is just given by the mean spacing of individual particles.

Then on the low frequency/ plain wave side the self-energy evaluates to

$$\Sigma^{(cross)} \propto \gamma^2 \omega^{2d} \tag{2.116}$$

, which assists the instanton in a frequency dependent modulation of the sound wave. However the instanton contribution is independent of γ, hence the irreducible self-energy part is negligible with respect to the instanton in case of weak disorder. Also this frequency dependence can not affect the Boson peak, which comes from a static renormalization of the sound velocity through the SCBA. In contrast no static renormalization appears from (2.116).

On the other hand at large frequencies beyond the localization threshold the Green's function is safely given by

$$G_r \sim \frac{c^{d-2}\rho_0 e^{-\frac{c^4\omega^3}{2\gamma c^3\rho_0}A}}{3\omega^d k^2}$$

yielding

$$\Sigma^{(cross)} \propto \gamma^2 \frac{c^d \rho_0}{\omega^d} e^{-\frac{3c^4\omega^3}{2\gamma c^3\rho_0}A}$$

which vanishes at large frequencies.

Additionally the Keldysh self-energy

$$\Sigma_K = \gamma \nabla^2 \langle u_{cl} u_{cl} \rangle \nabla^2 = \nabla S \nabla \tag{2.117}$$

is just related to the dynamical structure factor and can be used to construct the Boltzmann equation.

The third order term is in charge of contributing deviations to the instanton function.

$$\langle \delta u_q \rangle = i \langle \delta u_{cl} \rangle = 2\gamma G_r G_a + \mathcal{O}(\gamma^2) \tag{2.118}$$

So in general mean-field theory is well established in case of large frequencies, while small frequency deviations can be calculated for small γ. As the instanton factor vanishes $\frac{c^4\omega^3}{2\gamma c^3 \rho_0} A \ll 1$, the propagator will be of sound wave type and destroy short range order.

2.7 Non-linear Sigma Model

The Keldysh-action

$$\begin{aligned} iS = \frac{i}{2} \int d^d x dt \left[\mathbf{u}_q \circ (-\partial_t^2 + c\Delta + i\epsilon) \mathbf{u}_{cl} + \mathbf{u}_{cl} \circ (-\partial_t^2 + c\Delta - i\epsilon) \mathbf{u}_q \right] \\ -\frac{\gamma}{2} \int dt \int dt' d^d x \nabla \circ \mathbf{u}_q(t) \nabla \circ \mathbf{u}_{cl}(t) \nabla \circ \mathbf{u}_{cl}(t') \nabla \circ \mathbf{u}_q(t') \end{aligned} \tag{2.119}$$

is naturally of the same structure as the one studied by Stone and McKane (52) in their ground breaking non-linear Sigma model approach to localization in electronic systems.

This is because electrons start to move diffusively in presence of weak disorder, and the quantity which describes the localization transition is a short range density-density response function

$$\phi^2 \phi^2 \propto G_r G_a \tag{2.120}$$

. Hence McKane and Stone started their discussion from a path-integral representation with two degrees of freedom, referring to the retarded and advanced channel, but

used the replica expansion for both channels, instead of referring to the special kind of Keldysh contour.

The reason is, that they worked with an action for the sum of the retarded and advanced Green's function, while the Keldysh-action operates with the difference, and hence is normalization free. Therefore also their disorder term is a quadratic average of the replicated combination $\phi_+^2 + \phi_-^2$, while the complete Keldysh action is build up from $\phi_+^2 - \phi_-^2$ without additional replicas.

In ϕ^4 theory $G_r G_a$ is the quantity which contributes directly to the instanton, describing localization as we found in equation (2.118).

As usually the theory is reformulated in terms of the strain correlation by means of the Fadeev-Popov identity

$$S_F = i\mathrm{Tr}\left[\Lambda_{\alpha\beta}(Q_{\beta\alpha} - \nabla \circ \mathbf{u}_\beta(t')\nabla \circ \mathbf{u}_\alpha(t))\right] \tag{2.121}$$

with the Keldysh matrices

$$\Lambda = \begin{pmatrix} 0 & \Lambda_a \\ \Lambda_r & \Lambda_k \end{pmatrix}, Q = \begin{pmatrix} Q_k & Q_r \\ Q_a & 0 \end{pmatrix}, \tag{2.122}$$

yielding the action

$$S = \frac{1}{2}\mathrm{Tr}\ln\left[i(G_0^{-1} - \overleftarrow{\nabla}\Lambda\nabla\circ)\right] - \frac{\gamma}{2}\mathrm{tr}[Q_r\delta_{x-y}Q_r + Q_a\delta_{x-y}Q_a] + i\mathrm{Tr}[\Lambda Q] \tag{2.123}$$

The small tr just refers to the space-time integration, the large Tr refers to the additional matrix-trace. Multiplication of space-time operators automatically means convolution.

One can use projectors in order to write the mass term in form of the usual square,

$$P_l Q = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} \begin{pmatrix} Q_k & Q_r \\ Q_a & 0 \end{pmatrix} = \begin{pmatrix} p^l_{11}Q_k + p^l_{12}Q_a & p^l_{11}Q_r \\ p^l_{21}Q_k + p_{22}Q_a & p_{21}Q_r \end{pmatrix} \tag{2.124}$$

$$QP_r = \begin{pmatrix} Q_k & Q_r \\ Q_a & 0 \end{pmatrix} \begin{pmatrix} p^r_{11} & p^r_{12} \\ p^r_{21} & p^r_{22} \end{pmatrix} = \begin{pmatrix} Q_k p^r_{11} + Q_r p^r_{21} & Q_k p^r_{12} + Q_r p^r_{22} \\ Q_a p^r_{11} & Q_a p^r_{12} \end{pmatrix} \tag{2.125}$$

The mapping

$$Q_L = \begin{pmatrix} Q_a & 0 \\ Q_k & Q_r \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} Q_k & Q_r \\ Q_a & 0 \end{pmatrix} \tag{2.126}$$

$$Q_R \begin{pmatrix} Q_r & Q_k \\ 0 & Q_a \end{pmatrix} = \begin{pmatrix} Q_k & Q_r \\ Q_a & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.127}$$

achieves matrices with the structure of the Fermionic Green's function/self-energy, which could be of great help, if one likes to compare this expansion with the Keldysh Sigma model for the disordered electrons.

The mass term of the theory can be written into the matrix form by means of

$$\frac{\gamma}{2}\mathrm{tr}[Q_r Q_r + Q_a Q_a] = \frac{\gamma}{2}\mathrm{Tr}[Q_L^2] = \frac{\gamma}{2}\mathrm{Tr}[Q_R^2] \tag{2.128}$$

.

Variation with respect to Q and Λ yields exact equations of motion for density and self-energy

$$\langle Q \rangle = i\langle \overleftarrow{\nabla} \frac{1}{G_0^{-1} - \overleftarrow{\nabla}\Lambda\nabla} \nabla \rangle \tag{2.129}$$

$$\langle \Lambda_{r,a} \rangle = -2i\gamma\delta(\mathbf{x}-\mathbf{y})\langle Q_{r,a}\rangle \tag{2.130}$$

$$\langle \Lambda_k \rangle = 0 \tag{2.131}$$

.

Note that these equations of motion do not fix the Keldysh component of the self-energy field and also not the Keldysh component of the Greens function.

The identification of the self-energy operator in Dyson's equation with the average of the Λ ghost field, is equivalent with replacing the average over the resolvent in eq. (2.129), with the resolvent of the average. This is again the self-consistent Born approximation.

$$\Lambda_r = \gamma \int_{-\infty}^{\infty} dk \frac{k^4}{-\omega^2 + i\epsilon + c^2k^2(1-\Lambda_r(\omega))} \approx \gamma \frac{\omega^2}{c^2(1-\Lambda_r(\omega))} \tag{2.132}$$

$$\Lambda_r^2(\omega) = \gamma\omega^2(1-\Lambda_r) \tag{2.133}$$

The approximation (2.133) gives the self energy within the form of Wigner's semi-circle, which refers to random matrix eigenstates. The density of states in self-consistent Born approximation has been subject to intensive investigations (80, 67) and will not be discussed within this work.

The exact equation (2.130) states that Λ is a linear field in the disorder parameter, while for small γ, Q is a field of order 1. Therefore, deviations from this saddle-point render the action as a power series in γ

$$\mathrm{Tr}\ln(iG_0^{-1} - i\overleftarrow{\nabla}\Lambda\nabla - i\overleftarrow{\nabla}\delta\Lambda\nabla) = \mathrm{Tr}\ln(1 + \frac{1}{G_0^{-1} - i\overleftarrow{\nabla}\Lambda\nabla}\overleftarrow{\nabla}\delta\Lambda\nabla) = i\mathrm{Tr}\left[\bar{Q}\delta\Lambda\right] - \frac{1}{2}\mathrm{Tr}\left[(\bar{Q}\delta\Lambda)^2\right] + ... \tag{2.134}$$

$$S \approx S_0 - \frac{1}{2}\mathrm{Tr}\left[(\bar{Q}\delta\Lambda)^2\right] - \frac{\gamma}{2}\mathrm{Tr}[\delta Q_L^2] + \frac{i}{2}\mathrm{Tr}[\delta\Lambda\delta Q] + \gamma\mathrm{Tr}\left[\langle Q_L\rangle Q_L\right] \tag{2.135}$$

$$= S_0' - \frac{1}{2}\mathrm{Tr}(\bar{Q}\delta\Lambda)^2 - \frac{\gamma}{2}\mathrm{Tr}[\delta Q_L^2] + \frac{i}{2}\mathrm{Tr}[\delta\Lambda\delta Q] \tag{2.136}$$

as an expansion with respect to the Λ field is an expansion with respect to γ.

The source term in equation (2.136) can be integrated away as follows. The second order within the self-energy field has to be brought into the quadratic form:

$$\mathrm{Tr}\left[(\bar{Q}\delta\Lambda)^2\right] = \mathrm{Tr}\left[\delta\Lambda\bar{Q}\bar{Q}\delta\Lambda\right] + \mathrm{Tr}\left[[\delta\Lambda, \bar{\mathrm{Q}}]\bar{\mathrm{Q}}\delta\Lambda\right]. \tag{2.137}$$

The last term has to vanish, as it is the product of the trace full $\bar{Q}\delta\Lambda$ and the trace-less commutator, hence the second term should vanish, we evaluate this:

$$\mathrm{Tr}\left[\left(\delta\Lambda\bar{Q} - \bar{Q}\delta\Lambda\right)\bar{Q}\delta\Lambda\right] = \mathrm{Tr}\left[\delta\Lambda\bar{Q}\bar{Q}\delta\Lambda\right] - \mathrm{Tr}\left[\bar{Q}\delta\Lambda\bar{Q}\delta\Lambda\right] = \tag{2.138}$$

$$\mathrm{Tr}\left[(\bar{Q}\delta\Lambda)(\delta\Lambda\bar{Q})\right] - \mathrm{Tr}\left[(\bar{Q}\delta\Lambda)(\bar{Q}\delta\Lambda)\right] \tag{2.139}$$

Evaluation of the trace in detail yields

$$\mathrm{Tr}\left[\left(\delta\Lambda\bar{Q} - \bar{Q}\delta\Lambda\right)\bar{Q}\delta\Lambda\right] = tr\left\{(\bar{Q}_r\delta\Lambda_a - \delta\Lambda_r\bar{Q}_a)\bar{Q}_r\delta\Lambda_a + (\bar{Q}_a\delta\Lambda_r - \delta\Lambda_a\bar{Q}_r)\bar{Q}_a\delta\Lambda_r\right\} \tag{2.140}$$

$$+tr(-\delta\Lambda_a\bar{Q}_k + \delta\Lambda_k\bar{Q}_a)(\bar{Q}_k\delta\Lambda_r + \bar{Q}_r\delta\Lambda_k) \tag{2.141}$$

$$= tr\left\{(\bar{Q}_r\delta\Lambda_a)^2 - (\bar{Q}_a\delta\Lambda_r)^2 - \delta\Lambda_r(\bar{Q}_a\bar{Q}_r + \bar{Q}_r\bar{Q}_a + \bar{Q}_k\bar{Q}_k)\delta\Lambda_a\right\} \tag{2.142}$$

$$+tr\left\{\delta\Lambda_k\bar{Q}_a\bar{Q}_r\delta\Lambda_k - \delta\Lambda_a\bar{Q}_k\bar{Q}_r\delta\Lambda_k + \delta\Lambda_k\bar{Q}_a\bar{Q}_k\delta\Lambda_r\right\} \tag{2.143}$$

.

All terms until the last two in equation (2.143) are vanishing, because a trace over the product of retarded and advanced terms has to vanish by definition as $\Theta(t)\Theta(-t) = 0$. The last two terms vanish due to time reversal symmetry.

Then the Λ field can be integrated out yielding the action in terms of the Q field:

$$S_{det} = -\frac{1}{2}\mathrm{Tr}\left[\delta Q(\bar{Q}\bar{Q})^{-1}\delta Q\right] \tag{2.144}$$

$$= -\frac{1}{2}\mathrm{Tr}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\delta \mathrm{Q_L}(\bar{\mathrm{Q}}\bar{\mathrm{Q}})^{-1}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\delta \mathrm{Q_L}\right] \tag{2.145}$$

$$S_{nl\sigma m} = -\frac{1}{2}\mathrm{Tr}\left[\sigma_x \delta Q_L(\bar{Q}\bar{Q})^{-1}\sigma_x\delta Q_L + \gamma\delta Q_L^2\right] \tag{2.146}$$

Although the theory is quadratic to this level, it cannot simply be integrated out further, because the expansion of the $\mathrm{Tr}\ln$ term requires fluctuations of the Q field to be small. The mass term is Gaussian $\frac{\gamma}{2}\mathrm{Tr}[\delta Q_L^2]$ and roughly constrains the fields to $|\delta Q| < \frac{1}{\gamma}$. However there are fluctuations sufficiently larger within the integral, which would require higher terms of the Trace-log. Therefore, it is reasonable that for "small" γ, e. g. all fields are a power-series of γ, the effective action is sufficient.

This is what goes wrong in a strong coupling theory. According to Dyson equation, re summation of the perturbation series in ϕ^4 theories always yields to functions of the form $\frac{1}{g(x)+\gamma f(x)}$, which for "large" γ can be of the order $\frac{1}{\gamma}$, canceling the prefactor in (2.136) at every single power. However, note that within the sound-wave problem, Q and hence δQ is a strain-correlation function, which will be small for long wavelength, e. g. the hydrodynamic limit. Therefore, if one studies the spectrum which consists of long wavelength extended states, e. g. low frequency, the quadratic approximation can be guessed as being sufficient regardless of the strength of the parameter γ.

Investigating the exact form of the Q field smallness of γ means exactly $\gamma\Lambda(\omega) \ll 1$.

As $\lim_{\omega\to 0}\omega^2\Lambda''(\omega) \propto \omega^n$ the quadratic approximation is exact in the low frequency limit.

This is interesting for scaling arguments. If one manages to derive an exact scaling relation, f.e. from the exact equation (2.129), a solution to the quadratic theory can be expected to be exact for low frequencies, high frequency properties could be safely be calculated from the scaling approach.

We continue to follow the "Gold-stone" approach to localization within the Keldysh-language.

If the saddle-point is an accepted solution to the field theory, one frequently studies "low energy" excitations from this solutions, which are those who render the full mass term invariant. In the present theory they can be parametrized according to

$$\delta Q_L = e^W \begin{pmatrix} \bar{Q}_r & \bar{Q}_k \\ 0 & \bar{Q}_a \end{pmatrix} e^{-W} - \begin{pmatrix} \bar{Q}_r & \bar{Q}_k \\ 0 & \bar{Q}_a \end{pmatrix} \tag{2.147}$$

, which is slightly different from the electronic problem.

If one wants to evaluate the partition function one has to single out configurations which commute with the mean-field value of $\bar{Q}$

$$W = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \tag{2.148}$$

$$0 \neq - \begin{pmatrix} w_{11}^c & w_{12}^c \\ w_{21}^c & w_{22}^c \end{pmatrix} \begin{pmatrix} \bar{Q}_r & \bar{Q}_k \\ 0 & \bar{Q}_a \end{pmatrix} + \begin{pmatrix} \bar{Q}_r & \bar{Q}_k \\ 0 & \bar{Q}_a \end{pmatrix} \begin{pmatrix} w_{11}^c & w_{12}^c \\ w_{21}^c & w_{22}^c \end{pmatrix} \tag{2.149}$$

$$0 \neq \begin{pmatrix} [Q_r, w_{11}^c] + \bar{Q}_k w_{21}^c & \bar{Q}_r w_{12}^c - w_{12}^c \bar{Q}_a + \bar{Q}_k w_{22}^c - w_{11}^c \bar{Q}_k \\ \bar{Q}_a w_{21}^c - w_{21}^c \bar{Q}_r & [\bar{Q}_a, w_{22}^c] - w_{21}^c \bar{Q}_k \end{pmatrix} \tag{2.150}$$

. This would be a linear constraint, which can be included by means of an additional Lagrange-parameter.

However in order to leave the mass term invariant W must also commute with the projector matrix

$$\begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} = \begin{pmatrix} w_{12} - w_{21} & w_{11} - w_{22} \\ w_{22} - w_{11} & w_{21} - w_{12} \end{pmatrix} \tag{2.151}$$

Hence $w_{12} = w_{21}$, $w_{11} = w_{22}$.

. Now W equals

$$W = \begin{pmatrix} v & w \\ w & v \end{pmatrix} \tag{2.152}$$

and the constraint reads

$$0 \neq \begin{pmatrix} [Q_r, v] + Q_k w & \bar{Q}_r w - w\bar{Q}_a + [\bar{Q}_k, v] \\ \bar{Q}_a w - w\bar{Q}_r & [\bar{Q}_a, v] - w\bar{Q}_k \end{pmatrix} \tag{2.153}$$

.

As at least the fluctuations have been chosen to commute with the projector matrix the ordinary sigma expression

$$S = -\frac{1}{2}\mathrm{Tr}\left[\sigma_x \delta Q_L D \delta Q_L\right] \tag{2.154}$$

$$D = (\bar{Q}\bar{Q})^{-1}\sigma_x + \sigma_x * \gamma\delta(x-y)* \tag{2.155}$$

$$= \begin{pmatrix} 0 & d_{ra} = G_r^{-1}G_a^{-1} \\ d_{ra} & 0 \end{pmatrix} + \sigma_x * \gamma\delta(x-y)* \tag{2.156}$$

holds.

Then to fourth order

$$\delta Q = (1 + W + \frac{W^2}{2!} + \frac{W^3}{3!} + \frac{W^4}{4!})\bar{Q}(1 - W + \frac{W^2}{2!} - \frac{W^3}{3!} + \frac{W^4}{4!}) - \bar{Q} = \tag{2.157}$$

$$(1 + W + \frac{W^2}{2!} + \frac{W^3}{3!} + \frac{W^4}{4!})\bar{Q} + \bar{Q}(-W + \frac{W^2}{2!} - \frac{W^3}{3!} + \frac{W^4}{4!}) - \bar{Q}$$

$$+(W + \frac{W^2}{2!} + \frac{W^3}{3!} + \frac{W^4}{4!})\bar{Q}(-W + \frac{W^2}{2!} - \frac{W^3}{3!} + \frac{W^4}{4!}) \tag{2.158}$$

$$= [W + \frac{W^3}{3!}, \bar{Q}] + \{\frac{W^2}{2!} + \frac{W^4}{4!}, \bar{Q}\}$$

$$+WQ(-W + \frac{W^2}{2!} - \frac{W^3}{3!}) + \frac{W^2}{2!}Q(-W + \frac{W^2}{2!}) - \frac{W^3}{3!}QW + ... \tag{2.159}$$

$$= [W + \frac{W^3}{3!}, \bar{Q}] + \{\frac{W^2}{2!} + \frac{W^4}{4!}, \bar{Q}\}$$

$$-WQW + \frac{WQW^2}{2!} - \frac{WQW^3}{3!} - \frac{W^2}{2!}QW + \frac{W^2}{2!}Q\frac{W^2}{2!} - \frac{W^3}{3!}QW \tag{2.160}$$

$$= W^{(1)} + W^{(2)} + W^{(3)} + W^{(4)} \tag{2.161}$$

Another exact equation of motion is just $\langle Q \rangle = \langle \nabla \circ \mathbf{u} \nabla \circ \mathbf{u} \rangle$.

Hence to lowest order the average of the commutator $\delta Q = \langle \sigma_x [W, \bar{Q}] \rangle$ is the fluctuation of the strain field from the mean-field value

$$\langle \delta Q \rangle = \langle \begin{pmatrix} \bar{Q}_a w - w\bar{Q}_r & [\bar{Q}_a, v] - w\bar{Q}_k \\ [Q_r, v] + Q_k w & \bar{Q}_r w - w\bar{Q}_a + [\bar{Q}_k, v] \end{pmatrix} \rangle \tag{2.162}$$

. Requiring the quantum quantum component to vanish yields the equation of motion

$$[\bar{Q}_k, \langle v \rangle] + \bar{Q}_r \langle w \rangle - \langle w \rangle \bar{Q}_a = 0 \tag{2.163}$$

.

From (2.162) in case of vacuum physics $\bar{Q}_k = 0$ we can read of a possible instanton solution.

In Chapter 5 a possible instanton configuration had the property

$\langle \phi_{cl} \phi_{cl} \rangle = -\langle \phi_q \phi_q \rangle = \langle \phi_q \phi_{cl} \rangle$. Such a configuration is obtained in case of vacuum-physics

by

$$0 \neq \langle \bar{Q}_a w - w\bar{Q}_r \rangle = \langle [\bar{Q}_a, v] \rangle = \langle [\bar{Q}_r, v] \rangle$$

, which is, as we will see, a possible solution to the field theory.

With

$$W^{(1)} = [W, \bar{Q}] = \begin{pmatrix} [Q_r, v] + Q_k w & \bar{Q}_r w - w\bar{Q}_a + [\bar{Q}_k, v] \\ \bar{Q}_a w - w\bar{Q}_r & [\bar{Q}_a, v] - w\bar{Q}_k \end{pmatrix} \tag{2.164}$$

$$W^{(2)} = \frac{1}{2}\{W^2, \bar{Q}\} - W\bar{Q}W = \frac{1}{2}\left(W^2 Q + Q W^2\right) - \frac{1}{2}W\bar{Q}W - \frac{1}{2}W\bar{Q}W \tag{2.165}$$

$$= \frac{1}{2}\{W, [W, Q]\} = \frac{1}{2}\{W, W^{(1)}\} = \frac{1}{2}\left(\begin{pmatrix} w & v \\ v & w \end{pmatrix}\begin{pmatrix} w_{11}^{(1)} & w_{12}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} \end{pmatrix} + \begin{pmatrix} w_{11}^{(1)} & w_{12}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} \end{pmatrix}\begin{pmatrix} w & v \\ v & w \end{pmatrix}\right) \tag{2.166}$$

$$= \begin{pmatrix} \{w, w_{11}^{(1)}\} + v w_{21}^{(1)} + w_{12}^{(1)} v & v w_{22}^{(1)} + w_{11}^{(1)} v + \{w, w_{12}^{(1)}\} \\ w_{22}^{(1)} v + v w_{11}^{(1)} + \{w, w_{21}^{(1)}\} & \{w, w_{22}^{(1)}\} + v w_{12}^{(1)} + w_{21}^{(1)} v \end{pmatrix} \tag{2.167}$$

$$w_{11}^{(2)} = \{w, [Q_r, v] + Q_k w\} + v(\bar{Q}_a w - w\bar{Q}_r) + (\bar{Q}_r w - w\bar{Q}_a + [\bar{Q}_k, v])v \tag{2.168}$$

$$w_{12}^{(2)} = v([\bar{Q}_a, v] - w\bar{Q}_k) + ([Q_r, v] + Q_k w)w + \{w, \bar{Q}_r w - w\bar{Q}_a + [\bar{Q}_k, v]\} \tag{2.169}$$

$$w_{21}^{(2)} = ([\bar{Q}_a, v] - w\bar{Q}_k)v + v([Q_r, v] + Q_k w) + \{w, \bar{Q}_a w - w\bar{Q}_r\} \tag{2.170}$$

$$w_{22}^{(2)} = \{w, [\bar{Q}_a, v] - w\bar{Q}_k\} + v(\bar{Q}_r w - w\bar{Q}_a + [\bar{Q}_k, v]) + (\bar{Q}_a w - w\bar{Q}_r)v \tag{2.171}$$

$$W^{(3)} = \frac{1}{6}[W^3, \bar{Q}] + \frac{1}{2}W[\bar{Q}, W]W \tag{2.172}$$

$$W^{(4)} = \frac{1}{24}\{W^4, \bar{Q}\} - \frac{1}{6}W\{\bar{Q}, W^2\}W + \frac{1}{4}W^2\bar{Q}W^2 \tag{2.173}$$

,

and

$$\delta\bar{Q} = W^{(1)} + W^{(2)} + W^{(3)} + W^{(4)} \tag{2.174}$$

follows the sigma model action to fourth order

$$-2S_{nl\sigma m} = \mathrm{Tr}\left[W^{(1)}DW^{(1)} + W^{(2)}DW^{(2)} + \{W^{(1)}, D\}(W^{(2)} + W^{(3)})\right] \tag{2.175}$$

.

