

From waves to trajectories: some aspects of time in quantum problems

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Abstract. In stationary quantum mechanical problems time is absent. However time comes back if an experiment is performed on a stationary wave function. This property is demonstrated for a real experiment (photodetachment). The wave function is shown to set the stage for mutually exclusive experimental results, each of them having its own history of Feynman paths.

1. From philosophy to physics

The 18th century philosopher Immanuel Kant (1724 – 1804) who lived in Königsberg (now Kaliningrad) in former Prussia wrote an influential book entitled 'Kritik der reinen Vernunft' (Critique of Pure Reason). The book is tough reading but it contains, among other things, an interesting idea: time and space are not elements of external reality. They exist in our minds. Time forms the stage for events to happen, whereas the idea of space allows us to relate real objects. Kant's idea was fascinating but not correct. Time and space are elements of our universe and, as Einstein taught us, they can be influenced by motion and gravitation. Depending on the level of approach and language, there are still many questions left about the character of space and time. In this note we will point out some properties of time in non-relativistic quantum mechanics.

2. Quantum mechanics without time

Let us consider a quantum system where a constant stream of negative ions is hit by a monochromatic i. e. infinitely long laser beam (see Fig. 1).

In the interaction region, photoionization will take place, leading to the release of a constant stream of monochromatic electrons. Negative ions allow for a simple description of the outgoing electron wave because there is no Coulomb interaction between the emitted electron and the neutral atom that is left behind. In addition, we consider a low-current situation where the emitted electrons are so far separated from each other that their mutual Coulomb interaction can be neglected. Near threshold, the photoelectrons have little kinetic energy and, hence, a very large de Broglie wavelength. Having the situation of Fig. 1 in mind, we assume the de Broglie wavelength to be large compared to the spatial extension of the interaction region between laser beam and atomic beam (the dot in Fig. 1). Therefore all electrons can be treated as coming from the same point, say \mathbf{r}' . Finally, using O^- where bound p -electrons are the candidates for photoionization, we know from Wigner's threshold law that these electrons leave the atom near

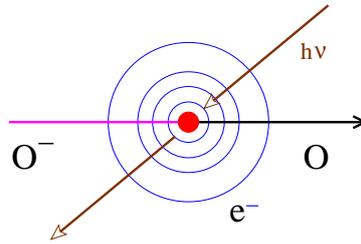


Figure 1. Example of a stationary quantum system: a constant beam of negative ions (here: O^-) is radiated by a monochromatic (i. e. very long) laser beam of energy $h\nu$. In the interaction region monochromatic electrons are released at a constant rate in form of a stationary wave.

threshold in an s -wave continuum.

In the absence of a final-state interaction, the electrons are then released in form of a free, stationary spherical s -matter wave which originates from $\mathbf{r} = \mathbf{r}'$. A particularly useful outgoing wave is the *Green function*

$$G_0(\mathbf{r}, \mathbf{r}'; E) = -\frac{m}{2\pi\hbar^2} \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}. \quad (1)$$

which is a solution of the inhomogeneous Schrödinger equation

$$[E - H_0]G_0(\mathbf{r}, \mathbf{r}'; E) = \delta^3(\mathbf{r} - \mathbf{r}') \quad (2)$$

for a free electron with H_0 being its Hamiltonian. The outgoing-wave Green function is the analytical solution of our little problem where photo-electrons are generated at $\mathbf{r} = \mathbf{r}'$. The δ -function on the right hand side of Eq.(2) represents a point source of unit strength for photoelectrons. By multiplying G_0 with a stretch factor C one can simulate point sources with variable strength.