The action has two basic terms

$$\mathrm{Tr}\left[LDR\right] = \mathrm{Tr}\left[\sigma_x L \begin{pmatrix} d_{ra} & 0 \\ 0 & d_{ra} \end{pmatrix} R + \gamma L \delta R\right] \tag{2.176}$$

$$= tr\left(\sum_{ijk}(1-\delta_{ij})L_{jk}d_{ra}R_{ki} + \gamma\sum_{ij}L_{ij}\delta R_{ji}\right) \tag{2.177}$$

$$= tr\left[L_{22}d_{ra}R_{21} + L_{21}d_{ra}R_{11} + L_{12}d_{ra}R_{22} + L_{11}d_{ra}R_{12} + \gamma\sum_{ij}L_{ij}\delta R_{ji}\right] \tag{2.178}$$

and

$$\mathrm{Tr}\left[\{L, D\}R\right] = \mathrm{Tr}\left[\sigma_x L \begin{pmatrix} d_{ra} & 0 \\ 0 & d_{ra} \end{pmatrix} R + L \begin{pmatrix} d_{ra} & 0 \\ 0 & d_{ra} \end{pmatrix} \sigma_x R + \gamma\left(L\delta R + R\delta L\right)\right] \tag{2.179}$$

$$= \left(\sum_{ijk}(1-\delta_{ij})L_{jk}d_{ra}R_{ki} + \sum_{ijk}L_{ij}d_{ra}(1-\delta_{jk})R_{ki} + 2\gamma\sum_{ij}L_{ij}\delta R_{ji}\right) \tag{2.180}$$

$$= tr\left[L_{22}d_{ra}R_{21} + L_{21}d_{ra}R_{11} + L_{12}d_{ra}R_{22} + L_{11}d_{ra}R_{12}\right] \tag{2.181}$$

$$+tr\left[L_{12}d_{ra}R_{11} + L_{11}d_{ra}R_{21} + L_{22}d_{ra}R_{12} + L_{21}d_{ra}R_{22}\right] \tag{2.182}$$

$$+2\gamma tr\left[L_{11}R_{11} + L_{12}R_{21} + L_{21}R_{12} + L_{22}R_{22}\right] \tag{2.183}$$

The kinetic quadratic part of the action reads

$$\mathrm{Tr}\left[W^{(1)}DW^{(1)} - 2\gamma W^{(1)}W^{(1)}\right] = tr\left[w_{22}^{(1)}d_{ra}w_{21}^{(1)} + w_{21}^{(1)}d_{ra}w_{11}^{(1)} + w_{12}^{(1)}d_{ra}w_{22}^{(1)} + w_{11}^{(1)}d_{ra}w_{12}^{(1)}\right] \tag{2.184}$$

$$= \mathrm{Tr}\left[\sigma_x \begin{pmatrix} 0 & 0 \\ w_{21}^{(1)} & w_{22}^{(1)} \end{pmatrix} \begin{pmatrix} d_{ra} & 0 \\ 0 & d_{ra} \end{pmatrix} \begin{pmatrix} w_{11}^{(1)} & 0 \\ w_{21}^{(1)} & 0 \end{pmatrix} + \sigma_x \begin{pmatrix} w_{11}^{(1)} & w_{12}^{(1)} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} d_{ra} & 0 \\ 0 & d_{ra} \end{pmatrix} \begin{pmatrix} 0 & w_{12}^{(1)} \\ 0 & w_{22}^{(1)} \end{pmatrix}\right] \tag{2.185}$$

$$= \mathrm{Tr}\left[\sigma_x \begin{pmatrix} w_{11}^{(1)} & w_{12}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} \end{pmatrix} \begin{pmatrix} d_{ra} & 0 \\ 0 & d_{ra} \end{pmatrix} \begin{pmatrix} w_{11}^{(1)} & w_{12}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} \end{pmatrix}\right] \tag{2.186}$$

.

Hence to quadratic order the action is given by

$$S_{nl\sigma m}^{(2)} = -\frac{1}{2}\mathrm{Tr}\left[\sigma_x W^{(1)}d_{ra}W^{(1)} + W^{(1)}2\gamma\delta_x W^{(1)}\right] \tag{2.187}$$

with $d_{ra} = \Delta^{-4}(-\partial_t^2 + c^2\Delta)^2$. This has no singularities, because a fluctuation of the strain field satisfies $\delta Q \propto \Delta$, hence $v, w \propto \Delta$.

Next we rewrite this in terms of the v, w - fields.

The instanton calculated within the single particle picture did not depend on the initial state. Hence we simplify by setting $\bar{Q}_k = 0$, and determine the Keldysh component from the initial condition, after the calculation of the response function.

Then using $\bar{Q}_{r/a}^2 = \bar{Q}_{r/a}$ expansion in terms of the w and v fields yields

$$-2S_{nl\sigma m}^{(2)}[w,w] = -\gamma\bar{Q}_a' w\delta_x w + \gamma\left[\bar{Q}_a(\{w\bar{Q}_r w, \delta_x\} + w\{\bar{Q}_r, \delta_x\})w - 2(\bar{Q}_a\delta\bar{Q}_a)'ww\right] \tag{2.188}$$

$$-2S_{nl\sigma m}^{(2)}[v,v] = -\gamma 2\bar{Q}_a' v\delta_x v + \gamma\left[\bar{Q}_r v\{\bar{Q}_r, \delta_x\})v + \bar{Q}_a v\{\bar{Q}_a, \delta_x\})v - 2(\bar{Q}_a\delta_x\bar{Q}_a)'vv\right] \tag{2.189}$$

$$-2S^{(2)}_{nl\sigma m}[w,v] = -w(\bar{Q}_a\bar{Q}_a^{-1} + \bar{Q}_a\bar{Q}_r^{-1})v + 2\bar{Q}'_r w(\bar{Q}_a^{-1} + \bar{Q}_r^{-1})v - (\bar{Q}_a\bar{Q}_r + \bar{Q}_r\bar{Q}_a)wd_{ra}v \quad (2.190)$$

$$-2S^{(2)}_{nl\sigma m}[v,w] = -v(\bar{Q}_r\bar{Q}_a^{-1} + \bar{Q}_a\bar{Q}_r^{-1})w + 2\bar{Q}'_r v(\bar{Q}_a^{-1} + \bar{Q}_r^{-1})w - (\bar{Q}_a\bar{Q}_r + \bar{Q}_r\bar{Q}_a)vd_{ra}w \quad (2.191)$$

.

The interaction coefficients can be further simplified:

$$\bar{Q}_r + \bar{Q}_a = 2\bar{\delta c}\Delta\delta(x-y)\delta(t-t') \quad (2.192)$$

$$\bar{Q}_r\bar{Q}_a^{-1} + \bar{Q}_a\bar{Q}_r^{-1} = \bar{Q}_r(\bar{Q}_a^{-1} - i\Lambda_a + i\Lambda_r) + \bar{Q}_a(\bar{Q}_r^{-1} - i\Lambda_r + i\Lambda_a) \quad (2.193)$$

$$= \delta + \delta - \bar{Q}_r i\Lambda_a - \bar{Q}_a i\Lambda_r \quad (2.194)$$

$$= \delta + \delta - 2\gamma(\bar{Q}_r\bar{Q}_a + \bar{Q}_a\bar{Q}_r) \quad (2.195)$$

$$\bar{Q}_r\bar{Q}_a + \bar{Q}_a\bar{Q}_r = -(\bar{Q}_r - \bar{Q}_a)^2 + (\bar{Q}_r + \bar{Q}_a) \quad (2.196)$$

$$= 4\bar{Q}''_r - 2\bar{\delta c}\Delta\delta(x-y)\delta(t-t') \quad (2.197)$$

Hence to second order in the v, w fields the non-linear sigma model action

$$S^{(2)}_{nl\sigma m} = S^{(2)}_p + S^{(2)}_d \quad (2.198)$$

consists of the two parts

$$S^{(2)}_p = -2\bar{Q}'_a\left[w(\bar{Q}_a^{-1} + \bar{Q}_r^{-1})v + \frac{\gamma}{2}(w\delta_x w + v\delta_x v)\right] + local\, dos\, terms \quad (2.199)$$

$$S^{(2)}_d = -(-4\bar{Q}''_r + 2\bar{Q}'_r)wd_{ra}v - 2(2\delta + \gamma\bar{Q}_r\bar{Q}_a)vw \quad (2.200)$$

.

S_p is just the one-particle sound wave propagator in presence of disorder, studied within the last section. In the electronic problem this part would be called the Cooperon

propagator.

The remaining terms describe diffusive motion in presence of disorder, as the quantity $d_{ra} \propto \Delta(\partial_t^2 - \Delta^2)$ has a diffusion pole at non-zero wave numbers. In the electronic problem this is called the Diffusion propagator. This type of excitations from the SCBA saddle-point describes diffusive heat transport. However, this is just the "re normalized" free diffusion process, which in case of electrons would be the quantum diffusion. The last part is the disorder induced diffusion part. A gradient expansion of $\bar{Q}_r \bar{Q}_a$ gives to second order a diffusion term whose Diffusion coefficient is proportional to γ.

Equation (2.199) can be identified with the reformulation of the instanton action of section 5 by means of $\bar{Q}_a' w = 1, \bar{Q}_a' v = v = \nabla \circ \mathbf{u} \nabla \circ \mathbf{u}$ yielding

$$S_p = -\int \mathbf{u} \circ (-\partial_t^2 + c^2 \Delta)\mathbf{u} + \frac{\gamma}{2} \int\int\int d^d x (\nabla \circ \mathbf{u} \nabla \circ \mathbf{u})_{t\mathbf{x}} (\nabla \circ \mathbf{u} \nabla \circ \mathbf{u})_{t'\mathbf{x}} \tag{2.201}$$

This is the main result of the present section. The instanton factor also appears in the Bosonized model. This dresses the SCBA Green's function at high frequencies according to

$$\langle \nabla \circ \mathbf{u} \nabla \circ \mathbf{u} \rangle = e^{S_p} \bar{Q} \propto e^{-|S_0(\omega)|} \bar{Q} \tag{2.202}$$

.

2.8 Outlook, Weak localization Ward-identity, Mode-coupling, Symmetry

Weak localization is the phenomenon where the (Heat-)Diffusion coefficient of eq. (2.200) is suppressed due to the higher order terms in (2.146). In the literature this is captured by a fourth order expansion of the non-linear sigma model action, selecting only certain terms via symmetry considerations, and apply a further gradient approx-

imation. For time-reasons we cannot perform this calculation within the present work, although it would be very interesting. We have already calculated the action up to fourth-order in terms of the v and w fields, which is given within the appendix. The detailed calculation is left for future work. A faster possibility which avoids the discussion of the vast number of terms is, to use the quadratic mass-less diffusion term in (2.200) and replicate the terms of the effective action in the work of McKane and Stone.

Another starting point for further investigations is the Ward-identity of the present model. The single particle representation

$$iS = \frac{i}{2}\int d^dx dt \left[\mathbf{u}_q \circ (-\partial_t^2 + c^2\Delta + i\epsilon)\mathbf{u}_{cl} + \mathbf{u}_{cl} \circ (-\partial_t^2 + c^2\Delta - i\epsilon)\mathbf{u}_q\right] \\ -\frac{\gamma}{2}\int dt \int dt' d^dx \nabla \circ \mathbf{u}_q(t)\nabla \circ \mathbf{u}_{cl}(t)\nabla \circ \mathbf{u}_{cl}(t')\nabla \circ \mathbf{u}_q(t') \tag{2.203}$$

yields the exact equation of motion

$$i(-\partial_t^2 + c\Delta)\langle \mathbf{u}_{cl}\mathbf{u}_q^T\rangle - \gamma \int dt \langle \nabla \left(\nabla \circ \mathbf{u}_{cl}(t)\nabla \circ \mathbf{u}_{cl}(t')\nabla \circ \mathbf{u}_q(t')\right)\mathbf{u}_q^T(t)\rangle = 0 \tag{2.204}$$

. The Ward-identity allows to re-express this into a closed equation for the two point function.

For the vacuum case, the action (2.203) is invariant with respect to exchange of the classical and quantum fields.

In contrast with the euclidean action the Keldysh action is build up from the difference $\phi_+^2 - \phi_-^2$, and hence is invariant with respect to the SL(2) transformation

$$\begin{pmatrix} \tilde{\phi}_+ \\ \tilde{\phi}_- \end{pmatrix} = \begin{pmatrix} \cosh\phi & -\sinh\phi \\ -\sinh\phi & \cosh\phi \end{pmatrix} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}$$

. This is much better than the euclidean replica model, as for the disordered Keldysh ac-

tion this is an exact symmetry, while the ordinary o(2) symmetry of the euclidean model was already broken by the regularization, and hence of the level of the euclidean action.

Within Keldysh rotation this just translates into a phase transformation $\phi_{cl} \to e^{\phi}\phi_{cl}, \phi_q \to e^{-\phi}\phi_q$

$$(1+\phi(t))\phi_{cl}(t)(1-\phi(t'))\phi_q(t') = \phi_{cl}\phi_q + \phi\phi\phi_{cl}\phi_q - \phi_q\phi_{cl})$$

and hence

$$\langle \epsilon\phi_{cl}\phi_q + ij_{cl}\phi_q - ij_q\phi_{cl}\rangle = 0$$
$$\langle \nabla\circ\mathbf{u}_{cl}\nabla\circ\mathbf{u}_q\rangle - \langle\nabla\circ\mathbf{u}_q\nabla\circ\mathbf{u}_{cl}\rangle = i\epsilon\int\langle\nabla\circ\mathbf{u}_{cl}(t)\nabla\circ\mathbf{u}_{cl}(t')\nabla\circ\mathbf{u}_q(t')\nabla\circ\mathbf{u}_q(t)\rangle \qquad (2.205)$$

Integrating (2.204) with respect to the spatial variable, and using the Ward-identity (2.205) within the equation of motion yields an exact equation for the density of vibrational states, which clearly should be examined in future.

Secondly, another interesting working perspective is, to derive exact equations of motion for the two-point function, using the SL(2) symmetry of the vacuum theory. Comparing with the literature, e.g. Berges et al. (9), one finds that those effective equation of motion are structurally identical with those of Vollhardt et al. within the Mode-coupling approach onto localization. This has to be done within the future, in order to get rid of the complicated sigma model structure of the problem, and perform rigorous calculations of the density of states of glasses.

2.9 Localization for vectorial Models

The vector theory has previously been studied extensively.

We briefly quote the generalization of the instanton calculation onto the vectorial

model.

The energy operator of linear elastic media is given by

$$\hat{H} = \frac{1}{2} \int d^d x \left(\lambda \hat{u}_{ii} \hat{u}_{ii} + \mu \hat{u}_{ij} \hat{u}_{ji} \right) \tag{2.206}$$

, with λ the bulk and μ the shear modulus, and $u_{ij} = \frac{1}{2} \left(\partial_i u_j + \partial_j u_i \right)$ the linear strain tensor. If $\vec{u}$ is decomposed into a longitudinal ($\nabla \times \vec{u}_l = 0$) and a transverse polarized ($\nabla \circ \vec{u}_t = 0$) component this reads

$$\hat{H} = -\frac{1}{2} \int d^d x \left(c_l^2 \hat{\vec{u}}_l \circ \Delta \hat{\vec{u}}_l + c_t^2 \hat{\vec{u}}_t \circ \Delta \hat{\vec{u}}_t \right) \tag{2.207}$$

with $c_l^2 = \lambda + 2\mu$ and $c_t^2 = \mu$ the longitudinal and transverse sound velocity. Modeling a glass averaging (2.206) is more reasonable then (2.207). The reason is, that the bulk modulus is much larger then the shear modulus in usual glasses, and hence the shear modulus is the quantity which is likely to fluctuate (63).

Averaging (2.206) over a Gaussian distribution within the Keldysh prescription hence yields

$$\begin{aligned} iS = \frac{i}{2} \mathrm{Tr} \left[\sigma_x \begin{pmatrix} 0 & \left(-\vec{u}^q \partial_t^2 \vec{u}^{cl} - \lambda u_{ii}^q u_{ii}^{cl} - \mu u_{ij}^q u_{ji}^{cl} \right) \\ \left(-\vec{u}^q \partial_t^2 \vec{u}^{cl} - \lambda u_{ii}^q u_{ii}^{cl} - \mu u_{ij}^q u_{ji}^{cl} \right) & \vec{u}_q G^{-1} \vec{u}_q \end{pmatrix} \right] \\ -\frac{\gamma}{2} \int \int u_{ij}^q(t) u_{ji}^{cl}(t) u_{lm}^q(t') u_{ml}^{cl}(t') \end{aligned} \tag{2.208}$$

. The equation of motion with instanton ansatz $iu_q = u_{cl} = u$ yields

$$-\partial_t^2 u_i + \lambda \partial_i u_{ii} + (\mu - 3\gamma \int_0^t dt' u_{lm}(t') u_{ml}(t')) \partial_j u_{ji} = 0 \tag{2.209}$$

. If there is a localized solution to (2.209) this translates into a monotonously lowered

sound velocity, which drops to zero at the center of localization.

Decoupling into longitudinal and transverse sound waves, yielding

$$-\partial_t^2 u_l + c_l^2(1 - \frac{6\gamma}{c_l^2}\int_0^t dt'(\nabla \circ u_l)^2 \Delta u_l = 0 \tag{2.210}$$

$$-\partial_t^2 u_t + c_t^2(1 - \frac{3\gamma}{c_t^2}\int_0^t dt'|\nabla \times u_t|^2) \Delta u_t = 0 \tag{2.211}$$

, where in agreement with the previous theory we ignore terms which couple longitudinal and transverse modes via the disorder term. This could be done rigorously by constraining the disorder-average onto configurations which respect this separation, e. g. by means of additional Lagrange parameters. Within this further "approximation" (technical convenience) the Keldysh partition function is just a product of longitudinal and transverse degrees of freedom, and the density of states reads

$$g(\omega) = e^{-\frac{\omega^d}{\rho_0 \bar{\mu}^d \gamma} A_l} g_l(\omega) + 2e^{-\frac{\omega^d}{\rho_0 \bar{\mu}^d \gamma} A_t} g_t(\omega) \tag{2.212}$$

$$A_t = \int d^d x |\tilde{u_t} \circ \tilde{\Delta} \tilde{u_t}|^2 \tag{2.213}$$

$$A_l = 4A_t \tag{2.214}$$

.

Within the Bosonized version the Sigma model reads

$$S = \frac{1}{2}\ln(i(G_0^{-1})_{ij}^{\alpha\beta} + i\partial_{ij}\Lambda_{ijlm}^{\alpha\beta}\partial_{lm}) + i\Lambda_{ijlm}^{\alpha\beta}Q_{mlji}^{\beta\alpha} - \frac{1}{2}Q_{ijlm}^{\alpha\beta}Q_{mlji}^{\beta\alpha} \tag{2.215}$$

.

Analogously with the scalar model this yields to

$$g_l(\omega) = \mathrm{Tr}\left[\frac{1}{\omega^2 + i\epsilon + (c_l^2 - \Sigma(\omega) - 6\gamma|u_l \Delta u_l|)\Delta}\right]'' \tag{2.216}$$

$$g_t(\omega) = \mathrm{Tr}\left[\frac{1}{\omega^2 + i\epsilon + (c_t^2 - 2\Sigma(\omega) - 3\gamma|u_t \Delta u_t|)\Delta}\right]'' \tag{2.217}$$

and the SCBA-equation generalizes to

$$\Sigma(\omega) = \frac{\gamma}{2}\mathrm{Tr}\left[\frac{e^{-\frac{\omega^d}{\rho_0 \bar{\mu}^d \gamma} A_l}\Delta}{\omega^2 + i\epsilon + (c_l^2 - \Sigma(\omega) - \gamma 6|u_l \Delta u_l|)\Delta} + \frac{e^{-\frac{\omega^d}{\rho_0 \bar{\mu}^d \gamma} A_t}\Delta}{\omega^2 + i\epsilon - (c_t^2 - 2\Sigma(\omega) - \gamma 3|u_t \Delta u_t|)\Delta}\right] \tag{2.218}$$

.

.

3 Results and discussion

We will solve the instanton equations for the longitudinal and transverse modes numerically. For simplification we use the frequency diagonal approximation and seek for solutions which only depend on the spatial modulus $r = |\mathbf{x}|$.

3.1 One-dimensional longitudinal model

We also sketched the solution method in section 2. The one-dimensional instanton equation is given by

$$\left(\omega^2 + (c^2 - 3\gamma\partial_x u \partial_x u)\partial_x^2\right) u(\omega, x) = 0 \tag{3.1}$$

. For numerical evaluation, we introduce the scaling ansatz $u \equiv \sqrt{\frac{1}{\gamma c^2 \omega^2}}\tilde{u}(\omega x)$ yielding the dimensionless equation

$$\left(1 + (1 - 3\partial_y \tilde{u} \partial_y \tilde{u})\partial_y^2\right) \tilde{u}(y) = 0 \tag{3.2}$$

, which is equivalent with the system of equations

$$\partial_y v(y) = -\frac{\tilde{u}(y)}{(1 - 3v(y)v(y))} \tag{3.3}$$

$$\partial_y \tilde{u} = v \tag{3.4}$$

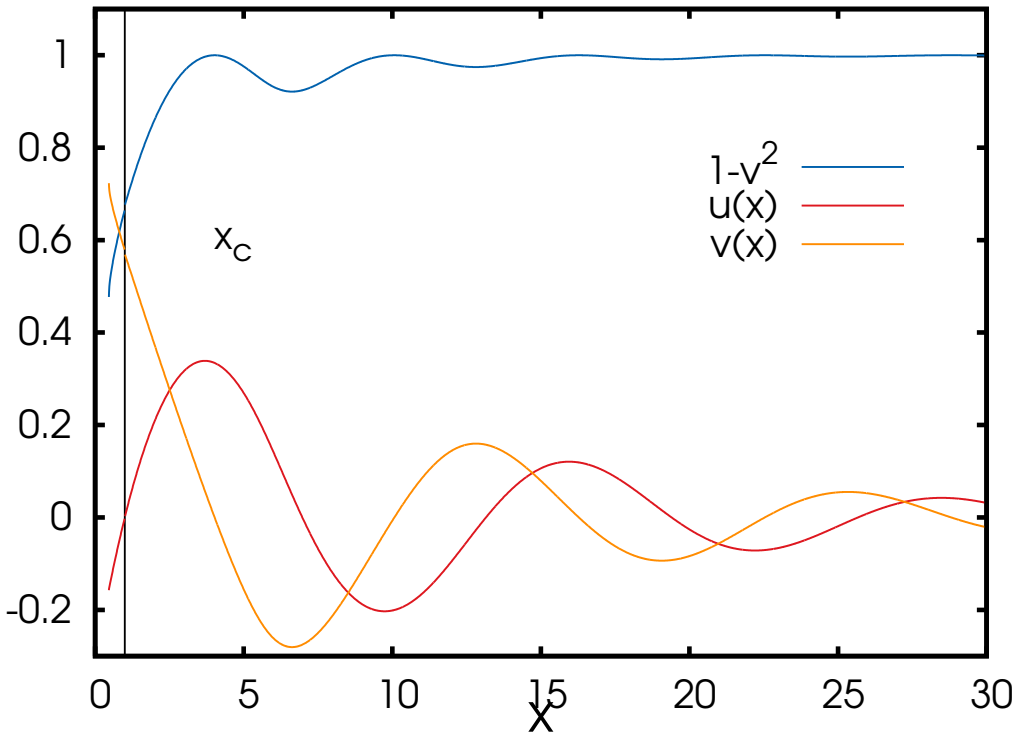

Figure 3.1: Solution to the one-dimensional instanton equation with $v(x_c) = \sqrt{\frac{1}{3}}, u(x_c) = 0$

, which is easily evaluated by means of the third order Runge-Kutta algorithm.

A unique solution is obtained by the initial conditions $v(x_c) = \sqrt{\frac{1}{3}}, u(x_c) = 0$. x_c is the point of zero sound velocity, which divides the oscillatory form strictly monotonous behavior of the instanton. The instanton factor A evaluates numerically to 0.1574.

3.2 Density of states for the vectorial model

We solve

$$\omega^2 u_l + \frac{c_l^2}{r^2}(1 - \frac{6\gamma}{c_l^2 r^2}(\partial_r(r u_l))^2)\partial_r(r^2 \partial_r u_l) = 0 \tag{3.5}$$

$$\omega^2 u_t + \frac{c_t^2}{r^2}(1 - \frac{3\gamma}{c_t^2 r^2}(\partial_r(r u_t))^2)\partial_r(r^2 \partial_r u_t) = 0 \tag{3.6}$$

, where the ansatz has been $\mathbf{u}_l \equiv u_l(\omega, r)\mathbf{e}_\mathbf{r}, \mathbf{u}_t \equiv u_t(\omega, r)\mathbf{e}_{\phi/\theta}$. Introducing the reduced units $v_{t/l} \equiv \sqrt{\frac{\gamma}{c_l^2 \omega^2}}\partial_r(r v_{t/l}(\omega r))$, $x = r\omega$, $u_{l/t} = c_{l/t}^2 u_{l/t}$ yields

$$u_l + \frac{1}{x^2}(1 - 6\left(\frac{u_l}{x} + v_l\right)^2)\partial_x(x^2 v_l) = 0 \tag{3.7}$$

$$u_t + \frac{1}{x^2}(1 - 3\left(\frac{u_t}{x} + v_t\right)^2)\partial_x(x^2 v_t(x)) = 0 \tag{3.8}$$

and hence

$$\partial_x v_l = -\frac{u_l}{(1 - 6\left(\frac{u_l}{x} + v_l\right)^2)} - \frac{1}{x}v_l \tag{3.9}$$

$$\partial_x v_t = -\frac{u_t}{(1 - 3\left(\frac{u_t}{x} + v_t\right)^2)} - \frac{1}{x}v_t \tag{3.10}$$

. Forward integration of equation (3.9) with the boundary conditions u(1)=0.2, v(1)=0 again yields to oscillating behavior which drops of faster then the volume measure $\int dx x^2$ as depicted in figure 3.2 . Integration with respect to arbitrary boundary conditions always produces localized states, due to the motion in a self-induced non-linear environment of lowered force constants.

A unique solution is obtained from the self-consistent requirement that at the critical point x_c where sound-velocity zero is reached, also the amplitude has to turn to zero, hence $u_{l/t}(x_c) = 0,\ v_{l/t}(x_c) = \sqrt{\frac{1}{6}}/\sqrt{\frac{1}{3}}$.
The instanton factor evaluates to $A_l = 2,2297$.

3.3 Comparison with experiments

We compare the theory with the measurement of Baldi et al. (5) on vitreous silica. Using the disorder parameter of the previous SCBA-calculation which is close to the critical region $\gamma = 0.99\gamma_c,\ \gamma_c = 0.1764$, the tail fits most of the data points in the frequency-region beyond the Boson peak. At large frequencies, the experimental data drops of faster than the Lifshitz tail of the present theory. This feature is beyond the scope of the present phenomenological discussion. Clearly, the experimental data shows a transi-

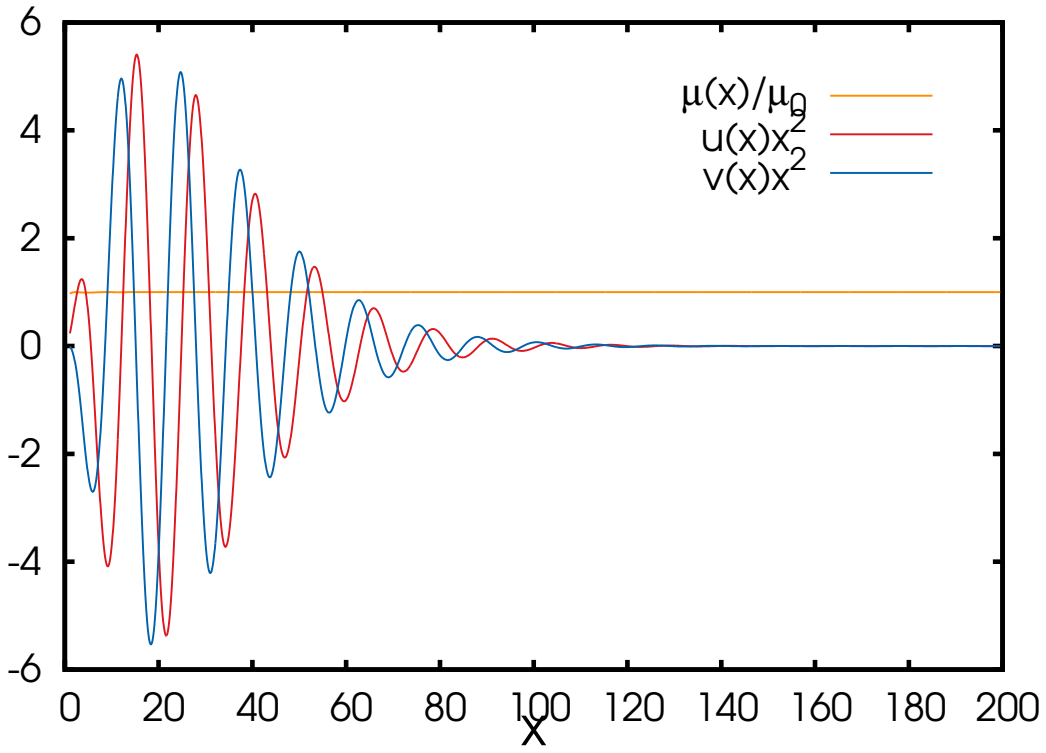

Figure 3.2: Solution of the longitudinal instanton equation in 3 dimensions with initial conditions u(1)=0.2, v(1)=0

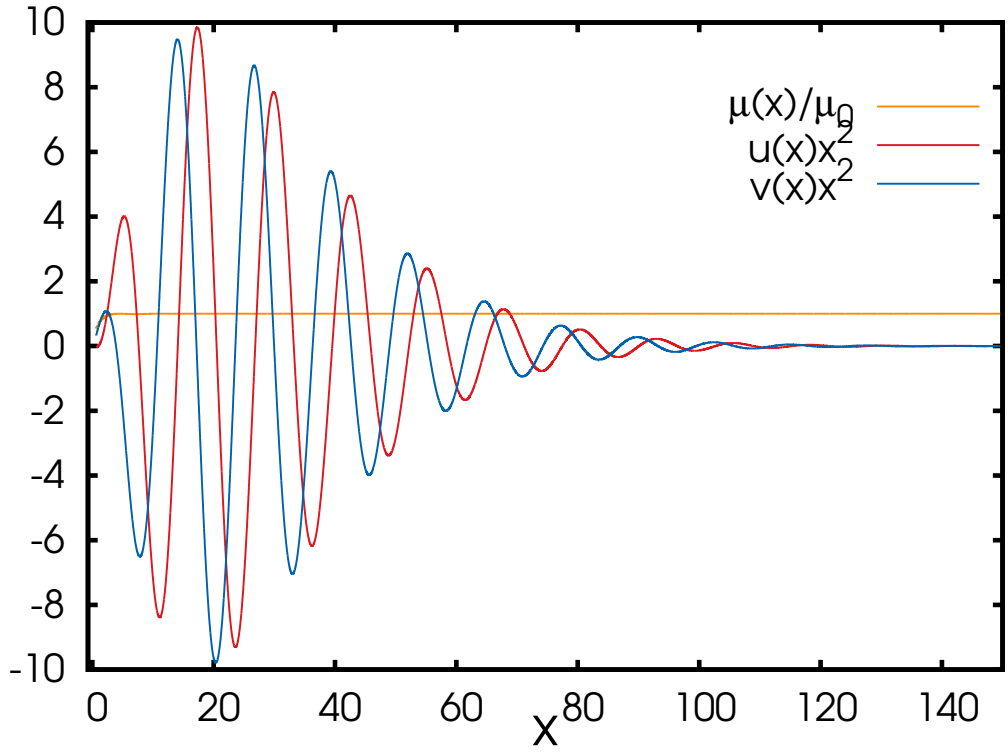

Figure 3.3: Solution of the longitudinal instanton equation in 3 dimensions with initial conditions $u(1) = 0$, $v(1) = \sqrt{\frac{1}{6}}$

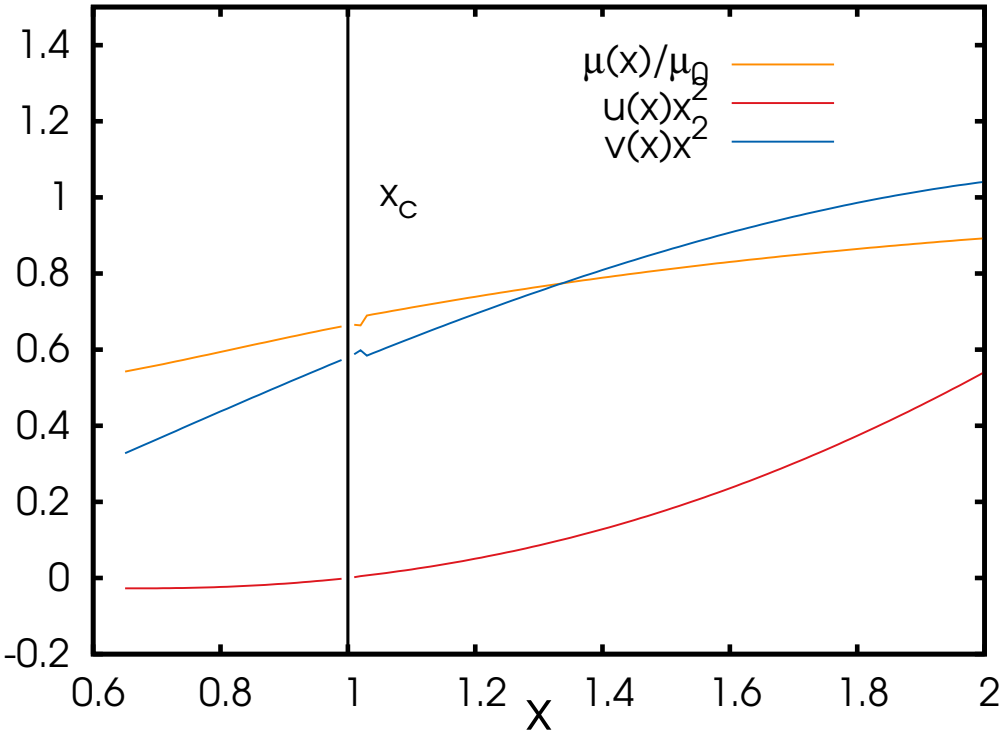

Figure 3.4: Solution of the longitudinal instanton equation in 3 dimensions with initial conditions $u(1) = 0$, $v(1) = \sqrt{\frac{1}{6}}$

tion to a slower decrease beyond 3.2 THz. Most of the other density of states, shown within the introduction show up such a transition to a slower or faster drop-off regime at high frequencies. This is a detail which can-not be deduced from a Lifshitz exponent which is a polynomial of the frequency and hence can not be explained in the present framework. However the interesting feature is, that an exponential drop-off far beyond the Boson-peak is related to a disorder parameter close to criticality. The Boson-peak its-self only exists at disorder parameters which do not deviate from the critical by a factor of 0.1. It may be hence understood as a preliminar of the localization transition: at such large critical values of the disorder parameter the density of states is dominated by "strong" disorder-induced scattering, in which the SCBA collects all processes which are analytic in the disorder parameter and the instanton collects scattering processes of order $\frac{1}{\gamma}$.

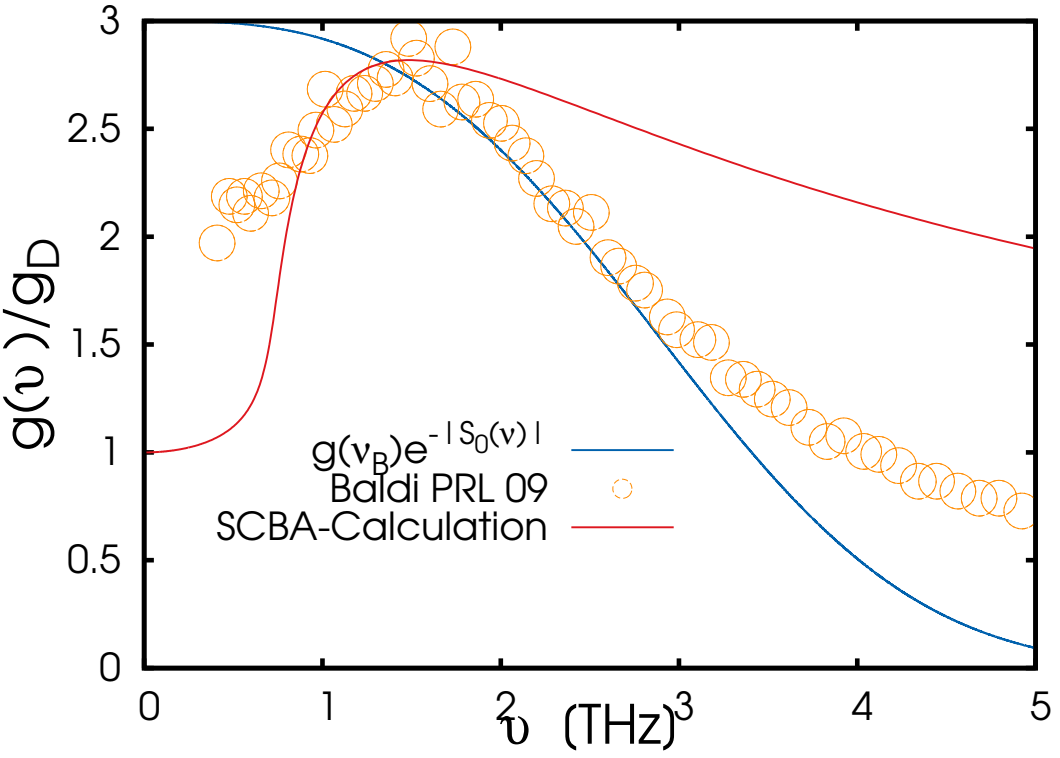

Figure 3.5: Comparison of the Lifshitz-exponential with dimensionless disorder parameter $\gamma = 0.99\gamma_c$, $\gamma_c = 0.1764$ with the measurement of Baldi et al. (5). The red line shows a previous SCBA-calculation.

3.4 Summary and conclusion

Within the present work, we established a consistent phenomenological theory of the frequency dependent density of vibrational states of glassy systems in terms of "weakly" fluctuating force constants.

The low-frequency region is dominated by propagating wave-like modes, which can be altered by additional anharmonic scattering effects, which already explained further low-frequency deviations from the usual Debye density of states. At intermediate frequencies, a transition to random-matrix eigenstates occurs which is followed by strongly localized modes. The Boson-peak and hence the random-matrix regime can be understood as preliminar of the strongly localized high frequency modes.

Although this phenomenological theory is in quite nice agreement with the experimental data, we found that it would be worth to formulate it on a more rigorous level in future. We hope that the present work can be helpful within this direction. The main issue for future investigations is now, that both the Boson-peak and the localized modes

are somehow related to isolated points within the material where the force-constants drop to zero. The theory of this drop-off is a theory of non-Gaussian distributed force constants, and is relevant in order to investigate the nature of the high-frequency eigenstates in the deep localized regime. We also found that at the Gaussian level, fluctuations within the present mean-field formalism yields to a vast number of terms which makes further argumentation very complicated.

In the future investigations this mean-field picture should really be withdrawn, and rediscovered within a larger machinery. Clearly the Keldysh method has very much potential in order to achieve this goal. The non-equilibrium formalism allows to re-express this theory not only on the level of Gaussian fluctuations, but as a coupled system of equations of motions where the information of the local sound-velocity is encoded in non-equilibrium response functions of the elastic media. These equations of motion can be expanded in a symmetry-expansion, due to the fact that the whole theory has to satisfy the fluctuation-dissipation relation and hence the SL(2) symmetry as outlined in section 2.8. The result will be something like a mode-coupling approach onto the phonon-propagation in case of frozen non-trivial elastic constants, where one should be able to reduce this theory somehow to the simple one- and two-particle mean-field theories, which have been very successful in explaining vibriational excitations in disordered media within the last two decades.

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Appendix

A.I Gaussian integrals

The usual Gaussian integral for a single variable is believed to generalize to operators with real-valued eigenvalues

$$\int \mathcal{D}f(x)e^{-\int dx f(x)\hat{D}f(x)+\int dx j(x)f(x)} = e^{\mathbf{j}D^{-1}\mathbf{j}}\prod_{\lambda}\sqrt{(\frac{\pi}{\lambda})}\mathcal{N}$$

. The normalization factor $\mathcal{N}$ comes from the rotation to the eigen-functions of $\hat{D}$, which for an ordinary Fourier-expansion becomes independent of the eigenvalues. Frequently the functional determinant

$\sqrt{\det(A)}^{-1}$ is rewritten into $e^{-\frac{1}{2}\mathrm{Tr}\ln A}$.

This also holds if the integration variable is deformed onto the imaginary axis

$$\int \mathcal{D}f(x) e^{-i\int dx f(x)\hat{D}f(x)+\int dx j(x)f(x)} = e^{-i\mathbf{j}D^{-1}\mathbf{j}} \prod_{\lambda} \sqrt{(\frac{\pi}{i\lambda})}\mathcal{N}$$

.

A.II Free bosonic Particles

Introducing the rotation yields

$$S_{fp} = i\int_0^T dt \begin{pmatrix} x_{cl}(t) & x_q(t) \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 \\ -\partial_t^2 & 0 \end{pmatrix} \begin{pmatrix} x_{cl}(t) \\ x_q(t) \end{pmatrix} - a x_{cl}(0)x_{cl}(0) - a x_q(0)x_q(0)$$

with $\ln \rho(x_0^+, x_0^-) = \ln\left[\phi(x_{cl}(0)+x_q(0))\phi^*(x_{cl}(0)-x_q(0))\right] = -a x_{cl}(0)^2 - a x_q(0)^2$ for Gaussian initial states. The constraint to this integral is $x_{cl}(T) = y, x_q(T) = 0$

$$\begin{aligned}
S_{fp} &= \lim_{\delta\to 0} i\int_\delta^T dt \begin{pmatrix} x_{cl}(t) & x_q(t) \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 \\ -\partial_t^2 & 0 \end{pmatrix} \begin{pmatrix} x_{cl}(t) \\ x_q(t) \end{pmatrix} \\
&+\frac{i}{\delta^2}(x_q(\delta)-x_q(0))(x_{cl}(\delta)-x_{cl}(0)) - a x_{cl}(0)x_{cl}(0) - a x_q(0)x_q(0) - lnZ \\
&= \lim_{\delta\to 0}\int_\delta^T dt \begin{pmatrix} x_{cl}(t) & x_q(t) \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 \\ -\partial_t^2 & 0 \end{pmatrix} \begin{pmatrix} x_{cl}(t) \\ x_q(t) \end{pmatrix} \\
&+(x_q(\delta)-x_q(0))x_{cl}(\delta) - x_{cl}(0)(x_q(\delta)-x_q(0)) - a x_{cl}(0)x_{cl}(0) - a x_q(0)x_q(0) - lnZ \\
&= \int_0^T dt \begin{pmatrix} x_{cl}(t) & x_q(t) \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 \\ -\partial_t^2 & 0 \end{pmatrix} \begin{pmatrix} x_{cl}(t) \\ x_q(t) \end{pmatrix} + \lim_{\delta\to 0}\frac{i}{\delta}\partial_t x_q(0)\left(x_{cl}(0)+\frac{1}{a\delta}\partial_t x_q(0)\right) - a x_q(0)x_q(0) \\
&= \int_0^T dt \begin{pmatrix} x_{cl}(t) & x_q(t) \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 \\ -\partial_t^2 & 0 \end{pmatrix} \begin{pmatrix} x_{cl}(t) \\ x_q(t) \end{pmatrix} - a x_q(0)x_q(0)
\end{aligned}$$

, where we got an other constraint $\partial_t x_q(t)|_{t=0} = 0$. Note that

$$a^{-1} = \langle x_{cl}(0)x_{cl}(0)\rangle = G_r^{-1}G_r\langle x_{cl}(0)x_{cl}(0)\rangle G_a G_a^{-1} = G_r^{-1}\langle x_{cl}(t)x_{cl}(t')\rangle G_a^{-1} = G_K$$

hence one could write within the Keldysh-logic

$$S_{fp} = \int_0^T dt \begin{pmatrix} x_{cl}(t) & x_q(t) \end{pmatrix} \begin{pmatrix} 0 & -\partial_t^2 \\ -\partial_t^2 & \langle x_{cl}(t)x_{cl}(t)\rangle^{-1} \end{pmatrix} \begin{pmatrix} x_{cl}(t) \\ x_q(t) \end{pmatrix}$$

One can try to evaluate this integral again via semi-classical expansion. Varying with respect to the quantum component setting it to zero afterwards yields the classical equation of motion

$$\partial_t^2 x_{cl}(t) = 0$$

with solution $x_{cl}(t) = x + vt$. The fluctuations can again be expanded within a Fourier-series requiring the fluctuations $\delta x_{cl}, \delta x_q$ to vanish at the boundary yielding

$$S_{fp} = i\sum_n \begin{pmatrix} x_{cl}^n & x_q^n \end{pmatrix} \begin{pmatrix} 0 & \left(\frac{n\pi}{T}\right)^2 \\ \left(\frac{n\pi}{T}\right)^2 & G_K^{-1} \end{pmatrix} \begin{pmatrix} x_{cl}^n \\ x_q^n \end{pmatrix}$$

yielding

$$\prod_{n=1}^{\infty} e^{\mathrm{Tr}\ln\begin{pmatrix} G_K & \left(\frac{T}{n\pi}\right)^2 \\ \left(\frac{T}{n\pi}\right)^2 & 0 \end{pmatrix}} \int dx_q^0 dx_{cl}^0 e^{-x_q G x_q}$$

. The zero mode has to be singled out because it can not be evaluated by use of the

Gaussian formula.

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A.III Sigma-model terms

First of all to the $W^{(2)}DW^{(2)}$. In vacuum we obtain the matrix elements

$$\mathrm{Tr}[W^{(2)}DW^{(2)}] =$$

$\mathcal{O}(w^4, v^4)$

$$\gamma[\bar{Q}_a, v]\left(\delta[\bar{Q}_a, v]v^2 + \delta v[\bar{Q}_r, v]v + v\delta v[\bar{Q}_a, v] + v[\bar{Q}_r, v]\delta v\right)$$
$$+\gamma\{w, \bar{Q}_a w - w\bar{Q}_r\}\{\{w, \bar{Q}_r w - w\bar{Q}_a\}, \delta\}$$

$\mathcal{O}(wv^3)$

$$\left(d_{ra}[\bar{Q}_a, v]v + d_{ra}v[\bar{Q}_r, v] + v[\bar{Q}_a, v]d_{ra}\right)\left(\{w, [\bar{Q}_a, v]\} + v(\bar{Q}_r w - w\bar{Q}_a) + (\bar{Q}_a w - w\bar{Q}_r)v\right)$$
$$+\left(d_{ra}v[\bar{Q}_a, v] + v[\bar{Q}_r, v]d_{ra} + [\bar{Q}_a, v]vd_{ra}\right)\left(\{w, [\bar{Q}_r, v]\} + v(\bar{Q}_a w - w\bar{Q}_r) + (\bar{Q}_r w - w\bar{Q}_a)v\right)$$
$$+\gamma[\bar{Q}_a, v]v\{[\bar{Q}_r, v]w, \delta\} + \gamma v[Q_r, v]\{\delta, [\bar{Q}_r, v]w\}$$

$\mathcal{O}(w^3 v)$

$$\left(d_{ra}\{w, \bar{Q}_a w - w\bar{Q}_r\} + \{w, \bar{Q}_r w - w\bar{Q}_a\}d_{ra}\right)\left(\{w, [\bar{Q}_a, v]\} + v(\bar{Q}_r w - w\bar{Q}_a) + (\bar{Q}_a w - w\bar{Q}_r)v\right)$$
$$+\left(d_{ra}\{w, \bar{Q}_r w - w\bar{Q}_a\} + \{w, \bar{Q}_a w - w\bar{Q}_r\}d_{ra}\right)\left(\{w, [\bar{Q}_r, v]\} + v(\bar{Q}_a w - w\bar{Q}_r) + (\bar{Q}_r w - w\bar{Q}_a)v\right)$$
$$+\gamma[Q_r, v]w\delta\{w, \bar{Q}_a w - w\bar{Q}_r\} + \gamma\left(\{w, \bar{Q}_a w - w\bar{Q}_r\}\right)\delta[Q_r, v]w$$

$\mathcal{O}(w^2v^2)$

$$+[\bar{Q}_r,v]wd_{ra}\left(\{w,[\bar{Q}_a,v]\}+v(\bar{Q}_rw-w\bar{Q}_a)+(\bar{Q}_aw-w\bar{Q}_r)v\right)$$

$$+[\bar{Q}_r,v]w\left(\{w,[\bar{Q}_r,v]\}+v(\bar{Q}_aw-w\bar{Q}_r)+(\bar{Q}_rw-w\bar{Q}_a)v\right)d_{ra}$$

$$+\gamma\left(\{w,[\bar{Q}_r,v]\}+v(\bar{Q}_aw-w\bar{Q}_r)+(\bar{Q}_rw-w\bar{Q}_a)v\right)\delta\left(\{w,[\bar{Q}_r,v]\}+v(\bar{Q}_aw-w\bar{Q}_r)+(\bar{Q}_rw-w\bar{Q}_a)v\right)$$

$$+\gamma\left(\{w,[\bar{Q}_a,v]\}+v(\bar{Q}_rw-w\bar{Q}_a)+(\bar{Q}_aw-w\bar{Q}_r)v\right)\delta\left(\{w,[\bar{Q}_a,v]\}+v(\bar{Q}_rw-w\bar{Q}_a)+(\bar{Q}_aw-w\bar{Q}_r)v\right)$$

$$\gamma\left(v[\bar{Q}_r,v]+[\bar{Q}_a,v]v\right)\delta\{w,\bar{Q}_rw-w\bar{Q}_a\}+\gamma v[\bar{Q}_a,v]\delta\{w,\bar{Q}_aw-w\bar{Q}_r\}$$

$$+\gamma\{w,\bar{Q}_rw-w\bar{Q}_a\}\delta\left([\bar{Q}_a,v]v+v[Q_r,v]\right)+\gamma\left(\{w,\bar{Q}_aw-w\bar{Q}_r\}\right)\delta v[\bar{Q}_a,v]$$

$\mathrm{Tr}\left[W^{(1)}DW^{(2)}\right]$

$\mathcal{O}(vw^2)$

$$[2\bar{Q}'_r,w]d_{ra}\left(\{w,[2\bar{Q}'_r,v]\}+\{[2\bar{Q}'_r,w],v\}\right)$$

$$+[2\bar{Q}'_r,v]d_{ra}\{w,[2\bar{Q}'_r,w]\}+2\gamma[\bar{Q}_r,v]w\left(\bar{Q}_aw-w\bar{Q}_r\right)\delta$$

$\mathcal{O}(wv^2)$

$$[2\bar{Q}'_r,v]d_{ra}\left([\bar{Q}_r,v]w\right) \tag{3.11}$$

$$+2\gamma[\bar{Q}_r,v]\left(\delta\{w,[\bar{Q}_r,v]\}+\delta v(\bar{Q}_aw-w\bar{Q}_r)+\delta(\bar{Q}_rw-w\bar{Q}_a)v+\left(\bar{Q}_rw-w\bar{Q}_a\right)\delta v\right) \tag{3.12}$$

$$+2\gamma[\bar{Q}_a,v]\left(\delta\{w,[\bar{Q}_a,v]\}+\delta v(\bar{Q}_rw-w\bar{Q}_a)+\delta(\bar{Q}_aw-w\bar{Q}_r)v+v\left(\bar{Q}_rw-w\bar{Q}_a\right)\delta+\left(\bar{Q}_aw-w\bar{Q}_r\right)\delta v\right) \tag{3.13}$$