3. From waves to orbits

The stationary matter wave of Fig. 1 carries information on orbits that can be uncovered by experiment within the rules of quantum mechanics. A useful tool for extracting information on the dynamics of a quantum system in real space is the Laplace transform K of the Green function,

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{i\hbar} \lim_{\eta \rightarrow 0^+} \int_0^\infty dt e^{i(E+i\eta)t/\hbar} K(\mathbf{r}, t|\mathbf{r}', 0). \quad (3)$$

K is called time-dependent *propagator* because it represents the motion of a particle from one point \mathbf{r} in space to another point \mathbf{r}' in a given time t . It goes without saying that relativistic effects are of course beyond the scope of non-relativistic quantum mechanics. Mathematically speaking, K represents the time evolution matrix $U(t, t' = 0)$ in coordinate space

$$K(\mathbf{r}, t | \mathbf{r}', t' = 0) \equiv \langle \mathbf{r} | U(t, t' = 0) | \mathbf{r}' \rangle. \quad (4)$$

Wave propagation with fixed energy E is ruled by the energy dependent propagator $G(\mathbf{r}, \mathbf{r}'; E)$, usually called energy Green function in order to avoid confusion with the (time-dependent) propagator K .

Coming back to the photodetachment problem of section 2 where the outgoing wave can be

described in terms of the Green function (1), we should relate G to a real experiment. Such an experiment was carried out by Blondel et al.[1, 2] who recorded interference fringes in configuration space for photoelectrons that originate from near-threshold photodetachment (see Fig. 2). The situation here is somewhat different from the setup in Fig. 1 because the emitted electrons are exposed to a homogeneous electric force field, $F = e\mathcal{E}$.

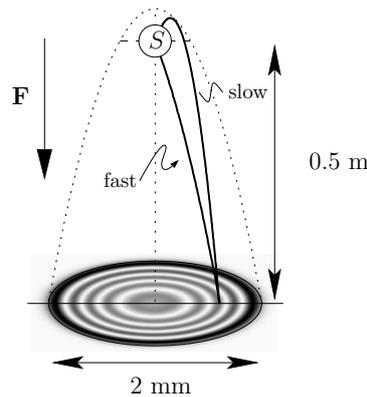


Figure 2. Near-threshold detachment of oxygen ions: $O^- \rightarrow O + e^-$ in the presence of a homogeneous electric force field $F = e\mathcal{E}$. The two possible classical trajectories for a photoelectron leading from the source (marked by S) to any destination will give rise to interference on a distant detector screen. The fringe pattern in the current distribution depends sensitively on the energy. By counting the number of fringes the binding energy E_0 of the outer electron can be determined from Einstein’s law [1, 2, 7].

Therefore the outgoing-wave Green function G_0 for a free electron must be replaced by the Green function G_{field} for the motion of an electron in a constant electric field. Let H_{field} be the corresponding field Hamiltonian; then Eq.(2) will be modified to

$$[E - H_{field}]G_{field}(\mathbf{r}, \mathbf{r}'; E) = \delta^3(\mathbf{r} - \mathbf{r}'), \quad (5)$$

where \mathbf{r}' is again the position of the electron source S . It certainly does not come as a surprise to see that the analytic solution [3, 4] is a wave that contains Airy functions. The mathematical details are not important here. Let us only point out that the experimental interference fringes are in perfect agreement with the theoretical description[5, 6, 7] based on G_{field} .

The interference fringes result from electrons that are generated in the source (interaction) region S at $\mathbf{r} = \mathbf{r}'$ and are registered at many different points \mathbf{r} . It goes without saying that the possibility of traveling to many different points in space means that an electron can experience many different histories. The histories are mutually exclusive since a given electron can only be registered at one point in space. For a rigorous definition of quantum mechanical histories we refer to [8, 9]. However each history itself contains many Feynman-path histories because Eq.(3) tells us that stationary wave propagation can be decomposed into infinitely many trajectories characterized by $K(\mathbf{r}, t|\mathbf{r}', 0)$.