$\mathcal{O}(v^3)$

$$[2\bar{Q}'_r,v]d_{ra}\left([\bar{Q}_a,v]v+v[\bar{Q}_r,v]\right)+[2\bar{Q}'_r,v]d_{ra}v[\bar{Q}_a,v]$$

$\mathcal{O}(w^3)$

$$2\gamma\left(\bar{Q}_a w - w\bar{Q}_r\right)\delta\{w, \bar{Q}_r w - w\bar{Q}_a\} + 2\gamma\left(\bar{Q}_r w - w\bar{Q}_a\right)\delta\{w, \bar{Q}_a w - w\bar{Q}_r\}$$

The fourth order term is given by $6\mathrm{Tr}\left[\{W^{(1)}, D\}W^{(3)}\right] =$

$\mathcal{O}(v^2w^2)$

$$2\gamma[Q_r, v]\delta\left(w[\bar{Q}_a, v]w - [\bar{Q}_r, v]w^2 + [v, (\bar{Q}_r w - w\bar{Q}_a)w] + w(\bar{Q}_a w - w\bar{Q}_r)v - (\bar{Q}_r w - w\bar{Q}_a)vw\right) \tag{3.14}$$

$$2\gamma\left(\bar{Q}_r w - w\bar{Q}_a\right)\delta\left([v, (\bar{Q}_a w - w\bar{Q}_r)v] + w[\bar{Q}_r, v]v + v[\bar{Q}_a, v]w - [\bar{Q}_a, v](wv + vw)\right) \tag{3.15}$$

$$2\gamma\left(\bar{Q}_a w - w\bar{Q}_r\right)\delta\left([v, (\bar{Q}_r w - w\bar{Q}_a)v] + w[\bar{Q}_a, v]v - [\bar{Q}_r, v]vw + [v, [Q_r, v]w]\right) \tag{3.16}$$

$$2\gamma[\bar{Q}_a, v]\delta\left(w[\bar{Q}_r, v]w - [\bar{Q}_a, v]w^2 + w(\bar{Q}_r w - w\bar{Q}_a)v - (\bar{Q}_a w - w\bar{Q}_r)vw + [v, (\bar{Q}_a w - w\bar{Q}_r)w]\right) \tag{3.17}$$

$\mathcal{O}(v^4)$

$$2\gamma\left([\bar{Q}_r, v]\delta[v, [\bar{Q}_r, v]v] + [\bar{Q}_a, v]\delta[v, [\bar{Q}_a, v]v]\right)$$

$\mathcal{O}(w^4)$

$$2\gamma\left(\bar{Q}_r w - w\bar{Q}_a\right)\delta\left(2w\bar{Q}_r w^2 - \{w^2, \bar{Q}_a\}w\right) + 2\gamma\left(\bar{Q}_a w - w\bar{Q}_r\right)\delta\left(2w\bar{Q}_a w^2 - \{w^2, \bar{Q}_r\}w\right)$$

$\mathcal{O}(wv^3)$

$$[2\bar{Q}'_r, v]d_{ra}\left([v, [2\bar{Q}'_r, w]v] + w[2\bar{Q}'_r, v]v + v[2\bar{Q}'_r, v]w - [2\bar{Q}'_r, v]\{w, v\}\right)$$
$$+[2\bar{Q}'_r, w]d_{ra}[v, [2\bar{Q}'_r, v]v]$$

$\mathcal{O}(vw^3)$

$$[2\bar{Q}'_r, w]d_{ra}\left([w, [2\bar{Q}'_r, v]]w + [v, ([2\bar{Q}'_r, w]w] + [w, [2\bar{Q}'_r, w]v]\right) + [2\bar{Q}'_r, v]d_{ra}[w, [2\bar{Q}'_r, w]]w$$

A.IV Introduction to the attached publications

In the appendix of the present thesis five publications (1, 2, 3, 4, 5) have been attached, which have been published after the completion of the author's diploma thesis. The recent publication *High-frequency vibrational density of states of a disordered solid* (5) comprises a shortened version of the contents of the present thesis. In the other papers (1, 2, 3, 4) the replica quantum field theory for vibrational excitations in disordered solids, based on weakly fluctuating elastic consants, which has been worked out in the author's diploma thesis, is applied to the case of correlated disorder and the combined presence of anharmonic and quenched-disordered interactions. These publications are intimately related to the subject-matter of the present work. They set the basis for understanding the anomalous vibrational spectrum at much lower frequencies than the Debye frequency, whereas the present work focusses on the disorder-induced band tail near or above the Debye frequency (Lifshitz tail). The saddle-point approximation used for the inverstigation of the lower-frequency regime relies on the smallness of the variance of the elasticity fluctuations, compared to the frequency at hand, whereas the investigation of the Lifshitz tail relies on the smallness of the inverse of the mentioned parameter. So these theories complement each other. In the following we briefly sketch the contents of the publications on the lower-frequency vibrationy properties.

A.IV.1 The role of correlations for the vibrational anomalies near the boson peak

The theory of the vibrational anomalies of glasses near the boson peak has been formulated by Schirmacher, 2006 (6). As the present thesis this description is based on the assumption that in a disordered solid the elastic constants exhibit spatial fluctuations, which are caused by the quenched structural disorder. In Schirmacher's theory it is assumed that the shear moduli have Gaussian fluctuations, which are uncorrelated. This theory gives a qualitative and in certain cases even a quantitative explanation of the vibrational anomalies (6, 7, 8), near the boson peak, (i.e. not near the upper band edge, but approximately at 1/10 of the Debye frequency) which are

- the enhancement of the density of states near 1/10 of the Debye frequency (bo-

son peak, BP);

- a cross-over from a Rayleigh-like ω^4 behavior to a ω^2 behavior of the sound attenuation coefficient near the BP frequency;
- a dip in the differential sound velocity near the BP frequency.

The question was now arising, which role elastic fluctuations with *correlated* disorder would play for the vibrational anomalies. In order to investigate this question numerically Baldi and Viliani (1, 3) simulated a two-dimensional system with spatially fluctuating harmonic interactions. The fluctuations were tailored in such a way that they had a correlation length which was chosen to have several different values. The theory of Schirmacher was now generalized for correlated disorder (1, 3), so that we were now able to discuss the numerical findings in the light of our theory. As to be expected the inverse correlation length acts as a cutoff in q space for the disorder fluctuations. Now this cutoff replaces the Debye ultraviolet cutoff, which had to be introduced into Schirmacher's theory. The self-consistent saddle-point equations for the self energy of the correlated theory exhibit a length scaling with the inverse correlation length. Such a scaling is, indeed, observed in the sound attenuation data of the simulated disordered two-dimensional system. It is very satisfactory that the scaled data of our self-consistent theory just lay on top of the simulated ones.

A.IV.2 Anharmonic elasticity theory

Within the author's Diploma thesis (9) the low-frequency sound attenuation of disordered solids had been discussed assuming generic anharmonicities introducing mode-Grüneisen parameters. However in our later inverstigations (2, 4) we realized that the nonlinear terms of the standard Lamé elasticity theory, which do not contribute to the anharmonic coupling in crystals, give rise to an appreciable anharmonic coupling in disordered solids in the presence of spatial fluctuations of the elastic constants. This effect is due to the absence of local momentum conservation in the disordered medium. The fact that the variance of the elasticity fluctuations are responsible both for the boson peak and the anharmonic sound attenuation reduces the set of adjustable parameters

in the theory. The combined anharmonic and disorder theory gives for the sound damping a so-called Akhiezer law $\Gamma(\omega) \propto \omega^2 T$, where T is the temperature. Such a frequency and temperature dependence is observed in a number of disordered solids in the GHz range, i.e below the boson peak. This anharmonic law masks the Rayleigh ω^4 contribution, which should be present at very low temperatures, at which the anharmonic contribution is suppressed.

A very interesting aspect, which arose from the work on anharmonic interactions is the fact that anharmonicity plays a crucial role for the case of marginal stability (10, 11). It turns out that small regions with very small positive or negative elastic constants exist in glasses and constitute patches of marginal stability. In these regions the anharmonic interaction as identified in the work developed in (2, 4) leads to a frequency-fractal dependence of the sound attenuation and density of states according to a $\omega^{3/2}$ law. Such a frequency dependence just below the boson peak can be identified experimentally in metallic glasses, in network glasses and computer simulations (10, 11).

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Vibrational excitations in systems with correlated disorder

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We investigate a d-dimensional model (d = 2,3) for sound waves in a disordered environment, in which the local fluctuations of the elastic modulus are spatially correlated with a certain correlation length. The model is solved analytically by means of a field-theoretical effective-medium theory (self-consistent Born approximation) and numerically on a square lattice. As in the uncorrelated case the theory predicts an enhancement of the density of states over Debye's ω^{d-1} law ("boson peak") as a result of disorder. This anomay becomes reinforced for increasing correlation length ξ. The theory predicts that ξ times the width of the Brillouin line should be a universal function of ξ times the wavenumber. Such a scaling is found in the $2d$ simulation data, so that they can be represented in a universal plot. In the low-wavenumber regime, where the lattice structure is irrelevant there is excellent agreement between the simulation at small disorder. At larger disorder the continuum theory deviates from the lattice simulation data. It is argued that this is due to an instability of the model with stronger disorder.

PACS numbers: 65.60

I. INTRODUCTION

The influence of quenched disorder on the dynamic properties of solids is enormous and is subject to widespread experimental and theoretical investigations [1]. The disorder leads to strong modifications of physical properties of the solid. On the other hand, the absence of lattice order in the solids and the corresponding breakdown of the Bloch theorem leads to appreciable difficulties for the theoretical interpretation of the disorder-induced phenomena. Here mean-field theories and particularly effective-medium theories have been of much help [2], as they very often lead, at least, to a qualitative understanding of the influence of the disorder. In particular the coherent-potential approximation [3] (CPA) and its small-disorder version, the self-consistent Born approximation (SCBA) [4], have proved to be useful for interpreting the electronic and other spectral properties of disordered solids. In many cases physically different situations can be mapped onto each other. So one can convert an electronical problem to a vibrational one by replacing the energy E by $-\omega^2$, where ω is the frequency parameter. If E is replaced by $i\tilde{\omega}$, one studies the mathematical analogous diffusion problem [2, 5, 6], where $\tilde{\omega}$ denotes the time Fourier parameter of the diffusion dynamics.

In the case of vibrational properties the disorder-induced excess in the density of states (DOS) over Debye's ω^{d-1} law (d is the dimensionality) ("boson peak") has been successfully explained for a lattice model by comparing a simulation of a disordered lattice system with the predictions of the lattice CPA [7]. The comparison showed once more that the CPA is a reliable theory of disorder. In this study it was shown that the boson peak anomaly marks the crossover from plane-wave like vibrational states to disorder-dominated states with increasing frequency ω. Near the crossover the effective sound velocity v becomes complex and frequency dependent. This corresponds to a dc-ac crossover in the analogous diffusion problem [6].

A similar but lattice-independent approach is the generalised elasticity theory in which the disorder is assumed to lead to spatial fluctuations of the elastic constants [8]. This model was solved by functional-integral techniques in which the SCBA plays the role of a saddle-point in a non-linear sigma-model treatment. This theory allowed for a generalization to include transverse degrees of freedom and to formulate a thermal transport theory [9]. Within this theory it was shown that the so-called plateau in the temperature dependence of the thermal conductivity [10] is caused by the boson-peak anomaly [9]. Furthermore, it has turned out [11] that the sound attenuation parameter (which is proportional to the imaginary part of $v(\omega)$) is related to the excess in the DOS in

the boson peak regime.

It should be noted that the model of spatially fluctuating elastic constants, treated in CPA and SCBA is by no means the only approach for explaining the boson-peak anomaly. In fact, an enormous number of possible explanations have been published in the literature, which can roughly grouped into three classes: *i*) defect models, *ii*) models associated with the glass transition and *iii*) models with spatially fluctuating elastic constants.

i): Defects with a heavy mass can produce resonant quasi-local resonant states within the DOS [12–14] and be thus the reason for the boson peak and the reduction of the thermal conductivity. Similarly defects with very small elastic constants, near which anharmonic interactions are important (soft potentials), can produce quasi-local states, which, if hybridized with acoustic excitations may produce a boson peak [15, 16] and a plateau in the thermal conductivity [17, 18] Inhomongeneities may also be the source of local vibrational excitations that contribute to the excess DOS [19]. Specifically in network glasses bond-angle distortions may also contribute to the boson-peak anomaly [20, 21]. In a recent study [8] the predictions of a defect model has been compared with those of a fluctuating elastic constant model. *ii*): In theories of the glass transition [22–26] the boson peak arises as a benchmark of the frozen glassy state. *iii*) In models with quenched disorder of elastic constants [5, 6, 8, 9, 11, 27–31] the boson peak marks the lower frequency bound of a band of irregular delocalized states with random mutual hybridization. These states are neither propagating nor localized [7]. The models have been solved with the help of numerical simulations as well as effective-medium theories.

A drawback of these models is that they are based on the model assumption of uncorrelated disorder, i.e. spatial fluctuations of the physical quantities are assumed to be uncorrelated. This assumption is only justified if the spatial correlation length is smaller or of the order of the natural length which appears in the system under consideration. In the present problem, namely vibrations in disordered solids, there are two important length scales. One is just the interatomic distance a, the other is the sound velocity, divided by the boson-peak frequency, which is in experimental data of the order of several interatomic distances. The wavenumber corresponding to this length scale is the maximum wavenumber wich can serve as a label for wave-like vibrational states. In any case it is a more sound procedure to start with a theory with *correlated disorder* and make the approximation of short correlations (if appropriate) only in the end. Such theories are available [32–34]. The aim of the present contribution is twofold: First we summarise the main features of the long-range-order SCBA. Secondly we present results of a two-dimensional simulation and compare them with those of the analytic theory.

II. MODEL AND SELF-CONSISTENT BORN APPROXIMATION (SCBA)

We start with the equation of motion for scalar wave-like excitations $u(\mathbf{r},t)$ in a d-dimensional disordered medium

$$\frac{\partial^2}{\partial t^2}\,u(\mathbf{r},t) = \nabla\cdot\, v^2(\mathbf{r})\,\cdot\nabla\, u(\mathbf{r},t) \tag{1}$$

Here $v(\mathbf{r})$ is a sound velocity (and $v^2(\mathbf{r})$ an elastic constant), which is supposed to exhibit random spatial fluctuations $v^2(\mathbf{r}) = v_0^2 + \Delta(\mathbf{r})$ with $v_0^2 = \langle v^2\rangle$ and

$$\begin{aligned} &\langle\Delta(\mathbf{r}+\mathbf{r}_0)\Delta(\mathbf{r}_0)\rangle = C(\mathbf{r}) = \langle\Delta^2\rangle e^{-r/\xi} \\ \Leftrightarrow\qquad &C(\mathbf{k}) = \langle\Delta^2\rangle C_0\,[k^2+\xi^{-2}]^{-\frac{d+1}{2}} \end{aligned} \tag{2}$$

with $C_0 = 2\pi(3d-5)/\xi$. In an effective-medium approximation the disordered system is mapped onto a homogeneous system, in which the influence of the disorder enters via a self-energy function $\Sigma(\mathbf{k},z)$ with $z=\omega+i\epsilon$. The dynamic susceptibility is given by

$$\chi(\mathbf{k},z) = \frac{k^2}{-z^2+k^2(v_0^2-\Sigma(\mathbf{k},z))} \tag{3}$$

In SCBA the self-energy function obeys the self-consistent equation [4, 32–34]

$$\Sigma(\mathbf{q},z) = \frac{1}{2}\int\limits_{|\mathbf{k}|<k_D}\left(\frac{\mathrm{d}\mathbf{k}}{2\pi}\right)^d C(\mathbf{q}-\mathbf{k})\chi(\mathbf{k},z) \tag{4}$$

with the Debye wavenumber $k_D = [2d\pi^{d-2}]^{1/2}/a$.

In the present study we are mainly interested in the low-frequency and -wavenumber properties, so we replace the self-energy by its $q\to 0$ limit $\Sigma(z)$ and obtain the SCBA equation

$$\Sigma(z) = \frac{\gamma}{2}\,\frac{v_0^4}{\varphi_d}\int\limits_{|\mathbf{k}|<k_D}\left(\frac{\mathrm{d}\mathbf{k}}{2\pi}\right)^d \frac{k^2C(k)/\langle\Delta^2\rangle}{-z^2+k^2\,(v_0^2-\Sigma(z))} \tag{5}$$

with the normalization constant $\varphi_d = \int\limits_{|\mathbf{k}|<k_D}(\mathrm{d}\mathbf{k}/2\pi)^d C(\mathbf{k})/\langle\Delta^2\rangle$ and the "disorder parameter" $\gamma = \langle\Delta^2\rangle\varphi_d/v_0^4$.

The DOS is given by

$$g(\omega) = \frac{2\omega}{\pi}\mathrm{Im}\left\{\int\left(\frac{\mathrm{d}\mathbf{k}}{2\pi}\right)^d \frac{1}{-z^2+k^2(v_0^2-\Sigma(z))}\right\} \tag{6}$$

In Fig. 1 we have plotted the "reduced DOS" $g(\omega)/\omega^2$ for $d=3$ and for three values of γ and two values of ξ. First we notice that, as in the uncorrelated case [7–9] there exists a critical amount of disorder $\gamma_c = 0.5$, beyond which the system becomes unstable. The "boson peak" becomes more pronounced and situated at lower frequencies as this value is approached. The interesting new feature in the correlated case is that the boson peak is re-inforced by the correlation and again shifted towards lower frequencies.

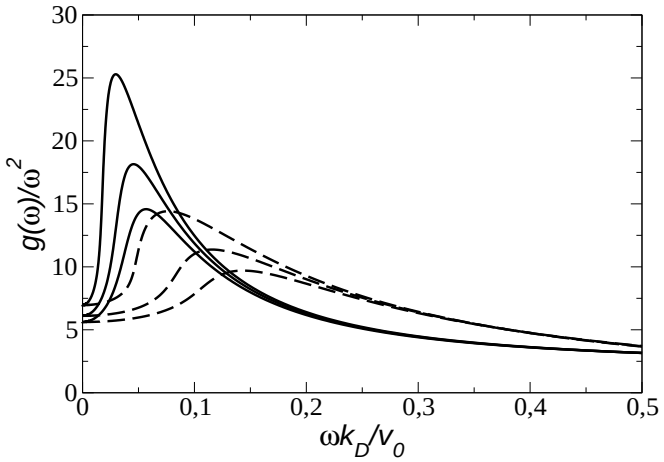

FIG. 1: Reduced DOS $g(\omega)/\omega^2$ for $\xi = 1/k_D$ (dashed lines) and $\xi = 5/k_D$ (full lines) and for three disorder parameters (from left to right) $\gamma = 0.49$, 0.47 and 0.45.

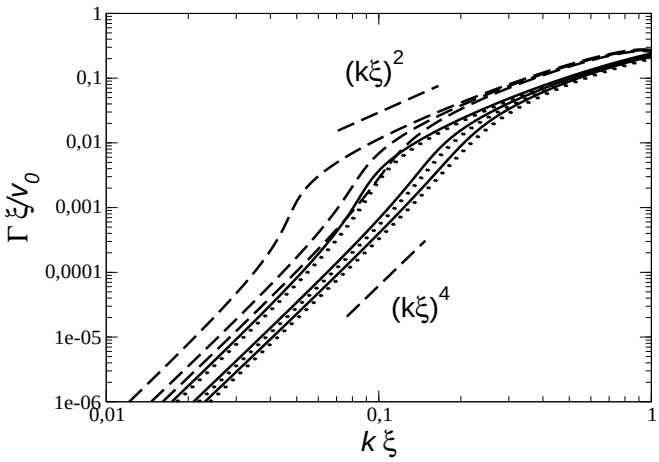

FIG. 2: Scaled Brillouin linewidth $\Gamma\xi/v_0$ against scaled wavenumber $q\xi$ for $\xi = 1/k_D$ (dashed lines) [36], $\xi = 5/k_D$ (full lines), $\xi = 10/k_D$ and $15/k_D$ (dotted lines). The disorder parameters γ are the same as in Fig. 1.

III. DYNAMIC STRUCTURE FACTOR AND DENSITY OF STATES

We now divide the self-energy function into a real and imaginary part $\Sigma(z) = \Sigma'(\omega \approx 0) + i\Sigma''(\omega)$ and define the *renormalised* sound velocity as $v^2 = v_0^2 - \Sigma'$. The dynamical structure factor $S(\mathbf{k}, \omega)$, which can be measured by inelastic neutron or X-ray scattering, and which is the Fourier transform of the dynamic density-density correlation function, is then given by the fluctuation-dissipation theorem [35] as

$$S(k,\omega) = \frac{k_B T}{\pi\omega}\mathrm{Im}\left\{\chi(k,z)\right\} \approx \frac{k_B T}{2\pi v^2}\frac{k^2\Sigma''(\omega)/2\omega}{[(kv-\omega)^2 + (k^2\Sigma''(\omega)/2\omega)^2]} \quad (7)$$

The Brillouin resonance is given by $\omega = kv$ and the line width (FWHM, sound attenuation parameter) is given by

$$\Gamma(k) = \frac{k}{v}\Sigma''(\omega = v\,k) \quad (8)$$

It can easily be shown that $\Sigma'' \propto \omega^d$ for $\omega \to 0$ so that $\Gamma \propto q^{d+1}$ for $q \to 0$ (Rayleigh law).

We now introduce the dimensionless variables $\tilde{\Sigma} = \Sigma/v_0^2$, $\tilde{C}_0 = C_0\xi = 2\pi(3d-5)$, $\tilde{z} = z\xi/v_0 = \tilde{\omega} + i\tilde{\epsilon}$ and $\tilde{k} = k\xi$. We then obtain

$$\tilde{\Sigma}(\tilde{z}) = \frac{\gamma}{2}\,\frac{\tilde{C}_0}{\varphi_d}\int\limits_{|\tilde{\mathbf{k}}|<\xi k_D}\left(\frac{\mathrm{d}\tilde{\mathbf{k}}}{2\pi}\right)^d \frac{\tilde{k}^2\,[1+\tilde{k}^2]^{-(d+1)/2}}{-\tilde{z}^2 + \tilde{k}^2(1-\tilde{\Sigma}(\tilde{z}))} \quad (9)$$

In this expression the correlation length ξ enters only via the upper $\tilde{k}$ cutoff. For the limit $\xi \gg a$ we therefore obtain the scaling relation

$$\tilde{\Gamma} = \Gamma\xi/v_0 = f(\gamma, \tilde{k}) \quad (10)$$

In Fig. 2 we have plotted $\tilde{\Gamma}$ against $\tilde{k}$ for $d = 3$, for the three γ values of Fig. 1 and for $\xi = 1/k_D$, $5/k_D$, $10/k_D$, and $15/k_D$. We see that the scaling is obeyed except for $\xi = 1/k_D$ [36] as expected. As in the uncorrelated case [11], the boson peak (see Fig. 1) marks the crossover from the Rayleigh regime $\tilde{\Gamma} \propto \tilde{k}^4$ to a behaviour $\tilde{\Gamma} \propto \tilde{k}^s$ with $s \approx 2$.

IV. SIMULATION

We now discretize (1) in $d = 2$ on a square lattice, which then takes the form of an equation of motion for unit masses connected by springs with spring constants $K_{ij} = \frac{1}{2a^2}(v^2(r_i) + v^2(r_j))$:

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\,u(\mathbf{r}_i,t) = \sum_{\ell\ n.N.} K_{i\ell}[u(\mathbf{r}_\ell,t) - u(\mathbf{r}_i,t)] \quad (11)$$

In the simulation [37] the force constants K_{ij} are extracted from a random distribution with mean K_0 and variance σ^2. The correlation is established following the Fourier filtering method (FFM) [38]. The network of random springs is created starting from a random set of $(2N)^2$ numbers uniformly distributed around zero obtained from a pseudo random number generator. The FFM method is then used to generate a $2N \times 2N$ two-dimensional lattice of "pair" random numbers $\{\eta_{ij}\}$ which obey a spatial correlation

$$\langle\eta_{00}\eta_{ij}\rangle \propto e^{-\frac{a}{2}(i+j)/\xi} \quad (12)$$

The random spring constants with mean K_0 and variance σ^2 are extracted from the pair numbers η_{ij}. The lattice spacing of masses-and-springs system is twice of that of the random-number lattice. Using this statistics the dynamic structure factor $S(k,\omega)$ of the model has been determined by the method of moments [39–41]. In Figs. 3a

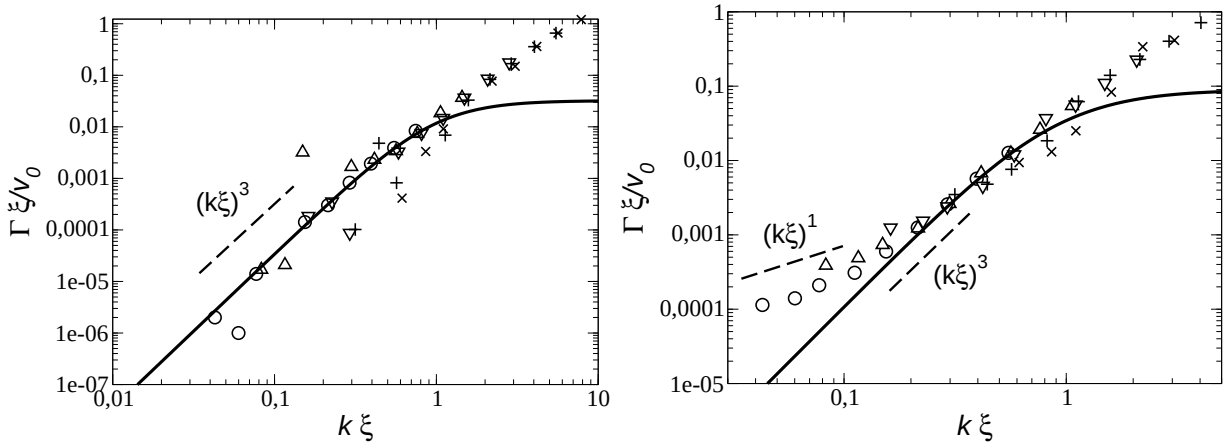

FIG. 3: Symbols: Linewidths Γ of the simulated Brillouin spectra, multiplied with the correlation length ξ and divided by the sound velocity v. $\circ : \xi = 2.79a$, $\Delta : \xi = 5.42a$, $\nabla : \xi = 10.56a$, $+ : \xi = 20.55a$, $\times : \xi = 40.0a$, Straight line: theory. The results of the left picture correspond to a disorder parameter $\gamma = 0.04$ that of the right picture to $\gamma = 0.111$.

and 3b the scaled widths of the Brillouin peak of samples with different correlation lengths have been plotted against the scaled wavenumber $\tilde{k}$. It is clearly seen that the simulated data follow the predicted scaling law. For the case with the lesser disorder ($\gamma = (\sigma/K_0)^2 = 0.04$) there is very good agreement with the theory ((9) with no cutoff in the integral) in the small wavenumber limit, where the lattice and continuum models should agree. In the high-wavenumber regime, of course, the lattice character of the simulated system becomes distinct.

Let us turn to the discussion of the data of Fig. 3b with the increased disorder $\gamma = 0.111$. The continuum theory in this case predicts the Rayleigh law $\tilde{\Gamma} \propto \tilde{k}^3$ (continuous line). We checked the stability of the system by investigating the simulated density of levels $g(\omega^2) = g(\omega)/2\omega$ and found that this quantity exhibits nonzero values for $\omega^2 < 0$, which means that the system is unstable. For this case it is known that the imaginary part of the self energy Σ'' is constant and passes continuously from positive to negative values of ω^2 in this case. Consequently the line width $\Gamma(\omega) \propto k\Sigma''$ shows a linear increase for small omega. Such a behavior is obviously an artefact of constructing a harmonic model with too much disorder, which leads to a small fraction of negative elastic constants. In a realistic physical system such "would-be" negative elastic constants are removed by the anharmonic interaction which causes relaxation of the system towards a stable situation. This has been nicely demonstratedby a model calculation of Gurevich et al [16].

V. CONCLUSION

We have investigated the vibrational properties of disordered systems with correlated disorder both analytically by the self-consistent Born approximation as well as by a simulation applying the method of moments and the Fourier-filtering method. The sound attenuation constant $\Gamma(k)$ (width of the Brillouin line) is found to scale with the correlation length ξ in such a way that $\xi\Gamma$ is a universal function of ξk. The enhancement of the density of states (boson peak) is found to be re-inforced by the correlations.

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Anharmonic elasticity theory for sound attenuation in disordered solids with fluctuating elastic constants

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Using anharmonic elasticity theory in the presence of spatially fluctuating elastic constants we derive a self-consistent theory for sound attenuation in disordered solids. In the low-frequency regime (below the boson peak frequency) we obtain a sound attenuation law proportional to $T\omega^2$, where T is the temperature and ω is the frequency. Together with the usual Rayleigh scattering mechanism this yields a crossover of the Brillouin linewidth from a ω^2 to a ω^4 regime. The cross-over frequency is fully determined by the boson peak frequency and the temperature. For network glasses like SiO_2 at room temperature this crossover is predicted to be situated one order of magnitude below the boson peak frequency.

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I. INTRODUCTION

The role of the phonon-phonon interaction in crystalline solids is very well understood. It accounts for a finite thermal conductivity, thermal expansion, as well as transverse ultrasound attenuation.[1,2] Landau and Rumer[3] realized that, due to energy and momentum conservation, a decay of the low-frequency density waves (longitudinal phonons) would be phase-space suppressed. In their theory only transverse phonons acquire a lifetime $\tau_T \propto \omega^{-1}$ at GHz frequencies. Akhiezer[4] solved the corresponding Boltzmann equation which results in a $\tau_T \propto 1/\omega^2 T$ behavior at substantially lower frequencies.[5]

The hydrodynamic modes are at the focus of interest in glass physics, because their physical properties appear to be independent of the specific underlying nonequilibrium static structure. Recent experiments showed the presence of an Akhiezer-like sound attenuation regime in the longitudinal channel,[6,7] however these authors claim different values of the cross-over frequency from the Akhiezer-like to the Rayleigh law. The authors refer to the old and frequently cited theory of Akhiezer.[4] However neither his approach nor that of Rumer/Landau[3] do apply, as they are only valid for the *low-frequency transverse* modes of *crystalline* solids. Fabian and Allen[8] performed simulations on a disordered lattice in the kinetic regime, they established the validity of an Akhiezer-like law for the longitudinal modes as well. In our analytical approach, it turns out that this observation is only possible in presence of disorder. In addition, our calculation is not limited to the kinetic regime. A treatment of anharmonic damping in disordered solids has been formulated some time ago,[9] but the focus was on weak and strong localization, so the applicability range is at very high frequencies above the boson peak.

We present an extension of the "fluctuating elastic constants" model,[11–14] to account for anharmonic sound damping of disordered solids at "low" frequencies (i.e., in the GHz-THz regime). This is achieved, using the fact, that the disorder-averaged spectral function $\chi''(\mathbf{q},\omega)$—which describes the vibrational spectrum of the disordered material—does not reflect momentum conservation anymore and exhibits a characteristic rapid increase in the THz frequency regime.[11–14] This phenomenon is frequently called "boson peak" (BP). The interaction of the irregular states near the BP produces, as we shall show an Akhiezer-like $T\omega^2$ law for the anharmonic sound attenuation. The prefactor is intimately related to the disorder-induced elasticity fluctuations, which produce the BP.

This paper is organized as follows: first we briefly review the theory for the spectrum of a harmonic disordered solid based on disorder-modified elasticity theory.[11–14] Then we introduce anharmonic interactions. Using standard quantum field-theoretical techniques we derive self-consistent mode-coupling equations, obtained from a saddle-point treatment of the disorder-averaged replica field theory,[10,15,16] which determine the phonon spectrum. For low enough temperatures and frequencies the nonself-consistent mode-decay approximation is sufficient, which results in the Akhiezer-like $\Gamma \propto T\omega^2$ law.

II. ANHARMONIC ELASTICITY THEORY WITH DISORDER

We start by reviewing the elasticity theory for a disordered solid. The starting point is Lamé's elasticity theory,[17] but with spatially fluctuating elastic constants. The dynamics of the displacement field $\mathbf{u}(\mathbf{x},t)$ is determined by the Lagrange density

$$\mathcal{L} = \frac{\rho}{2}\dot{\mathbf{u}}(\mathbf{x},\mathbf{t})^2 - \frac{1}{2}\lambda(\mathbf{x})\left(\sum_i u_{ii}(\mathbf{x},t)\right)^2 - \mu(\mathbf{x})\sum_{ij} u_{ij}(\mathbf{x},t)^2, \tag{1}$$

in which $u_{ij}=(\partial_i u_j+\partial_j u_i)/2$ is the usual strain tensor. Here λ and μ are Lamé's elastic constants and ρ is the mass density. As in our previous work we assume that the disorder affects the elastic properties only via μ:

$$\mu(\mathbf{x}) = \mu_0 + \delta\mu(\mathbf{x}) \quad \mu_0 = \langle\mu(\mathbf{x})\rangle,$$

$$\lambda(\mathbf{x}) = \lambda_0 = \langle\lambda(\mathbf{x})\rangle, \tag{2}$$

i.e., the spatial fluctuations of λ are neglected. The fluctuations $\delta\mu(\mathbf{x})$ are characterized by a correlation function $\langle\delta\mu(\mathbf{x})\delta\mu(\mathbf{x}')\rangle=K_\mu(|\mathbf{x}-\mathbf{x}'|)$; Higher moments of $\delta\mu(\mathbf{x})$ are discarded. The correlation function is given in terms of the variance of the shear modulus Δ^2 and the correlation length ξ (Ref. 18)

$$K_\mu(|\mathbf{x}-\mathbf{x}'|) = \Delta^2 \exp\left(-\frac{|\mathbf{x}-\mathbf{x}'|}{\xi}\right), \tag{3}$$

and has the Fourier transform

$$K_\mu(\mathbf{k}) = \int \mathrm{d}^3\tilde{\mathbf{x}} e^{-i\mathbf{k}\tilde{\mathbf{x}}} K_\mu(\tilde{\mathbf{x}}) = \frac{8\pi\xi^3\Delta^2}{[1+(k\xi)^2]^2}. \tag{4}$$

The quantities Δ^2 and ξ are the two phenomenological parameters, which characterize our model. As noted in,[11–14] there exists a critical amount of disorder Δ_c^2, depending only on the ratio of the squared sound velocities $(v_L/v_T)^2$, beyond which the system becomes unstable. This criticality arises, because a too large variance Δ^2 allows for negative values of the shear modulus $\mu(\mathbf{x})$, which is unphysical.

Performing standard field theoretical methods[10,16] the following set of self-consistent equations for the disorder-averaged longitudinal ($i=L$) and transverse ($i=T$) dynamical susceptibilities has been derived:[11–14]

$$\chi_i(q,z) = \frac{q^2}{-z^2 + q^2[v_{i,0}^2 - \Sigma_{i,\mathrm{dis}}(z)]}, \tag{5}$$

where $z=\omega+i\epsilon$ and $\epsilon\to+0$. Because only fluctuations of μ have been considered, we have $\Sigma_{L,\mathrm{dis}}=2\Sigma_{T,\mathrm{dis}}$. $\Sigma_{T,\mathrm{dis}}(z)$ is given by

$$\Sigma_{T,\mathrm{dis}}(z) = \frac{1}{V}\sum_{\mathbf{k}} \frac{K_\mu(\mathbf{k})}{\rho^2}[\chi_L(k,z) + \chi_T(k,z)]. \tag{6}$$

These mean-field equations arise from a saddle point within an effective replica field theory. The self-energy is evaluated in the long wavelength limit $\Sigma_{T,\mathrm{dis}}(z)=\Sigma_{T,\mathrm{dis}}(\mathbf{q}\to 0,z)$, in agreement with similar approximation schemes, e.g., the coherent potential approximation or dynamical mean field theory (DMFT).[19] The dynamical structure factor then follows from the fluctuation-dissipation theorem

$$S(q,\omega) = \frac{1}{\pi}\frac{1}{1-e^{\beta\omega}}\mathrm{Im}\{\chi_L(q,z)\}. \tag{7}$$

with $\beta=\hbar/k_BT$. The real part of the self energies $\Sigma_{i,\mathrm{dis}}$ renormalizes the sound velocities $v_i^2=v_{i,0}^2-\Sigma'_{i,\mathrm{dis}}(\omega)$ and their imaginary parts give the (harmonic) sound attenuation. In particular, the Brillouin linewidth of $S(q,\omega)$ is given by Ref. 12,

$$\Gamma(k) = \frac{\omega_k}{v_L^2}\Sigma''_{L,\mathrm{dis}}(\omega=\omega_k) \quad \omega_k = v_L k. \tag{8}$$

In the case of a short correlation length the function $K_\mu(k)$ is constant in the relevant wave-number range and one recovers the *uncorrelated* version of the self-consistent Born approximation (SCBA),[11,12] which has been shown to explain the excess density of states (DOS) [boson peak (BP)] and the dip in the temperature dependence of the thermal conductivity as a consequence of strong disorder-induced scattering. The Brillouin linewidth has been shown to vary as ω^2 in the BP regime and to be related to the excess DOS.[12] In the case of a *finite* correlation length ξ the ratio between DOS and Debye DOS is not limited to a factor 2 (see Ref. 12) but increases indefinitely with ξ.[13,14] Within this description (uncorrelated *and* correlated) the BP marks the crossover of the vibrational spectrum from a weakly scattered plane-wave regime to a disorder-dominated regime, where k does no more label the modes.

We turn now to the consideration of anharmonic elasticity. In the general theory of elasticity[17,20] the strain tensor contains nonlinear terms. Inserting the full nonlinear strain tensor into the elastic Lagrangian yields an additional anharmonic interaction

$$\mathcal{L}_{\mathrm{an}} = \lambda_0\left(\sum_i u_{ii}\right)\sum_{ij} v_{ij}v_{ij} + \mu(\mathbf{x})\sum_{ij\ell} u_{ij}v_{i\ell}v_{\ell j}, \tag{9}$$

where $v_{ij}=\frac{1}{2}(\partial_j u_i-\partial_i u_j)$ is the rotation tensor.

Further anharmonic terms would be due to anharmonic potential contributions yielding mode-Grüneisen-type couplings (cf., e.g. Refs. 17 and 21). In a system without spatial fluctuations of elastic constants translational invariance leads to a phase-space suppression of the anharmonic damping channel via Eq. (9) due to momentum conservation and a linear sound dispersion.[3,22] In the older treatments of anharmonic sound damping,[3,4] therefore, the mode-Grüneisen terms were taken as dominant anharmonic coupling which couple one transverse with two longitudinal phonons. As momentum conservation does not apply in the present situation, a finite phonon lifetime $\Gamma\{\mu(\mathbf{x})\}$ can already be calculated for a given configuration $\{\mu(\mathbf{x})\}$ from the interaction (9). The configurationally averaged lifetime $\langle\Gamma\rangle_{\{\mu(\mathbf{x})\}}$ would be nonzero in general. However it is more useful to work out the effect of the anharmonic interaction in terms of the effective fields χ_i,Σ_i, as they are important entities describing harmonic vibrations in glasses.

Using the standard replica field theory of disordered solids[15,16] we are able to show that the interaction (9) induces a third-order term in the effective theory for the fields representing the dynamic susceptibilities. A replica diagonal,

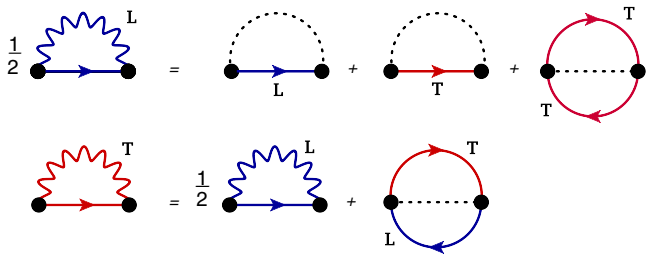

FIG. 1. (Color online) Diagrammatic representation of the anharmonic mean-field equations: blue=L, red=T; full lines are susceptibilities, dashed lines represent the correlation function; winding lines are the full self energies.

translation, and rotational invariant saddle point has been chosen, which yields the following self-consistent equations for the full self energies:

$$\Sigma_L(\omega_n) = \Sigma_{L,\mathrm{dis}}(z = i\omega_n) + 2\Sigma_{T,T,\mathrm{an}}(\omega_n), \tag{10}$$

$$\Sigma_T(\omega_n) = \frac{\Sigma_L(\omega_n)}{2} + \Sigma_{L,T,\mathrm{an}}(\omega_n), \tag{11}$$

$$\Sigma_{ij,\mathrm{an}}(\omega_n) = \frac{k_B T}{6V^2\rho^3}\sum_{\mathbf{k},\mathbf{q},m} \chi_i(\mathbf{k}, i\omega_{n-m}) K_\mu(\mathbf{k}-\mathbf{q})\chi_j(\mathbf{q}, i\omega_m). \tag{12}$$

Such equations have been shown[21] to be mathematically equivalent to mode-coupling equations.[23,24]

Indeed, these saddle-point equations resemble the structure of a calculation of the self-energy to first order in the anharmonic and disorder-induced interaction. The corresponding diagrams are shown in Fig. 1. The saddle-point equations contain self-energy dressed propagators instead of free ones.

III. MODE-DECAY APPROXIMATION AND RESULTS

In the following, we exploit this analogy for justifying the most obvious approximation to Eqs. (10)–(12), the *mode-decay approximation*. Our interest is the anharmonic effect on the dynamical structure factor and hence we are investigating the anharmonic effect on the longitudinal self-energy. We treat the anharmonic interaction as small perturbation and split the self-energy into harmonic and anharmonic parts $\Sigma_L = \Sigma_{\mathrm{dis}} + \Sigma_{\mathrm{an}}$. The propagators χ_i are approximated by the solution of the linearized equations, which are just the harmonic SCBA Eqs. (5) and (6).

Σ_{an} is then represented by the last self-energy diagram of the longitudinal channel in Fig. 1, in which the full transverse susceptibilities are replaced by the disorder-dressed ones.

We now represent $\mathbf{k}$ sums by

$$\sum_{\mathbf{k}} = \frac{V}{(2\pi)^3}\int_{|\mathbf{k}|<k_D} \mathrm{d}^3\mathbf{k},$$

and Matsubara sums by[25]

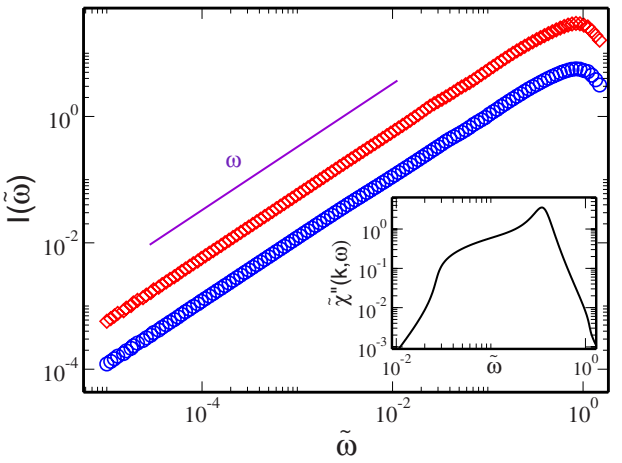

FIG. 2. (Color online) Frequency dependence of the anharmonic self-energy correction, for $\Delta^2 = 0.99\Delta_c^2$, $\xi = 2/k_D$ and $\Delta^2 = 0.9999\Delta_c^2$, $\xi = 1.5/k_D$. Inset: the function $\chi''(k=0.5k_D, \omega)$.

$$\sum_{\omega_m} A(i\omega_m) = \frac{\beta}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega \coth\frac{\beta\omega}{2}\mathrm{Im}\{A(z=\omega+i\epsilon)\}.$$

The anharmonic contribution to the Brillouin linewidth is then given by:

$$\Gamma_{\mathrm{an}}(k) = \frac{\omega_k}{v_L^2}\Sigma''_{\mathrm{an}}(\omega=\omega_k) \quad \omega_k = v_L k,$$

$$\Sigma''_{\mathrm{an}}(\omega) = \frac{\hbar}{6(2\pi)^7\rho^3}\int_{k_D} \mathrm{d}^3q\,\mathrm{d}^3k \int_0^\infty \mathrm{d}\bar{\omega}\coth\left(\frac{\beta\bar{\omega}}{2}\right) \times \chi''_T(\mathbf{k},\bar{\omega})K(\mathbf{q}-\mathbf{k})[\chi''_T(\mathbf{q},\bar{\omega}+\omega) - \chi''_T(\mathbf{q},\bar{\omega}-\omega)]. \tag{13}$$

The behavior of the susceptibility can be estimated from the inset of Fig. 2, it resembles the shape of the momentum independent self-energy, only the position of Brillouin peak is momentum dependent. We replace the correlation function $K_\mu(\mathbf{k})$ by its maximal value $8\pi\xi^3\Delta^2$. This approximation is robust, as it reflects the anharmonic expression we would have obtained in an uncorrelated framework. In addition we apply the classical (high temperature) limit in which we can replace the hyperbolic cotangent by its inverse argument. Then the self-energy is given by

$$\tilde{\Sigma}''_{\mathrm{an}}(\tilde{\omega}) = g(\Delta^2,\xi,k_BT)I(\Delta^2,\xi,\tilde{\omega}), \tag{14}$$

$$g(\Delta^2,\xi,k_BT) = \frac{\Delta^2 k_B T}{3\xi^3\pi^4\rho^3 v_T^4}, \tag{15}$$

$$I(\Delta^2,\xi,\tilde{\omega}) = \int_0^\infty \int_0^{\xi k_D} \mathrm{d}\tilde{k}\tilde{k}^2 \int_0^{\xi k_D} \mathrm{d}\tilde{q}\tilde{q}^2 \frac{\mathrm{d}\tilde{\bar{\omega}}}{\tilde{\bar{\omega}}} \times \tilde{\chi}''_T(\tilde{\mathbf{q}},\tilde{\bar{\omega}})[\tilde{\chi}''_T(\tilde{\mathbf{k}},\tilde{\bar{\omega}}+\tilde{\omega}) - \tilde{\chi}''_T(\tilde{\mathbf{k}},\tilde{\bar{\omega}}-\tilde{\omega})], \tag{16}$$

with g the interaction parameter in units of a squared sound

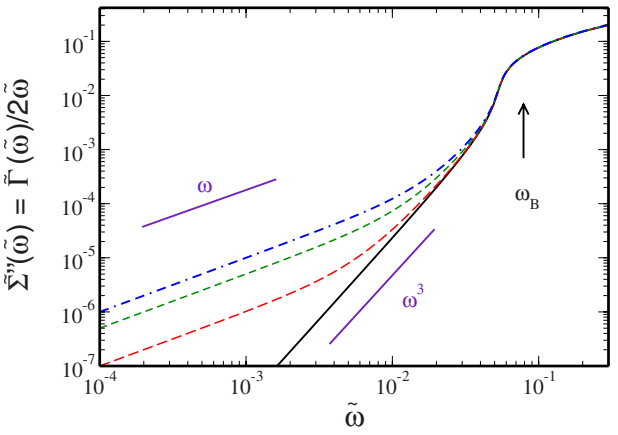

FIG. 3. (Color online) Brillouin linewidth, divided by frequency $\tilde{\Sigma}'' \cdot \alpha$ including disorder and anharmonicity for $\xi = 2/k_D$, $\Delta^2/\Delta_c^2 = 0.99$, $\alpha = (v_L/v_T)^2 = 2.52$ for different temperatures $T/T_0 = 0$ (full, black), 0.001 (long dashes, red), 0.005 (short dashes, green), 0.01 (dash-dots, blue). T_0 is defined by $\tilde{\Sigma}''_{\mathrm{an}}(\tilde{\omega}) = (T/T_0)\tilde{\omega}$ in the linear region.

velocity and a dimensionless integral I.[26] For small external frequencies, the integral kernel scales such as

$$\chi''_T(\mathbf{k}, \bar{\omega} + \omega) - \chi''_T(\mathbf{k}, \bar{\omega} - \omega) = \omega \partial_{\bar{\omega}} \chi''_T(\mathbf{k}, \bar{\omega}), \tag{17}$$

the Brillouin linewidth satisfies an Akhiezer-like sound attenuation law

$$\Sigma''_{\mathrm{an}}(\omega) \propto \omega T \Rightarrow \Gamma_{\mathrm{an}}(k) \propto \omega_k^2 T. \tag{18}$$

The validity of this ω^2 behavior has been tested by evaluating the full integral (16) instead of using Eq. (17). The result is shown in Fig. 3.

The self-energy behaves linearly in the whole frequency range, and not just at the lower band-edge $\omega \to 0$, as one would naively expect. This happens because the main contribution to the integral I, for frequencies below the BP, comes from the band of irregular delocalized high-frequency modes; these states contribute a wide $\chi'' \propto \omega$ regime, situated above the BP, to the disordered spectral density (see the inset of Fig. 2), for which the approximation (16) becomes exact.

Further, we estimate the amount of the attenuation induced by anharmonicity as compared with the disorder-induced one. The ratio $R(\omega) = \Gamma_{\mathrm{an}}(\omega)/\Gamma_{\mathrm{dis}}(\omega) \propto I(\tilde{\omega})/\tilde{\omega}$, which becomes frequency-independent beyond the BP, determines the crossover frequency. This ratio is fixed by the parameters Δ^2 and ξ, which set up the BP position, and the temperature. For example SiO_2 requires $\Delta^2 = 0.99\Delta_c^2 = 0.401\rho^2 v_T^4$ and $\xi = 2/k_D$. The ratio of the squared sound velocities is $(v_L/v_T)^2 = 2.52$ and the Debye cutoff $1.6 \times 10^{10}/m$.[12] At room temperature $k_B T k_D^3/\rho v_T^2 = 0.6$ and the ratio $I(\tilde{\omega})/\tilde{\omega} \approx 50$ is evaluated numerically for these parameters. We obtain $\Sigma''_{\mathrm{an}}(\tilde{\omega}) \approx 0.005\tilde{\omega}$, i.e., $T_0 = 7.3 \cdot 10^5$ K. Figure 3 shows the full Brillouin linewidth due to disorder and anharmonicity. The anharmonic corrections already lead to deviations from the disordered contribution slightly below the shoulder of the BP, the highest frequency, where the Akhiezer-like behavior is present in SiO_2 is therefore predicted to be one order of magnitude below the BP, i.e., in the 100 GHz regime. In general, for observing the Rayleigh law one needs to go to low enough temperature, which shifts the crossover toward lower frequencies.

IV. DISCUSSION AND CONCLUSIONS

Let us now discuss the possible role of potential-induced anharmonicity. There is no problem to introduce interactions involving longitudinal and transverse mode-Grüneisen parameters $g_{L,T}$ into the theory. In the longitudinal case one just has to replace Δ^2 by $(1+g_L^2)\Delta^2$ in the saddle point Eqs. (10)–(12). This will shift the crossover from Akhiezer-like to Rayleigh scattering upwards and reduce the "Rayleigh window" between the Akhiezer-Rayleigh crossover and the BP. Within our continuum description it is not possible to judge the importance of the mode-Grüneisen parameters $g_{L,T}$, because they are effective constants which have to be calculated from a certain microscopic theory, taking into account the material-specific details of the interaction. It has been pointed out by Fabian *et al.*,[8] that the Grüneisen parameters which they have extracted from their simulations are unusually strong, compared to the bare crystalline couplings. However, a suitable choice of the parameters for the Weber-Stillinger potential[27] used in their simulations[28] should account for the nonlinear part of the strain tensor as well. Hence, their strong Grüneisen parameters γ_i, should not be confused with our nonlinear couplings $g_{L,T}$, which may as a first guess be identified with their rather weak crystalline counterparts,[1,2] as long as one deals with weak disorder. However it cannot be excluded, that strong disorder or impurities drive these constants toward a strong-coupling regime within a renormalization-group approach. Therefore, for a particular material it has to be determined by experiment, whether our "minimal" description is sufficient, or one has to deal with mode-Grüneisen parameters. In any case our estimate of the Akhiezer-Rayleigh crossover serves as a lower bound.

The measurements on vitreous SiO_2, performed by Masciovecchio *et al.*,[6] exhibits the Akhiezer-Rayleigh crossover around 100 GHz, which fits our estimates quite well. In contradiction Devos *et al.*[7] claim the crossover to take place near 400 GHz. However they performed their measurements on amorphous thin films of SiO_2, prepared by chemical vapor deposition. Such materials—in comparison to glasses quenched from the liquid state—are known to have a wealth of additional defects such as voids and dangling bonds. It is at the heart of impurity physics that defects give rise to additional effective interactions, i.e., anharmonicities. This can lead to enhanced mode-Grüneisen parameters $g_{L,T}$, which then have to be taken into account.

In several experiments dealing with vibrational spectra near and below the glass transition[29,30] one observes an increase of the DOS in the BP regime. Within the mode-decay approximation one can account for the trends but not numerically reproduce such spectra.[31] We believe that one has to solve the full mode-coupling Eqs. (10)–(12) in order to be able to do so.

In conclusion, we developed a consistent perturbative treatment of the anharmonic contribution to the Brillouin

linewidth in disordered solids. Our treatment solely in terms of elasticity parameters, which enter into the mean values and correlation functions, suggests a correlation between the boson peak position and the Akhiezer-Rayleigh crossover at temperatures scaled with the Debye temperature. Further developments in experimental techniques are required to explore this extremely interesting frequency window in the upper GHz regime.

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CONDENSED MATTER PHYSICS

Sound attenuation and anharmonic damping in solids with correlated disorder

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We study via self-consistent Born approximation a model for sound waves in a disordered environment, in which the local fluctuations of the shear modulus G are spatially correlated with a certain correlation length ξ. The theory predicts an enhancement of the density of states over Debye's ω^2 law (boson peak) whose intensity increases for increasing correlation length, and whose frequency position is shifted downwards as $1/\xi$. Moreover, the predicted disorder-induced sound attenuation coefficient $\Gamma(k)$ obeys a universal scaling law $\xi\Gamma(k) = f(k\xi)$ for a given variance of G. Finally, the inclusion of the lowest-order contribution to the anharmonic sound damping into the theory allows us to reconcile apparently contradictory recent experimental data in amorphous SiO_2.

Key words: *sound attenuation, vibrational properties of disordered solids, boson peak, anharmonic interactions*

PACS: *63.50.-x, 43.20.+g, 65.60.+a*

The vibrational properties of disordered solids at THz frequencies are subject of an enormous attention both from the experimental and from the theoretical side [1], due to the related anomalies observed in the specific heat and thermal conductivity of glasses [2]. The origin of an excess of the vibrational density of states (DOS) over the Debye prediction ("boson peak") at THz frequencies and its relation to the rather anomalous sound attenuation in the same frequency regime is in focus of a lively debate [3–5]. In particular, the origin of the dispersion and attenuation of sound-like excitation in the THz frequency range has been a matter of controversy quite recently [6, 7]. In spite of this debate, nowadays many authors agree that the boson peak and the frequency dependence of the sound attenuation are the related phenomena dictated by the structural disorder, rather than by anharmonic interactions, and occur at frequencies at which the wavevector k looses its significance for labeling the transverse vibrational states (Ioffe-Regel regime) [8].

The way the disorder controls the thermophysical properties, however, is still not fully understood, and the experimental phenomenology is not completely reproduced by the current fluctuating-elastic-constant (FE) approaches [6, 9, 10], which are based on zero-range correlations.

The FE approach has been recently applied to low-frequency Raman scattering and for the first time accounted for the experimentally observed frequency dependence, which is different from incoherent neutron scattering [11]. In this study and in a recent comparison of a scalar FE model with a simulation of a simple model having correlated disorder [12] it was realized that the *finite*

correlation length ξ of the elasticity fluctuations plays an important role discussing the vibrational anomalies. A similar conclusion was drawn from molecular-dynamics simulations of quenched Lennard-Jones Argon and SiO_2 [13]. In the latter study it emerged that these correlations exist over an extended number of inter-atomic distances. This verifies a conjecture of Elliott [14] quite a time ago.

In the present paper we use the full vector FE approach [10] to study the effect of a finite correlation length and the presence of anharmonic interactions. We find that the BP becomes strongly enhanced with increasing correlation length, a result which emphasizes the importance of this latter property in real systems. We further demonstrate that ξ times the disorder-induced sound attenuation constant is a universal function of ξk (where k is the wavenumber).

We consider an elastic continuum, in which the shear modulus G fluctuates in space around its mean value G_0 (the bulk modulus K_o is supposed to be constant): $G(\mathbf{r}) = G_0 + \Delta G(\mathbf{r})$, we also assume that the correlation function of $\Delta G(\mathbf{r})$, $C(\mathbf{r}) = \langle \Delta G(\mathbf{r}+\mathbf{r}_0)\Delta G(\mathbf{r}_0)\rangle$ and its Fourier transform are of the forms

$$\begin{aligned} C(\mathbf{r}) &= \langle \Delta G^2 \rangle \mathrm{e}^{-r/\xi}, \\ C(\mathbf{k}) &= \left\langle \Delta G^2 \right\rangle (8\pi/\xi) \left[k^2 + \xi^{-2}\right]^{-2}. \end{aligned} \tag{1}$$

The corresponding mean-field equation for the low-wavenumber self energy $\Sigma(\omega) = \Sigma(q=0,\omega)$ (self-consistent Born approximation, SCBA) takes the form [11, 12, 15, 16]

$$\Sigma(\omega) = \frac{\gamma}{2\varphi_3 \ \langle \Delta G^2 \rangle} \int\limits_{|\mathbf{k}|<k_\mathrm{D}} \left(\tfrac{\mathrm{d}\mathbf{k}}{2\pi}\right)^3 C(k) \big[\chi_L(k,\omega) + \chi_T(k,\omega)\big]$$

with

$$\chi_L(k,\omega) = k^2 \big[-\omega^2 + k^2(v_{L,0}^2 - 2\Sigma(\omega))\big]^{-1}, \tag{2}$$

$$\chi_T(k,\omega) = k^2 \big[-\omega^2 + k^2(v_{T,0}^2 - \Sigma(\omega))\big]^{-1}. \tag{3}$$

Here $\gamma = \langle \Delta G^2 \rangle \varphi_3 / v_0^4$. is the "disorder parameter", $v_{L,0}$, $v_{T,0}$, are the (unrenormalized) sound velocities, and $\varphi_3 = \int\limits_{|\mathbf{k}|<k_\mathrm{D}} (\mathrm{d}\mathbf{k}/2\pi)^3 C(\mathbf{k})$ is a normalization constant. k_D is the usual Debye-cutoff, typical values have been elaborated in [6].

The DOS, given by

$$g(\omega) = \frac{2\omega}{3\pi} \int\limits_{|\mathbf{k}|<k_\mathrm{D}} \left(\tfrac{\mathrm{d}\mathbf{k}}{2\pi}\right)^3 \frac{1}{k^2} \mathrm{Im}\left\{\chi_L(k,\omega) + 2\chi_T(k,\omega)\right\} \tag{4}$$

is reported in figure 1. Here we have plotted the "reduced DOS" $g(\omega)/g_\mathrm{D}(\omega)$ (where g_D is Debye's DOS) for three values of γ and five values of ξ. First we notice that, similarly to the uncorrelated case ($\xi \to 0$) [6, 9, 10] there exists a critical amount of disorder γ_c, beyond which the system becomes unstable. The "boson peak" becomes more pronounced and is located at lower frequencies as this value is approached. However, at variance with the experimental data, the maximum amplitude of the boson peak predicted from the $\xi = 0$ case is a factor larger than the Debye expectation. The interesting feature appearing in the correlated case ($\xi > 0$) is that the boson peak amplitude increases and its position shifts towards lower frequencies with increasing ξ. In figure 1 – where we have taken the frequencies scaled by v_T/ξ in order to show that the boson peak frequencies scales as $1/\xi$ – one can see that the boson peak amplitude can reach the value as high as ten with still reasonable ξ value.

The sound attenuation constant (i.e., the width of the Brillouin line in $\chi_L''(k,\omega)$) is given in terms of the imaginary part of the self-energy $\Sigma''(\omega)$ as [6]

$$\Gamma(k) = 2\frac{k}{v_L}\Sigma''(\omega = k/v_L), \tag{5}$$

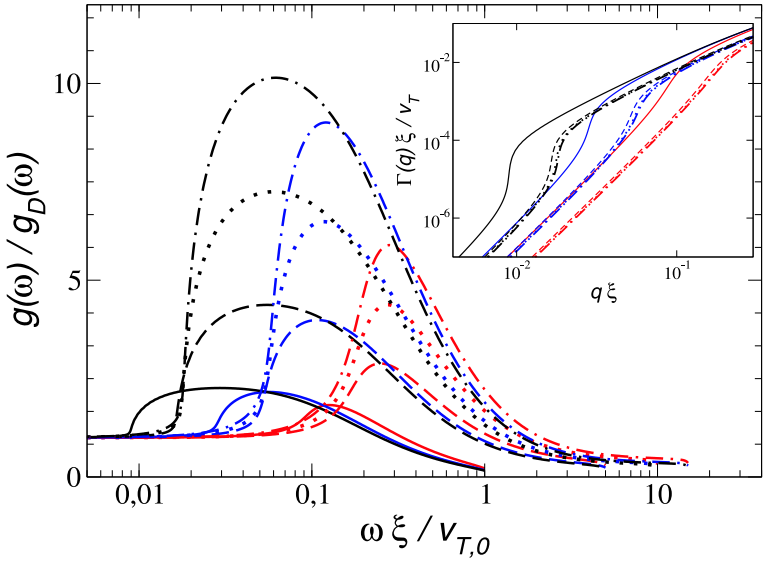

Figure 1. Reduced DOS $g(\omega)/g_{\rm D}(\omega)$ against scaled frequency $\omega\xi/v_{T,0}$ for $\xi = 1/k_{\rm D}$ (full lines) $\xi = 5/k_{\rm D}$ (dashed lines), $\xi = 10/k_{\rm D}$ (dotted lines), $\xi = 15/k_{\rm D}$ (dash-dotted lines), for three disorder parameters (from left to right) $\gamma - \gamma_{\rm c} = 0.0001$ (black), 0.001 (blue) and 0.01 (red). Inset: Scaled Brillouin linewidth $\Gamma\xi/v_0$ against scaled wavenumber $q\xi$ for the same parameters and with the same line and color codes.

where $v_L = [v_{L,0}^2 - 2\Sigma'(\omega = 0)]^{1/2}$ is the *renormalized* longitudinal sound velocity. In particular, the relation between Γ and the excess DOS derived for $\xi = 0$ (see equation (5) in [6]) – and this has been found to be in agreement with the experimental data [6] – remains the same also for $\xi > 0$. If one now introduces the dimensionless variables $\tilde{\Sigma} = \Sigma/v_{T,0}^2$, $\tilde{\omega} = \omega\xi/v_{T,0}$ and $\tilde{k} = k\xi$ and inserts these into the SCBA equation (2) one realizes that the correlation length only appears via the upper cutoff $\tilde{k}_{\rm D} = k_{\rm D}\xi$. This means that for large enough ξ (in which case the cutoff does not play any role) $\tilde{\Sigma}$ and $\tilde{\Gamma}$ does not depend on ξ. This implies, in turn, that $\tilde{\Gamma} = \Gamma\xi/v_{T,0}$ is - for a fixed disorder parameter γ – a universal function of k. $\tilde{\Sigma}$ (and, in fact Σ as well) is – within our approach – a universal function of $\xi\omega/v_L$ or ξk.

In the inset of figure 1 we have plotted $\tilde{\Gamma}$ against $\tilde{k}$ for $d = 3$, for the three γ values of figure 1 and for $\xi = 1/k_{\rm D}$, $5/k_{\rm D}$, $10/k_{\rm D}$, and $15/k_{\rm D}$. We see that the scaling is obeyed except for $\xi = 1/k_{\rm D}$ as expected. The crossover from the Rayleigh regime $\tilde{\Gamma} \propto \tilde{k}^4$ to a behavior $\tilde{\Gamma} \propto \tilde{k}^s$ with $s \approx 2$, occurring at the low frequency edge of the boson peak [6, 10], is now understood to be a universal feature independent of the magnitude of the correlation length (see figure 1).

In real amorphous solids, the relation $\Gamma(k) \propto k^2$ holds – at frequencies around the boson peak frequency – for almost all glasses. This is in agreement with the present theory, which predicts $\Gamma(k) \propto k^2$ in the boson peak for all values of γ and ξ. On the contrary, a clear-cut Rayleigh scattering law ($\Gamma(k) \propto k^4$) is seldomly observed. Generally, at much lower frequencies, one finds a sound attenuation proportional to k^2, which increases with temperature and is therefore attributed to anharmonic effects. Some evidence of a possible transition between k^2 and k^4 behavior has been found for vitreous silica [17].

In order to account for this contribution we consider a cubic anharmonic interaction of the form [19]

$$\mathcal{V}_{\rm an} = \lambda_0 \sum_{ij} u_{ii} v_{ij} v_{ij} + G(\mathbf{x}) \left(\sum_{ij\ell} u_{ij} v_{i\ell} v_{\ell j} + g_1 \sum_i u_{ii}^3 \right) \tag{6}$$

with the linearized strain- $u_{ij} = \frac{1}{2}(\partial_j u_i + \partial_i u_j)$ and rotation $v_{ij} = \frac{1}{2}(\partial_j u_i - \partial_i u_j)$ tensor and g_1 a phenomenological mode-Grüneisen-like parameter. Using a replica field formalism at finite temperature T, a set of mode-coupling-like self consistency equations for the full dynamical sus-

ceptibilities has been derived [20]. This treatment involving an Akhiezer-like 'mode-coupling' parameter $g(\langle\Delta G^2\rangle, \xi, k_{\rm B}T) = (1+g_1^2)\langle\Delta G^2\rangle k_{\rm B}T/3\xi^3\pi^4\rho^3\bar{v}_T^4$. In a perturbative regime, the relevant anharmonic contribution to the attenuation of density fluctuations can be reduced to

$$\Sigma''_{\rm an,i}(0,\tilde{\omega}) = g\int_0^\infty \int_0^{\xi k_{\rm D}} {\rm d}\tilde{k}\tilde{k}^2 \int_0^{\xi k_{\rm D}} {\rm d}\tilde{q}\tilde{q}^2 \frac{{\rm d}\tilde{\bar{\omega}}}{\tilde{\bar{\omega}}} \tilde{\chi}''_T(\tilde{\mathbf{q}},\tilde{\bar{\omega}}_+)\left[\tilde{\chi}''_T(\tilde{\mathbf{k}},\tilde{\bar{\omega}}+\tilde{\omega}) - \tilde{\chi}''_T(\tilde{\mathbf{k}},\tilde{\bar{\omega}}-\tilde{\omega})\right], \qquad (7)$$

where the full susceptibilities are replaced with their harmonic disorder-modified counterparts (2). The specific form of the correlation function enters the anharmonic sound attenuation function only indirectly through the harmonic susceptibilities. The latter ones, are only weakly effected by a change from exponential to Gaussian correlations. At room temperature, the integral (7) scales like $T\omega$ for $\omega \ll \omega_{\rm B}$. This is already suggested by the specific form of the integral kernel, and has been confirmed numerically [20].

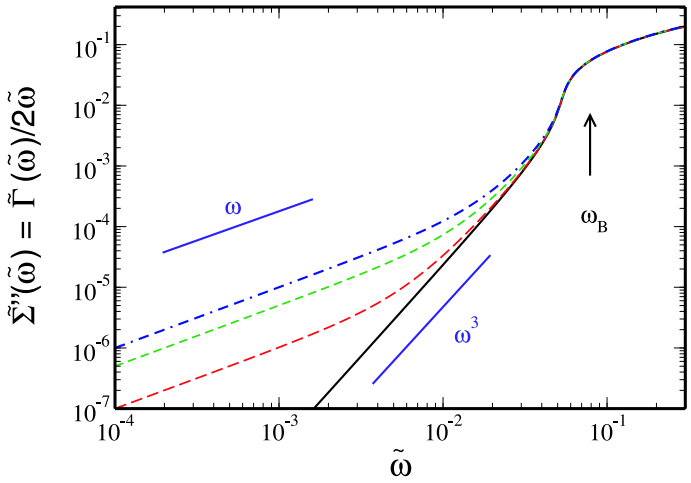

Figure 2. Brillouin linewidth, divided by frequency $\tilde{\Sigma}''\cdot\alpha$ including disorder and anharmonicity for $\xi = 2/k_{\rm D}$, $\gamma/\gamma_{\rm c} = 0.99$, $\alpha = (v_L/v_T)^2 = 2.52$ for different temperatures T/T_0=0 (full,black), 0.001 (long dashes, red), 0.005 (short dashes, green), 0.01 (dash-dots, blue). T_0 is defined by $\tilde{\Sigma}''_{\rm an}(\tilde{\omega}) = (T/T_0)\tilde{\omega}$ in the linear region.

Figure 2 shows the full Brillouin linewidth due to disorder and anharmonicity with the known parameters of SiO_2 [6] $\gamma = 0.99$, $\Delta G_{\rm c}^2 = 0.401$, $\rho^2 v_T^4$, $\xi = 2/k_{\rm D}$, $(v_L/v_T)^2 = 2.52$,$k_{\rm D} = 1.6\times10^{10}/m$, $T = 300$ K, $g_1 \approx 0$. The anharmonic corrections already lead to deviations from the disordered contribution slightly below the shoulder of the BP, the highest frequency, where the Akhiezer-like behavior is present in SiO_2, is therefore predicted to be one order of magnitude below the BP, i.e., in the 100 GHz regime.

This compares qualitatively with some recent inelastic UV light scattering data of vitreous SiO_2 by Masciovecchio et al. [17]. They observed the crossover from a ω^2 to a very steep increase – compatible with a ω^4 law – around 100 GHz.

More recently Devos et al. [18] reported on the results of the measurements of sound absorption on thin films of SiO_2 produced by chemical vapor deposition (CVD). These $\Gamma(k)$ data are found to be different from the data of [17]. The authors of [18], implicitly assuming that the structure of the materials investigated in the two sets of experiments are the same, claim that the data sets reported in [17] must be in error.

As it is well known, the structure of disordered solids crucially depends on the preparation method [21]. A glass, which is quenched from the melt, is known to have a much more relaxed structure than an amorphous material evaporated onto a cold substrate from the gaseous phase. Therefore, we believe that both the anharmonic coupling strength as well as the correlation length of differently prepared materials can differ considerably. This may be the reason that the Akhiezer-Rayleigh-crossover might occur at different frequencies in differently prepared materials.

In conclusion, we have combined a model in which the shear modulus exhibits spatially correlated fluctuations with an anharmonic interaction. By this we are able to discuss these phenomena in terms of the structure of the materials and to solve an apparent contradiction recently reported in the literature. More importantly, we have at hand a theory capable of quantitatively reproducing most of the phenomena related to the high frequency vibrations in glasses, such as the existence of a boson peak and the puzzling k dependent behavior of the sound attenuation.

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Послаблення звуку та ангармонічне загасання у твердих тілах зі скорельованим безладом

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За допомогою самоузгодженого наближення Борна ми досліджуємо модель для звукових хвиль у невпорядкованому оточенні, де локальні флуктуації модуля зсуву G є просторово скорельовані з певною кореляційною довжиною ξ. Теорія передбачає зростання густини станів понад законом Дебая ω^2 (бозонний пік), чия інтенсивність зростає із збільшенням кореляційної довжини та частота зсувається в область низьких частот як $1/\xi$. Крім того, передбачено, що коефіцієнт викликаного безладом послаблення звуку $\Gamma(k)$ задовільняє універсальному закону скейлінґу $\xi\Gamma(k) = f(k\xi)$ для заданої варіації G. Врешті, врахування внеску найнижчого порядку до ангармонічного загасання звуку в теорії дозволяє нам узгодити наявні суперечливі недавні експериментальні дані для аморфного SiO_2.

Ключові слова: *послаблення звуку, вібраційні властивості невпрорядкованих твердих тіл, бозонний пік, ангармонічні взаємодії*

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Replica field theory for anharmonic sound attenuation in glasses

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ABSTRACT

A saddle-point treatment of interacting phonons in a disordered environment is developed. In contrast to crystalline solids, anharmonic attenuation of density fluctuations becomes important in the hydrodynamic regime, due to a broken momentum conservation. The variance of the shear modulus Δ^2 turns out to be the strength of the disorder enhanced phonon–phonon interaction. In the low-frequency regime (below the boson peak frequency) we obtain an Akhiezer-like sound attenuation law $\Gamma \propto T\omega^2$. Together with the usual Rayleigh scattering mechanism this yields a crossover of the Brillouin linewidth from a ω^2 to a ω^4 regime. The crossover frequency ω_c is fully determined by the boson peak frequency and the temperature. For network glasses like SiO_2 at room temperature this crossover is predicted to be situated one order of magnitude below the boson peak frequency.

1. Introduction

Theories for sound-wave propagation in inhomogeneous media (e.g. a spatially fluctuating sound velocity) have served as a common tool for explaining the anomalous vibrational properties of disordered solids for at least two decades [1–12]. However, less is known about the role of the anharmonic interaction in such models. In a previous phenomenological approach, involving only the longitudinal modes, a *Mode-Grüneisen* like 3 phonon interaction has already been incorporated [13]. During the recent years, the detailed vector theory [5], based on Lame's elasticity theory with spatially fluctuating elastic moduli, has gained importance, because it establishes the connection with Raman scattering data [8]. From first principles of elasticity theory, this vector model allows for the inclusion of a phonon–phonon interaction, which depends only on the constants that characterize the harmonic medium, and requires no additional parameters. In the present paper we present the derivation of the generalized anharmonic saddle-point equations within the *replica formalism* [14–16]. We evaluate the anharmonic corrections on the Brillouin linewidth within a perturbative regime. At room temperature the theory predicts anharmonic sound attenuation at the THz scale. This is in agreement with previous simulations [17,18], which report on strong effective Grüneisen parameters, compared with their rather weak crystalline counterparts; in the present treatment the relevant expansion parameter of the anharmonic vertex is just the fluctuation of the shear modulus Δ^2 which typically is of the order $\approx 0.1\rho^2 v_T^4$, whereas the Grüneisen parameters of crystalline solids are much smaller and lead to anharmonic sound attenuation at and below several GHz [19] ($v_{L/T}$ is the longitudinal/transverse sound velocity). Recent experiments [20,21] showed already the existence of anharmonic sound attenuation at the THz scale in SiO_2, e.g. the Brillouin linewidth exhibits an additional ω^2 regime below the disorder-induced Rayleigh ω^4 law, but disagree about the precise value of the crossover frequency separating both regimes. In addition it was widely believed that these anharmonic effects coincided with those of the corresponding crystalline phase, and several authors consulted an old kinetic description of anharmonic solids [22]. However, this kinetic theory only applies to transverse phonons, due to energy and momentum conservation, as we explain in the second section. In contrast, the anharmonic sound attenuation emerging from the present calculation relies crucially on the presence of disorder. The Brillouin linewidth satisfies an Akhiezer-like law, with a prefactor related to the disorder-dressed spectral function. This is more reasonable, because the vibrational degrees of freedom of a glass are assumed to be at thermal equilibrium throughout the whole literature, whereas the kinetic description only applies to non-equilibrium phonon distributions.

2. Theory of anharmonic sound attenuation in glasses

2.1. Anharmonic elasticity

The usual textbook derivation [23,24] of elasticity theory starts with the non-linearized strain tensor,

$$u_{ij}(\mathbf{x},t) = \frac{1}{2}\left(\partial_i \mathbf{u}_j(\mathbf{x},t) + \partial_j \mathbf{u}_i(\mathbf{x},t) + \frac{1}{2}\sum_k \partial_i \mathbf{u}_k(\mathbf{x},t)\partial_j \mathbf{u}_k(\mathbf{x},t)\right) \quad (1)$$

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which measures the deformation of a differential volume element. The elastic free energy functional $\mathcal{F}_{el}$ to quadratic order

$$\mathcal{F}_{el} = \sum \left(\frac{\lambda}{2} u_{ii}^2 + \mu(\mathbf{x}) u_{ij} u_{ij} \right) \tag{2}$$

is built up from the translation and rotational invariant contractions of the strain tensor. If the displacement of the individual atoms from their equilibrium position is small e.g. $\nabla \cdot \mathbf{u} \ll 1$, the non-linear part of Eq. (1) can be neglected. Even then, the residual third order contributions of Eq. (2) and possible third order contractions with independent elastic moduli (Grüneisen-like parameters) have to be taken into account, for explaining other physical properties of solids, likewise a finite thermal conductivity or thermal expansion [25]. As we explain in the next paragraph, the anharmonicities included in Eq. (2) cannot lead to thermalization of the density modes in the crystalline phase.

2.2. Absence of sound attenuation in the hydrodynamic regime

In case of a spatially independent shear modulus $\mu(\mathbf{x}) = \mu_0$ the wave number $\mathbf{k}$ is a good quantum number. According to the continuity equation, longitudinal phonons are density fluctuations $\rho(\mathbf{x}, t) = \rho_0 \nabla \cdot \mathbf{u}(\mathbf{x}, t)$. The absorption of a density wave through an energy and momentum conserving three phonon collision obeys the conservation laws

$$\omega_L + \omega_i^{(1)} = \omega_i^{(2)} \tag{3}$$

$$\mathbf{k}_L + \mathbf{k}_i^{(1)} = \mathbf{k}_i^{(2)}. \tag{4}$$

Applying the triangular inequality to Eq. (4) and inserting Eq. (3) leads to Eq. (6)

$$|\mathbf{k}_L| \geq \left| \mathbf{k}_i^{(2)} \right| - \left| \mathbf{k}_i^{(1)} \right| \tag{5}$$

$$\frac{1}{v_L} \geq \frac{1}{v_i}, \tag{6}$$

which states that density fluctuations can only be absorbed by longitudinal phonons. (In a solid $v_L \geq v_T$!) In that case Eq. (3) equals

$$|\mathbf{k}_L| + \left| \mathbf{k}_L^{(1)} \right| = \left| \mathbf{k}_L^{(2)} \right|, \tag{7}$$

only collisions with parallel aligned momenta occur. To calculate an extensive decay probability via Fermi's golden rule, the number of possible final states has to be of the order of total degrees of freedom (the number of degrees of freedom is bounded through the Debye cutoff $k_D = \sqrt[3]{6\pi^2 N / V}$). Anharmonic attenuation of density fluctuations would therefore not be observable in the thermodynamic limit ($V \to \infty$ with finite density), in a translationally invariant system. This series of arguments has been already used by Landau and Rumer in 1936 [26]. In their theory transverse phonons acquire a lifetime due to collisions with thermalized phonons. In 1939 Akhiezer developed the corresponding kinetic theory [22], which takes into account scattering at phonons in a non-equilibrium state. In crystalline solids the Akhiezer regime is reported at frequencies below 1 GHz [19]. Both theories only apply to transverse phonons, and cannot account for high-frequency deviations observed in Brillouin light scattering experiments, which are probing the longitudinal modes.

2.3. Replica field theory

The imaginary time quantum dynamics [27] of the present model emerge from the Euclidean action Eq. (8), in which $u_{ij} = \frac{1}{2}(\partial_i \mathbf{u}_j(\mathbf{x}) + \partial_j \mathbf{u}_i(\mathbf{x}))$ is the linearized strain and $v_{ij} = \frac{1}{2}(\partial_i \mathbf{u}_j(\mathbf{x}) - \partial_j \mathbf{u}_i(\mathbf{x}))$ the linearized rotation tensor.

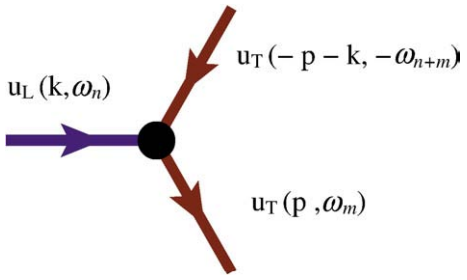

Fig. 1. 3-phonon vertex, the Fourier modes $\mathbf{u}_i(\mathbf{k}, \omega_n)$ are defined through Eq. (21).

$$S\left[u_{ij}(\mathbf{x}, \tau)\right] = \int_0^\beta d^4x \left(\frac{\rho}{2} u_{ii} \partial_\tau^2 u_{ii} + \frac{\lambda}{2} u_{ii}^2 + \mu(\mathbf{x}) u_{ij} u_{ij} + \lambda u_{ii} v_{ij} v_{ij} + \mu(\mathbf{x}) u_{ij} v_{il} v_{lj} \right), \tag{8}$$

Eq. (8) contains an interaction between longitudinal and transverse phonons, for which the perturbation theory can be developed from the elementary vertex shown in Fig. 1.

The probability to absorb or emit a longitudinal phonon vanishes in a translationally invariant model, as the creation of a virtual transverse phonon pair satisfies Eq. (4). However this is not true for a spatially dependent shear modulus, averaging the inverse lifetime $\Gamma[\mu(\mathbf{x})]$ over a certain distribution of $\mu(\mathbf{x})$ yields a finite Brillouin linewidth Γ, as we are averaging strictly positive numbers. Therefore Γ should in general depend only on the local fluctuations $\langle \delta\mu(\mathbf{x}) \delta\mu(\mathbf{x}) \rangle$, rather than the average $\langle \mu(\mathbf{x}) \rangle = \mu_0$, as $\Gamma[\mu_0] = 0$. We assume a Gaussian distribution of the shear modulus $\langle \delta\mu(\mathbf{x}) \delta\mu(\mathbf{x}') \rangle = K_\mu(\mathbf{x} - \mathbf{x}')$, and carry out the disorder average applying the replica trick [7,8]. The spatial fluctuations of λ are neglected. This yields the euclidean action in replica space:

$$\begin{aligned} S\left[u_{ij}^a(\mathbf{x}, \tau)\right] = & \int_0^\beta d^4x \sum_a \left(\frac{\rho}{2} u_{ii}^a \partial_\tau^2 u_{ii}^a + \frac{\lambda}{2} (u_{ii}^a)^2 + \lambda u_{ii}^a v_{ij}^a v_{ij}^a + \mu_0 u_{ij}^a v_{il}^a v_{lj}^a \right) \\ & + \sum_{ab} \int_0^\beta \frac{d^4x d^4x'}{2\hbar} \left(u_{ij}^a u_{ij}^a(\mathbf{x}, \tau) K_\mu(\mathbf{x} - \mathbf{x}') u_{lm}^b u_{lm}^b(\mathbf{x}, \tau') \right. \\ & \left. + u_{ij}^a(\mathbf{x}, \tau) v_{il}^a v_{lj}^a K_\mu(\mathbf{x} - \mathbf{x}') u_{hk}^b v_{hm}^b v_{mk}^b(\mathbf{x}', \tau') \right) \\ & + \sum_{ab} \int_0^\beta d^4x \int_0^\beta \frac{d^4x'}{\hbar} \left(u_{ij}^a(\mathbf{x}, \tau) u_{ij}^a K_\mu(\mathbf{x} - \mathbf{x}') u_{hk}^b v_{hm}^b v_{mk}^b(\mathbf{x}', \tau') \right) \end{aligned} \tag{9}$$

We now derive an effective action with the help of the pair modes

$$u_{ij}^a(x) u_{hk}^b(x') = \hbar Q_{ijhk}^{ab}(x, x') \tag{10}$$

$$v_{ij}^a(x) v_{hk}^b(x') = \hbar \tilde{Q}_{ijhk}^{ab}(x, x') \tag{11}$$

and their conjugate Lagrange multipliers Λ via the Fadeev–Popov transformation [28]:

$$\begin{aligned} S\left[u_{ij}^a(\mathbf{x}, \tau), Q, \tilde{Q}\right] = & \int_0^\beta d^4x \left(\frac{\rho}{2} u_{ii}^a \partial_\tau^2 u_{ii}^a + \frac{\lambda}{2} (u_{ii}^a)^2 + \lambda u_{ii}^a \tilde{Q}_{ijij}^{aa}(x, x) + \mu_0 u_{ij}^a \tilde{Q}_{ilij}^{aa}(x, x) \right) \\ & + \frac{\hbar^2}{2} \int_0^\beta d^4x' d^4x \left(\frac{K_\mu(\mathbf{x} - \mathbf{x}')}{\hbar} Q_{ijlm}^{ab}(x, x')^2 \right. \\ & \left. + Q_{ijhk}^{ab}(x, x') \tilde{Q}_{ilmk}^{ab}(x, x') K_\mu(\mathbf{x} - \mathbf{x}') \tilde{Q}_{ljhm}^{ab}(x, x') \right) \\ & + \hbar^2 \int_0^\beta d^4x' d^4x Q_{ijkh}^{aa}(x, x) K_\mu(\mathbf{x} - \mathbf{x}') \tilde{Q}_{hmmk}^{bb}(x', x') u_{hk}^b(\mathbf{x}', \tau') + S_{F1} + S_{F2} \end{aligned} \tag{12}$$

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$$S_{F1} = \sum_{ijhkab} i\int d^4x \frac{d^4x'}{\hbar} \Lambda^{ab}_{ijhk}(x,x')\left(\hbar Q^{ab}_{ijhk} - u^a_{ij}(x)u^b_{hk}(x')\right) \tag{13}$$

$$S_{F2} = \sum_{ijhkab} i\int d^4x \frac{d^4x'}{\hbar} \tilde{\Lambda}^{ab}_{ijhk}(x,x')\left(\hbar \tilde{Q}^{ab}_{ijhk} - v^a_{ij}(x)v^b_{hk}(x')\right) \tag{14}$$

As the disorder average restores translational and rotational invariance, the mean field approximation has to reflect these symmetries. In addition we assume replica diagonal pair modes:

$$\tilde{Q}^{ab}_{ijlm}(x,x') = \delta_{ab}\left(\delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}\right)\chi_2(x-x') \tag{15}$$

$$\tilde{\Lambda}^{ab}_{ijlm}(x,x') = i\delta_{ab}\left(\delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}\right)\sum\nolimits_2(x-x') \tag{16}$$

$$Q^{ab}_{ijlm}(x,x') = \delta_{ab}\left(\delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}\right)\chi_1(x-x') \tag{17}$$

$$\Lambda^{ab}_{ijlm}(x,x') = i\delta_{ab}\left(\delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}\right)\sum\nolimits_1(x-x') \tag{18}$$

This ansatz removes the bare anharmonic interaction terms with μ_0 and Λ from the effective action in agreement with the previous scalar approach [13], and in addition the last term of Eq. (12).

We kept $\hbar$ explicitly for identifying the quantum contributions: the phonon dynamics are governed by the effective Lagrange density

$$\begin{aligned}\mathcal{L}_{eff} = {} & u^{(1)}_{ij}(x)G^{-1}_{0ijlm}(x-x')u^{(1)}_{lm}(x') \\ & -u^{(1)}_{ij}(x)i\Lambda^{(1)}_{ijlm}(x-x')u^{(1)}_{lm}(x') \\ & -v^{(1)}_{ij}(x)i\tilde{\Lambda}_{ijlm}(x-x')v^{(1)}_{lm}(x')\end{aligned} \tag{19}$$

in which the Lagrange multipliers Λ, $\tilde{\Lambda}$ enter as external fields. As far as their dynamics are independent of $\hbar$, we are just left with a classical continuum field theory, subjected to canonical statistics. This happens in the case of zero anharmonicity, in which the problem is reduced to the determination of the classical spectral function [5,8].

Proceeding with the mean field approach, a Matsubara decomposition of the euclidean action (12) is done with the following conventions:

$$\mathbf{u}_i(\mathbf{x},\tau) = \frac{1}{\sqrt{\beta V}}\sum_{n,\mathbf{k}} u_i(\omega_n,\mathbf{k})e^{i\omega_n\tau - i\mathbf{k}\cdot\mathbf{x}} \tag{20}$$

$$Q(x-x') = \frac{1}{\beta V}\sum_k Q(k)e^{i(k,x-x')} \tag{21}$$

Here we introduced the four-vector notation $k=(\mathbf{k},\omega_n)$, $(k,x)=i\omega_n\tau - i\mathbf{k}\cdot\mathbf{x}$. The imaginary time displacement field is integrated out leaving the effective action in terms of the composite fields.

Minimizing this effective action yields the saddle-point equations satisfied by the composite fields (22–25). Linearizing these equations leaves just the classical harmonic theory [5,7,8], in which the self energy satisfies the self consistent Born approximation. Therefore they establish a reasonable generalization of the harmonic theory.

$$\sum\nolimits_1(\mathbf{q},\omega_n) = \frac{1}{V}\sum_{\mathbf{k}} K_\mu(\mathbf{k}-\mathbf{q})(\chi_L(\mathbf{k},\omega_n) + \chi_T(\mathbf{k},\omega_n)) + \frac{\sum^L_{an}(\mathbf{q},\omega_n)}{2} \tag{22}$$

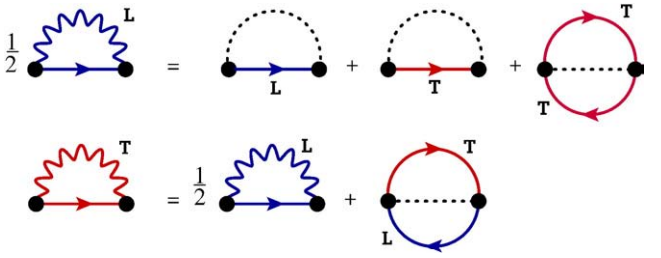

Fig. 2. Diagrammatic representation of the anharmonic mean field equations: blue = L, red = T; full lines are susceptibilities, dashed lines represent the correlation function; winding lines are the full self energies. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$\begin{aligned}\sum\nolimits_2(\mathbf{q},\omega_n) = {} & -\frac{\hbar}{6\beta V^2}\sum_{\mathbf{k},\mathbf{p},\omega_m}(\chi^*_T(\mathbf{p}+\mathbf{q},\omega_n-\omega_m) \\ & + \chi^*_L(\mathbf{p}+\mathbf{q},\omega_n-\omega_m))K_\mu(\mathbf{p}-\mathbf{k})\chi_T(\mathbf{k},\omega_m) \\ = {} & \frac{1}{2}\sum\nolimits^L_{an}(\mathbf{q},\omega_n) + \sum\nolimits^T_{an}(\mathbf{q},\omega_n) \\ = {} & -\frac{\hbar}{6\beta V}\sum_{\mathbf{k}}\left(\sum\nolimits_1(\mathbf{k}+\mathbf{q},\omega_{n-m}) - \frac{\sum^L_{an}(\mathbf{k}+\mathbf{q},\omega_{n-m})}{2}\right)\chi_T(\mathbf{k},\omega_m)\end{aligned} \tag{23}$$

$$\chi_L(\mathbf{q},\omega_m) = \frac{\mathbf{q}^2}{\rho\omega_n^2 + \mathbf{q}^2(\lambda + 2\mu_0 - 2\sum\nolimits_1(\mathbf{q},\omega_n))} = \mathbf{q}^2 G_L(\mathbf{q},\omega_m) \tag{24}$$

$$\chi_T(\mathbf{q},\omega_m) = \frac{\mathbf{q}^2}{\rho\omega_n^2 + \mathbf{q}^2(\mu_0 - \sum\nolimits_1(\mathbf{q},\omega_n) - \sum\nolimits_2(\mathbf{q},\omega_n))} = \mathbf{q}^2 G_T(\mathbf{q},\omega_m) \tag{25}$$

The quadratic (in χ) terms emerge from the disorder enhanced anharmonic interaction, all anharmonic terms vanish in the case of zero disorder $K_\mu \to 0$.

These saddle-point equations can be represented diagrammatically (Fig. 2). Indeed, they resemble the structure of a calculation of the self energy to first order in the anharmonic and disorder-induced interaction. In the following we exploit this analogy for justifying the most obvious approximation to Eqs. (22–25), the *mode-decay approximation*.

2.4. Mode-decay approximation

We choose an exponential correlation function $K_\mu((\mathbf{x}-\mathbf{x}')) = \Delta^2\exp\left(-\frac{|(\mathbf{x}-\mathbf{x}')|}{\xi}\right)$, with Δ^2 the variance of the shear modulus and ξ the correlation length. The small anharmonic corrections to the longitudinal phonon propagator are estimated by expanding Eqs.(22–25) around the solution of the linearized saddle-point equations:

$$\chi_i = \overline{\chi}_i + \delta\chi_i \tag{26}$$

$$\sum\nolimits_i = \overline{\sum}_i + \delta\sum\nolimits_i \tag{27}$$

The lowest order anharmonic correction to the longitudinal phonon self energy is represented through the last diagram of Fig. 2, but with the full susceptibilities replaced by the disorder-dressed ones $\overline{\chi}_i$:

$$\delta\sum\nolimits_L(\mathbf{q}\to 0,\omega_n) = -\frac{\hbar}{6\beta V^2}\sum_{\mathbf{k},\mathbf{p},\omega_m}\overline{\chi}_T(\mathbf{p},\omega_n-\omega_m)K_\mu(\mathbf{p}-\mathbf{k})\overline{\chi}_T(\mathbf{k},\omega_m) \tag{28}$$

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Eq. (28) is recasted by the Matsubara technique [29]:

$$\delta\sum_L(\mathbf{q}\to 0,\omega_n) = -\frac{\hbar}{12V^2\pi}\sum_{\mathbf{k},\mathbf{p}}\int_{-\infty}^{\infty}d\omega\coth\left(\frac{\beta\omega}{2}\right) \times \overline{\chi}_T(\mathbf{p},\omega_n - i\omega_+)K_\mu(\mathbf{p}-\mathbf{k})\overline{\chi}''_T(\mathbf{k},i\omega_+) \quad (29)$$

$$= -\frac{\hbar}{6V^2\pi}\sum_{\mathbf{k},\mathbf{p}}\int_0^{\infty}d\omega\,\coth\left(\frac{\beta\omega}{2}\right)\overline{\chi}''_T(\mathbf{k},i\omega_+) \times K_\mu(\mathbf{p}-\mathbf{k})(\overline{\chi}_T(\mathbf{p},\omega_n - i\omega) - \overline{\chi}_T(\mathbf{p},\omega_n + i\omega)) \quad (30)$$

$$\approx -\frac{\hbar\Delta^2\xi^3}{6\pi^4}\int_0^{\infty}d\omega\int_0^{k_D}dkk^2\int_0^{k_D}dpp^2\coth\left(\frac{\beta\omega}{2}\right) \times (\overline{\chi}_T(\mathbf{p},\omega_n - i\omega) - \overline{\chi}_T(\mathbf{p},\omega_n + i\omega))\overline{\chi}''_T(\mathbf{k},i\omega_+) \quad (31)$$

The Fourier transformed density-correlation function is linked to the dynamical longitudinal susceptibility, via the fluctuation–dissipation theorem:

$$\langle\rho^*(\mathbf{k},\omega)\rho(\mathbf{k},\omega)\rangle = \frac{1}{\pi}\coth\left(\frac{\beta\omega}{2}\right)\chi''_L(\mathbf{k},\omega_n = i\omega_+) = \frac{1}{\pi}\coth\left(\frac{\beta\omega}{2}\right)\chi''_L(k,\omega_+) \quad (32)$$

The Brillouin linewidth is then just the width of the longitudinal susceptibility at resonance

$$\Gamma(k) = k\sum''_L(\omega k)/\upsilon_L \quad \omega_k = \upsilon_L k. \quad (33)$$

At room temperature, the anharmonic contribution to the imaginary part of the self energy reads

$$\delta\sum''_L(\omega_n = i\Omega_+) = \frac{\Delta^2 k_B T\xi^3}{3\pi^4}\int_{(k,p,\omega)}\frac{k^2p^2}{\omega}\,\overline{\chi}''_T(\mathbf{k},\omega_+) \times (\overline{\chi}''_T(\mathbf{p},\omega_+ + \Omega) - \overline{\chi}''_T(\mathbf{p},\omega_+ - \Omega)). \quad (34)$$

The transverse susceptibility

$$\chi''_T(\mathbf{k},\omega_+) = \frac{1}{\rho\upsilon_T^2}\frac{\mathbf{k}^2\sum''(\omega_+)}{(-\omega_+^2 + \upsilon_T^2\mathbf{k}^2)^2 + \mathbf{k}^4\left(\sum''(\omega_+)\right)^2} \quad (35)$$

consists not only of a Brillouin-peak, but resembles the shape of the self energy in self consistent Born approximation (Fig. 3).

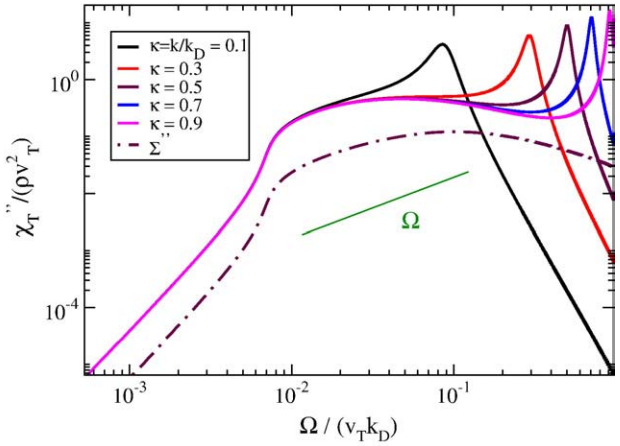

Fig. 3. The spectral density function $\chi''_T(\mathbf{k},\omega_+)$ for various wave numbers.

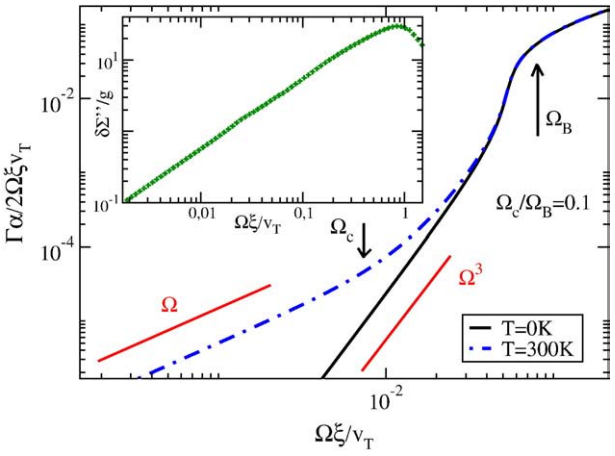

Fig. 4. Full Brillouin linewidth due to disorder and anharmonicity for $(\upsilon_L/\upsilon_T)^2 = 2.52$, $\Delta^2 = 0.99, \Delta_c^2 = 0.401\rho^2\upsilon_T^4, \xi = 2/k_D$ and $T = 300K$ inset: the anharmonic self energy integral (35) divided by the anharmonicity parameter $g = \Delta^2 k_B T/(3\pi^4\xi^3\rho^3\upsilon_T^4)$.

For numerical evaluation we introduce dimensionless quantities, $\tilde{\omega} = \frac{\omega\xi}{\upsilon_T}, \tilde{k} = k\xi, \tilde{\chi}'' = \chi''\rho\upsilon_T^2$.

$$\delta\sum''_L\left(\tilde{\Omega}_+\right) = \frac{\Delta^2 k_B T}{3\pi^4\xi^3\rho^3\upsilon_T^4}\int_0^{k_D\xi}d\tilde{k}\tilde{k}^2\int_0^{k_D\xi}d\tilde{p}\tilde{p}^2\int_0^{\infty} \times\frac{d\tilde{\omega}}{\tilde{\omega}}\left(\tilde{\chi}''_T(\tilde{\mathbf{p}},\tilde{\omega}_+ + \tilde{\Omega}) - \tilde{\chi}''_T(\tilde{\mathbf{p}},\tilde{\omega}_+ - \tilde{\Omega})\right)\tilde{\chi}''_T\left(\tilde{k},\tilde{\omega}_+\right) \quad (36)$$

The sound-attenuation function exhibits a linear behavior at frequencies below the boson peak and drops off above (see the inset of Fig. 4). This happens because the main contribution to the integral (36), for frequencies below the boson peak, comes from the band of irregular delocalized high-frequency modes; these states contribute a wide $\chi''_T \propto \omega$ regime, situated above the boson peak, to the disordered spectral density (see Fig. 3), for which the kernel $\tilde{\chi}''_T\left(\tilde{\mathbf{p}},\tilde{\omega}_+ + \tilde{\Omega}\right) - \tilde{\chi}''_T\left(\tilde{\mathbf{p}},\tilde{\omega}_+ - \tilde{\Omega}\right)$ can be replaced with $\tilde{\Omega}\partial\tilde{\omega}\tilde{\chi}''_T(\tilde{\mathbf{p}},\tilde{\omega}_+)$.

2.5. Estimation of the crossover frequency in SiO^2

We estimate the amount of the attenuation induced by anharmonicity as compared with the disorder-induced one. The ratio $R(\Omega) = \Gamma_{an}(\Omega)/\Gamma_{dis}(\Omega) \propto \delta\sum_L\left(\tilde{\Omega}\right)/\tilde{\Omega}$, which becomes frequency-independent beyond the boson peak, determines the crossover frequency. This ratio is fixed by the parameters Δ^2 and ξ, which set up the boson peak position, and the temperature. For example SiO_2 requires $\Delta^2 = 0.99\Delta_c^2 = 0.401\rho^2\upsilon_T^4$ and $\xi = 2/k_D$. The ratio of the squared sound velocities is $(\upsilon_L/\upsilon_T)^2 = 2.52$ and the Debye cutoff 1.6×10^{10}/m [6]. At room temperature $k_B T k_D^3/\rho\upsilon_T^2 = 0.6$ we obtain $\delta\sum''_L\left(\tilde{\Omega}\right) \approx 0.0045\,\tilde{\Omega}$, i.e. $T_0 = 7.3\cdot10^5 K$. Fig. 4 shows the full Brillouin linewidth due to disorder and anharmonicity. The anharmonic corrections already lead to deviations from the disordered contribution slightly below the shoulder of the boson peak, the highest frequency, where the Akhiezer-like behavior is present in SiO_2 is therefore predicted to be one order of magnitude below the boson peak, i.e. in the 100 GHz regime. In general, for observing the Rayleigh-law one needs to go to low enough temperature, which shifts the crossover towards lower frequencies.

Let us now discuss the possible role of potential-induced anharmonicity. There is no problem to introduce interactions involving longitudinal and transverse Mode-Grüneisen parameters $g_{L,T}$ into the theory. In the longitudinal case one just has to replace Δ^2 by $(1+g_L^2)\Delta^2$ in the saddle-point Eqs. (22–25). This will shift the crossover from Akhiezer-like to Rayleigh scattering upwards and

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reduce the "Rayleigh window" between the Akhiezer–Rayleigh crossover and the boson peak. Within our continuum description, it is not possible to judge the importance of the Mode-Grüneisen parameters $g_{L,T}$, because they are effective constants which have to be calculated from a certain lattice theory, taking into account the microscopic details of the interaction. It has been pointed out by Fabian et al. [17], that the Grüneisen parameters which they have extracted from their simulations are unusually strong, with respect to the bare crystalline couplings. However, a suitable choice of the parameters for the Stillinger–Weber potential [30] used in their simulations [18] should account for the non-linear part of the strain tensor as well. Hence their strong Grüneisen parameters γ_i, should not be confused with our non-linear couplings $g_{L,T}$, which may as a first guess be identified with their rather weak crystalline counterparts [25], as long as one deals with weak disorder. However it cannot be excluded, that strong disorder or impurities drive these constants to a strong coupling regime, in a renormalization group approach. Therefore, it has to be determined by experiment, whether our "minimal" description is sufficient, or one has to deal with Grüneisen parameters.

The SiO_2 measurement, performed by Masciovecchio et al. [20], exhibits the Akhiezer–Rayleigh crossover around 100 GHz, which fits our estimates quite well. In contradiction Devos et al. [21] claim the crossover to take place at 400 GHz, however they performed their measurements on vitreous SiO_2, which shelters several defects. It is at the heart of impurity physics, that defects give rise to additional interactions, e.g. anharmonicities. This can lead to enhanced Mode-Grüneisen parameters $g_{L,T}$, which then have to be taken into account. In several experiments dealing with vibrational spectra near and below the glass transition [31,32] one observes an increase of the DOS in the boson peak regime. Within the mode-decay approximation one can account for the trends but not numerically reproduce such spectra. We believe that one has to solve the full mode-coupling Eqs. (22–25) in order to be able to do so.

3. Conclusion

In conclusion we developed a consistent perturbative treatment of the anharmonic contribution to the Brillouin linewidth in disordered solids. Our treatment solely in terms of elasticity parameters, which enter into the mean values and correlation functions suggests a correlation between the boson peak position and the Akhiezer–Rayleigh crossover at temperatures scaled with the Debye temperature. Further developments in experimental techniques are required to explore this extremely interesting frequency window in the upper GHz regime.

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High-frequency vibrational density of states of a disordered solid

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Abstract
We investigate the high-frequency behavior of the density of vibrational states in three-dimensional elasticity theory with spatially fluctuating elastic moduli. At frequencies well above the mobility edge, instanton solutions yield an exponentially decaying density of states. The instanton solutions describe excitations, which become localized due to the disorder-induced fluctuations, which lower the sound velocity in a finite region compared to its average value. The exponentially decaying density of states (known in electronic systems as the Lifshitz tail) is governed by the statistics of a fluctuating-elasticity landscape, capable of trapping the vibrational excitations.

(Some figures may appear in colour only in the online journal)

1. Introduction

The density of states (DOS) of a disordered system is a quantity which has been vividly discussed [1–4]. Lifshitz was one of the first authors to calculate the disorder-induced corrections to the DOS, for electron and phonon systems [5]. By a phenomenological argument, he explained the occurrence of an exponential tail of the DOS in the vicinity of the band-edges, which is related to the localization of the one-particle states. As the penetrability of an arbitrarily shaped barrier tends towards zero at large energies [6], one expects the high-energy eigenstates of a system with a random fluctuating potential to be localized. The DOS is then proportional to the probability of the occurrence of wells, capable of trapping the single-particle states, which for weak fluctuations (e.g. low impurity concentrations) can always be approximated by an exponential function. The energy dependence of the exponent depends crucially on the energy of localization, from which some substantial corrections from the set of maximally crossed diagrams in the perturbation expansion arise, similar to the energy–momentum relation of a wave in a potential well, if the length scale set by the disorder parameter is of the order of the localization length. Such corrections can be treated in a field-theoretical approach by means of an ϵ-expansion of the nonlinear σ model in the vicinity of the localization energy [7, 8], or by self-consistent mode coupling expansion techniques [9], which lead to the potential-well analogy [10–13]. These corrections are important for the electronic problem, because the Lifshitz tail mostly consists of the ground states of such wells, for which the irreducible one-particle self-energy is energy dependent.

For phonons the situation is different, because one deals with fluctuating elastic constants instead of potentials, and localized states appear only at the upper band edge [14, 15] for positive values of ω^2 [16, 17], where ω is the vibrational excitation frequency. There is an extended amount of literature concerning the cross-over from the Debye type acoustic wave regime to a regime of diffusive, random-matrix type vibrational excitations ('boson peak' [18–20]), which has been accurately described within the σ-model approach by two non-crossing techniques, namely the self-consistent Born [21–24] and coherent-potential approximations [15, 25–27]. Instead, here we are interested in the behavior at large positive frequencies. In the σ-model approach one finds that the one-particle self-energy on the localized side becomes frequency independent, and the system can be assumed to be described by a renormalized Ginzburg–Landau theory [28, 29]. The states with the highest values of ω^2 within a region of constant elastic modulus, bounded by a mismatch, carry wavenumbers of the order of the Debye wavenumber. Hence these states dominate the Lifshitz tail. If one assumes further the fluctuations of the elastic constants to be small and the localization length to

scale with the inverse frequency, $\xi \propto \omega^{-1}$, as in elementary wave mechanics [6], the DOS should be proportional to $\exp(-a\omega^{4-d})$. Such a behavior of the exponent is suggested by recent experiments [30, 31], in which a linear exponential decay of the DOS in the high-frequency region is found.

In the remainder of this paper we will reformulate the field theoretic approach within the Keldysh formulation of quantum dynamics, in order to include the instanton contribution, from which the tail of the DOS can be extracted.

2. Keldysh formulation for weakly disordered phonons

The quantum dynamics for the displacement field $\mathbf{u}(\mathbf{x}, t)$ with spatially dependent elastic moduli will be calculated from the Keldysh partition function $1 = \int \mathcal{D}\mathbf{u}\ \mathrm{e}^{\mathrm{i}S}$, where the action involves the classical (symmetric) and quantum (antisymmetric) linear combinations of the two replicas acting left and right on the density matrix describing the initial state [32]. The reason for naming them classical and quantum is as follows: if the action is related to the Lagrangian of a simple non-relativistic one-particle system, the saddle-point solution of the field theory with $u_{\mathrm{q}} = u_+ - u_- = 0, u_{\mathrm{cl}} \equiv u_+ + u_- = u(t)$ yields Newton's equation of motion for the particle's trajectory $u(t)$. Quantum corrections like the appearance of a phase or tunneling contributions arise from the finite expectation values and higher correlations of the antisymmetric $u_+ - u_-$ linear combination, which is hence named the quantum component.

The action may involve arbitrary nonlinear terms, which in a classic kinetic approximation give rise to phonon thermalization, at least in three dimensions. For the vibrational spectra of disordered systems the anharmonic interactions are only important below the boson peak [33, 34]. For our purpose it is hence enough to approximate the Keldysh action to quadratic order in the displacement field,

$$S = \int \mathrm{d}^{d+1}x \left\{ -\mathbf{u}^{\mathrm{q}}\partial_t^2\mathbf{u}^{\mathrm{cl}} + 2\mu(\mathbf{x})u_{ij}^{\mathrm{q}}u_{ji}^{\mathrm{cl}} + \lambda(\mathbf{x})u_{ii}^{\mathrm{q}}u_{ii}^{\mathrm{cl}} \right\} + \int \mathrm{d}^{d+1}x\, \mathbf{u}^{\mathrm{q}}(G^{-1})_{\mathrm{K}}\mathbf{u}^{\mathrm{q}} \tag{1}$$

where $x = (\mathbf{x}, t)$, $u_{ij} = \frac{1}{2}\left(\partial_i u_j + \partial_j u_i\right)$ is the usual strain-tensor, and λ and μ are Lamé's elastic constants, which are assumed to fluctuate due to the structural disorder of the material [21–25]. We use units in which the mass density equals unity. The Keldysh component G_{K} characterizes the actual state of the system, which can be determined from knowledge of the retarded and advanced Green's functions and a proper initial condition. If one assumes that the disorder does not alter the thermalization process, the Keldysh component can safely be replaced by a thermal distribution. The formulation (1) ignores further initial correlations.

The advantage of Keldysh's closed time-contour is the absence of vacuum contributions to the partition function; hence, one can average it directly over an arbitrary distribution of elastic constants. This average can be performed formally by characterizing the probability distribution through its irreducible correlation functions

$$K(x_1, \ldots, x_n) \equiv \frac{\delta}{\delta x_1} \ldots \frac{\delta}{\delta x_n} \ln \int \mathrm{d}\mu\, P[\mu] \mathrm{e}^{(\mu, j)}, \tag{2}$$

which leads to an action of the form

$$\begin{aligned} S_{\mathrm{dis}} = S - S[\langle\mu\rangle, \langle\lambda\rangle] = \\ + \int_{x_1 x_2} K_\mu(\mathbf{x}_1, \mathbf{x}_2) u_{ij}^{\mathrm{q}}(x_1) u_{ji}^{\mathrm{cl}}(x_1) u_{lm}^{\mathrm{q}}(x_2) u_{ml}^{\mathrm{cl}}(x_2) \\ + \int_{x_1 x_2} K_\lambda(\mathbf{x}_1, \mathbf{x}_2) u_{ii}^{\mathrm{q}}(x_1) u_{ii}^{\mathrm{cl}}(x_1) u_{jj}^{\mathrm{q}}(x_2) \\ \times u_{jj}^{\mathrm{cl}}(x_2) + \cdots . \end{aligned} \tag{3}$$

For the Gaussian theory the structure of the action is the same as for a dissipative quantum system [35], in which the spectral function of the heat bath is replaced by two classical strain fields. Therefore the calculation of instanton solutions in disordered systems exhibits a strong resemblance to the calculation of thermal activation of a system attached to a heat bath [35].

Within this paper we do not want to perform technically detailed calculations. We rather want to demonstrate the general procedure of mapping the disordered bosonic system onto a disordered fermionic one within the Keldysh prescription. Of course this mapping is only possible between the pair modes of the bosonic and fermionic systems.

In general, the theory can be represented in terms of these two-point functions using the Faddeev–Popov transformation

$$\begin{aligned} F\left[u_{ij}^{\alpha}(x_1) u_{lm}^{\beta}(x_2)\right] = \int_{Q,\Lambda} \mathrm{e}^{\mathrm{i}\mathrm{Tr}[(\Lambda - uu^\dagger)Q]} \\ \equiv \int \mathcal{D}Q\mathcal{D}\Lambda F\left[Q_{ijlm}^{\alpha\beta}(x_1, x_2)\right] \\ \times \mathrm{e}^{\mathrm{i}\Lambda_{ijlm}^{\alpha\beta}\left(Q_{mlji}^{\beta\alpha} - u_{ml}^{\beta}(x_1) u_{ji}^{\alpha}(x_2)\right)}. \end{aligned}$$

Here Greek indices represent the Keldysh degrees of freedom. The following mapping achieves the same causality structure for the composite phonons as for the electrons [35]:

$$A_{\mathrm{R}} \equiv A \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad A_{\mathrm{L}} \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} A.$$

If the matrix A has the causality structure of a bosonic Green's function, A_{R} has the c.s. (causality structure) of a fermionic Green's function and A_{L} the c.s. of a fermionic self-energy. The advantage is now that the phonon nonlinear σ-model can be developed along the electronic counterpart. One can now write the disorder-induced nonlinear terms as

$$S_{\mathrm{dis}} = \sum_n \mathrm{Tr}\left[K_n^{\mu} Q_{\mathrm{R}}^n + K_n^{\lambda}(\chi Q_{\mathrm{R}})^n\right] \tag{4}$$

in which χ is a characteristic matrix defined according to $\chi Q_{ijlm} = \delta_{ij}\delta_{lm}Q_{ijlm}$.

For the sake of simplicity we will only consider a locally fluctuating shear modulus, $K_n^{\lambda} = 0$, $K_2^{\mu} = \gamma^{-1}\delta(\mathbf{x} - \mathbf{y})$, $K_{n\neq 2}^{\mu} = 0$.

In the absence of anharmonicities one can immediately integrate out the composite field Λ, which reduces the Faddeev–Popov procedure to the Hubbard Stratonovich

transformation. This could be the starting point to formulate the nonlinear σ model approach to phonon localization around the weakly disordered SCBA saddle-point [21].

However, as also discussed by Cardy [29], in the large energy regime, where the phonon energy is large compared to the energy-fluctuations set by the disorder potential, the semiclassical one-particle approximation of the partition function becomes valid. It is more convenient to discuss the Lifshitz tail in terms of the one-particle functions, as one avoids the complicated renormalization-group method. One would agree that the simple one-particle saddle-point is sufficient, as long as one is interested in the deep localization regime, where knowledge of the mobility edge is lost. In contrast, the universal properties of vibrations in a glass in the vicinity of the mobility edge [16, 17], must be developed from (4) within the usual Keldysh nonlinear σ model.

3. Instanton solutions

In the remainder we will use the simple instanton picture in order to calculate the exponential dependence of the vibrational density of states at high energies.

The first step is to express the partition function as an infinite product of discrete frequencies $1 = \prod_\omega Z(\omega)$, where $Z(\omega) = \mathrm{e}^{\mathrm{i}s(\omega)}$ and

$$s(\omega) = \int \mathrm{d}^d x \left[\omega^2 \vec{u}_\mathrm{q}\vec{u}_\mathrm{cl} + g_k \vec{u}_\mathrm{q}\vec{u}_\mathrm{q} + 2\mu u^\mathrm{q}_{ij} u^\mathrm{cl}_{ji} + \lambda u^\mathrm{q}_{ii} u^\mathrm{cl}_{ii}\right] + \int \mathrm{d}^d x\, \gamma \left(u^\mathrm{q}_{ij}(-\omega, x) u^\mathrm{cl}_{ji}(\omega, x)\right)^2. \quad (5)$$

If the frequency is sufficiently large, this field theory can be solved in the semiclassical saddle-point approximation by extremizing the action with respect to the classical and quantum components. In analogy to the theory of dissipative quantum systems there exist instanton solutions in which the expectation value of the quantum component $\langle u_i\rangle = \mathrm{i}v^\mathrm{q}_i$ is finite and purely imaginary.

From the equation of motion (6) one deduces that these solutions describe a situation in which condensation of strain, $\mathrm{i}v^\mathrm{q}_{ij} = -v_{ij} = -v^\mathrm{cl}_{ij}$, leads to a finite region with a sound velocity substantially lower than the average. The states are hence trapped in this finite region. There is a second instanton equation describing the other possibility, where the sound velocity is raised. We seek an instanton ansatz where the saddle-point solution satisfies

$$(\omega^2 - (\lambda + \mu[v])\nabla\nabla \circ -\mu[v]\Delta)\vec{v}(\omega, x) = 0$$
$$\mu[v] = \mu(1 - \gamma v_{ij} v_{ji}). \quad (6)$$

Reinsertion of this equation of motion (6) into (5) yields a finite action $\mathrm{i}f(\omega)$, and hence an exponential factor of the partition function $\mathrm{e}^{-f(\omega)}$, which is calculated via formula (11).

In order to calculate the density of states and the Green's function we have to expand (5) with respect to the fluctuations above this instanton saddle-point $u^\alpha_{ij} = v_{ij} + \delta u^\alpha_{ij}$. The irreducible retarded Green's function is by definition just the correlator of $\langle \delta u^\mathrm{cl}_i \delta_j u^\mathrm{q}\rangle$. Obviously, this quantity is proportional to the factor $\mathrm{e}^{-f(\omega)}$ which is nothing other than the exponential Lifshitz tail. The action (5) expanded around the instanton saddle-point reads

$$s(\omega) = \mathrm{i}f(\omega) + O\left[\delta u^3_{ij}, \delta u^4_{ij}\right] + \int \mathrm{d}^d x\, \omega^2 \delta\vec{u}_\mathrm{q}\delta\vec{u}_\mathrm{cl} + \int \mathrm{d}^d x \left(2\mu\left(1 - 2\frac{\gamma}{\mu}\right)\delta u^\mathrm{q}_{ij} v_{hk} v_{kh} \delta u^\mathrm{cl}_{ji} + \lambda \delta u^\mathrm{q}_{ii}\delta u^\mathrm{cl}_{ii}\right). \quad (7)$$

The next step is to use the bosonization-procedure (5) to express this action in terms of the pair modes $Q_\mathrm{R} = \langle \delta u^\mathrm{cl}_i \delta u^\mathrm{q}_j\rangle$. Using a further saddle-point approximation in order to determine Q_R yields the following set of equations:

$$\langle Q_\mathrm{R}(\omega, x)\rangle \equiv \mathrm{i}\gamma \mathrm{e}^{-f}\left([1]\left[G_0^{-1}(\omega, x) - \nabla\left(\Sigma + v_{ij}v_{ji}\right)_{\omega,x}\nabla^\mathrm{T}\right]^{-1} + \vec{v}\vec{v}^\mathrm{T}\right) \quad (8)$$

$$\Sigma_\mathrm{R}(\omega, x) \propto \mathrm{e}^{-f}\gamma \mathrm{Tr}\nabla \times \frac{1}{G_0^{-1}(\omega, x) - \nabla(\Sigma + v_{ij}v_{ji})_{\omega,x}\nabla^\mathrm{T}}\nabla^\mathrm{T} \quad (9)$$

$$f(\omega) = \int_\mathbf{x}\left\{\omega^2|\vec{v}(\omega, x)|^2 + 2\mu v_{ij}v_{ji} + \lambda v^2_{ii}\right\} \quad (10)$$

in which the field satisfies the exact equation of motion

$$\frac{\delta}{\delta v^\alpha} s(\omega) = \frac{\delta}{\delta v^\alpha}\left\{\vec{v}^\mathrm{T}\left(G_0^{-1} + \nabla\Sigma\nabla^\mathrm{T}\right)\vec{v} + S_\mathrm{dis}[v]\right\} = 0. \quad (11)$$

These equations have a rather simple interpretation: they allow for a self-consistent determination of the instanton solution in the Hartree-approximation and a further non-crossing approximation of the self-energy of the propagator, which has a frequency and spatially dependent sound velocity, due to the finite instanton amplitude. However, we are mostly interested in a discussion of the exponential factor and leave the numerical solution of this set of equations for future work.

From (8) it becomes clear that within this approximation the density of states is just the usual one in the SCBA approximation, multiplied by the instanton factor $\mathrm{e}^{-f(\omega)}$. In order to estimate the power law satisfied by the exponent of the DOS we look for a spherically symmetric solution with longitudinal polarization in three dimensions.

The equation for the radial part reads

$$\omega^2\Psi(r) + (1 - 4\gamma\,(\partial_r\Psi)^2)\Delta_r\Psi(r) = 0. \quad (12)$$

The frequency and the disorder parameter can immediately be scaled out according to $\phi = \frac{1}{\omega\sqrt{\gamma}}\Psi(\omega r)$, where the spatially dependent part $\Psi(y = \omega r)$ satisfies the reduced equation

$$\Psi(y) + (1 - 4(\partial_y\Psi)^2)\Delta_y\Psi(y) = 0. \quad (13)$$

For numerical solution one replaces (13) by the first-order system

$$\partial_r\Psi(r) = \phi(r)$$
$$\partial_r\phi(r) = \Psi(1 - 4\phi(r)^2)^{-1} - 2r^{-1}\phi(r)$$

which may readily be solved by means of a second-order Runge Kutta algorithm.

The phase can be estimated at large frequencies

$$\begin{aligned} f &= \int \mathrm{d}^d r\, \phi(r)(\omega^2 + \Delta_r^2)\phi(r) \\ &= \frac{1}{\gamma}\omega^{-d} \int \mathrm{d}^d y\, \Psi(y)(1+\Delta_y)\Psi(y) \\ &= \int_{q<q_\mathrm{D}\omega} \frac{\mathrm{d}^d q}{(2\pi)^3}\Psi(q)(1+q^2)\Psi(q) \\ \omega \to \infty : \frac{1}{\gamma}&\left(\frac{\omega}{\omega_\mathrm{D}}\right)^{4-d} \int \frac{\mathrm{d}^d q}{(2\pi)^3}\Psi(q)\Psi(q) \\ &= \frac{1}{\gamma}\left(\frac{\omega}{\omega_\mathrm{D}}\right)^{4-d}. \end{aligned} \tag{14}$$

From (13) it is clear that there exists a localized exponential solution, as long as the state has a single point where the condensed dimensionless strain exceeds the critical value $\partial_y \Psi(y) = \frac{1}{2}$, which can always be imposed as a boundary condition. Note that q is not the Fourier component of the spatial variable r, but of the frequency scaled variable $y = \omega r$.

In contrast to the electronic calculation, the phase is dominated by the small-distance behavior of the wavefunction. As a result we find the same power law of the exponent as predicted by the Lifshitz-argument.

Figure 1 shows a spherically symmetric transversely polarized solution $\vec{u}(y = \omega r) = \Psi \vec{e}_\theta$ to the instanton equation (5), together with its radial derivative $\phi(y = \omega r) = \partial_y \Psi(y)$. The one-particle states turn out to be localized, because they drop to zero faster than the spherically symmetric volume element (which is proportional to r^2). The corresponding localization length would be a number of the order of several wavelengths. The inset shows the density of vibrational states normalized to the Debye law, measured by Baldi *et al* [36] in vitreous silica. The red curve is a previous fit with the SCBA theory, which used the disorder parameter $\gamma = 0.99\gamma_\mathrm{c}$ close to the critical value $\gamma_\mathrm{c} = 0.1764$. The blue curve shows the Lifshitz tail with the same disorder parameter. The amplitude of the exponential has been adjusted so that the high-frequency density of states agrees with the measured one. It can be seen that the Lifshitz line fits the experimental data beyond the boson peak quite well. From a theoretical standpoint one may state that the boson peak and the strongly localized one-particle states are related, due to the fact that the SCBA collects a set of strong scattering processes which are analytic in γ, and the instanton approximation is obviously a resummation of scattering processes which are analytic in $1/\gamma$. In this sense the boson peak is the precursor of the localization transition.

The high-frequency deviation from the experimental data is not captured by the present phenomenological theory. A possible reason is that the localization is related to 'singular' points within the material, where the elastic constant drops to zero. To account for this, non-Gaussian effects have to be considered in order to prevent a negative elastic constant.

This corresponds to the fact that the SCBA cannot account quantitatively for the magnitude of the boson peak [36]. It has been shown recently, using the coherent-potential approximation (CPA), that indeed non-Gaussian distributions of elastic constants are able to account for the strong boson peak enhancement of the density of states in oxide glasses [27].

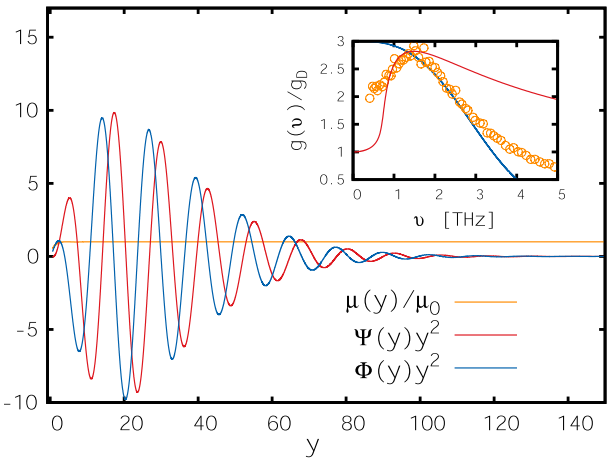

Figure 1. Numerical solution to the instanton equation (5); for details see the text. Inset: the density of states, divided by the Debye density of states, against the frequency $\nu = \omega/2\pi$. Symbols: spectral data measured in vitreous silica [36]; red line: previous calculation in the self-consistent Born approximation (SCBA) using the disorder parameter $\gamma = 0.99\gamma_\mathrm{c}$ with $\gamma_\mathrm{c} = 0.1764$ [23]; red line: Lifshitz tail calculated according to the present theory with the same γ value. For details see the text.

Let us make a general statement on the nature of the vibrational excitations in disordered materials. Below the boson peak these excitations are Debye waves due to the fact that for scales large compared to an interatomic distance the material is homogeneous and isotropic. For smaller length scales, i.e. higher frequencies, the boson peak indicates the breakdown of the wave concept [24]. The vibrational excitations are no longer described by the translational and rotational symmetry. Instead they can be characterized as random-matrix states, which obey the Gaussian-orthogonal-ensemble spectral statistics [15]. At even higher frequencies the localization transition occurs, which is a transition within the random-matrix scenario. This step-wise transition from wave physics first to diffusive motion and then to localization is well known for electrons in a random potential [37, 38].

4. Summary and conclusion

In this work we formulated the theory of weakly fluctuating elastic constants of a glass within the Keldysh-formalism, in order to propose an expression for the high-frequency behavior of the density of states of a glass. In three dimensions, where this approach is valid, it yields an exponentially decaying density of states. This exponential decay is expected by basic Lifshitz-like considerations, and has also been observed in recent experiments [30, 31]. If one measures this exponential decay in an experiment, it is therefore straightforward to extract the disorder parameter γ,

which can be compared with the values extracted from experiments and simulations for the description of the boson peak [21–25].

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