The contribution of the classically allowed trajectories to a history described by $G(\mathbf{r}, \mathbf{r}'; E)$, with \mathbf{r} and \mathbf{r}' fixed, is obtained from the stationary phase approximation to Eq. (3). Usually classically allowed orbits contribute most to the transition amplitude K . A glance at Fig. 2

shows that just as in Young's double-slit experiment, the fringe pattern in the current profile of the photoelectrons can be interpreted as interference between the two classical trajectories, here of a particle in a constant force field. However there are also classically forbidden trajectories that correspond to classically forbidden processes like tunneling. There is a time scale for the tunneling-time problem but no general answer that would be independent of an experiment. For a better understanding of quantum processes it can be quite useful to analyze problems that can be analytically solved (see, for example [3, 7, 10]). It is amazing to see how successful Green functions can be used as mathematical tools for describing a diverse range of problems in modern quantum technology

Relativity puts space and time on equal footing – in contrast to our intuition. We can travel back and forth in space but not in time. In this context it is interesting to see how much effort Einstein put into the problem of closed trajectories in time. At the turn of 1916 he wrote a letter[11] to the mathematician Constantin Carathéodory who worked at that time among other things¹ on mathematical properties of the Hamilton–Jacobi theory. In his letter Einstein wrote: 'Wouldn't you like to think about the problem of closed lines in time? Here lies the core of the still unsolved part of the space–time–problem.' (*Wollen Sie nicht noch etwas über das Problem der geschlossenen Zeitlinien nachdenken? Hier liegt der Kern dieses noch ungelösten Teiles des Raum-Zeit-Problems.*)

4. Pauli's footnote on time

The character of time in quantum mechanics has always been a matter of discussion. The famous 'Handbuch der Physik' article by Pauli on the 'Principles of Wave Mechanics' (*Die allgemeinen Prinzipien der Wellenmechanik*)[13] touched this problem in a footnote. There, Pauli used the Heisenberg equation of motion

$$\frac{\hbar}{i}\dot{F} = H F - F H \quad (6)$$

for an arbitrary Hermitean operator F to show that time cannot be represented by a Hermitean operator $t(p,q)$. Because, if such an operator t existed it would have to satisfy ($\dot{t} = 1$)

$$\frac{\hbar}{i} = [H, t]. \quad (7)$$

Pauli then remarks that the existence of such a commutation relation requires H to have a continuous energy spectrum ranging from $-\infty$ to $+\infty$ ². Realistic Hamiltonians don't have such a continuous energy spectrum. They possess a ground state (their spectra are bounded from below) along with discrete states. Therefore a time operator obeying commutation relation (7) doesn't make sense. Pauli concluded that *... die Zeit in der Quantenmechanik notwendig als gewöhnliche Zahl („c-Zahl“) betrachtet werden muß*, meaning that time in quantum mechanics must be necessarily considered as an ordinary number ('c-number').

5. Schrödinger's bright ideas

The Hamilton–Jacobi theory played an important role in the discovery of wave mechanics because it can be used to build a bridge from classical mechanics to geometrical optics and, as Schrödinger was convinced, to all kinds of wave phenomena. In his first of four

¹ Carathéodory is famous for his many contributions on variational theory. He laid the mathematical foundations to the field of 'Dynamical Optimization'[12].

² Indeed, it follows from Eq.(7) that if $|E\rangle$ is an eigenstate of H with energy E then $\exp(i\omega t)|E\rangle$ will be an eigenstate of H with energy $E + \hbar\omega$. Since ω is arbitrary, a continuum of energy eigenstates would be generated through this simple operation.

Mitteilungen (communications)[14], Schrödinger started from the time-independent Hamilton–Jacobi equation

$$H(q, p = \frac{\partial S}{\partial q}) = E \quad (8)$$

with $S(q, E)$ being the stationary action. In order to obtain a linear wave equation, Schrödinger substituted

$$S = \mathcal{K} \ln \psi \quad (9)$$

into Eq.(8). At this point \mathcal{K} was a constant that had to be determined later. Schrödinger used the last two equations to eliminate p

$$H(q, p = \frac{\mathcal{K}}{\psi} \frac{\partial \psi}{\partial q}) = E. \quad (10)$$

In three dimensions this formula reads explicitly

$$\left(\frac{\partial \psi^2}{\partial x} \right) + \left(\frac{\partial \psi^2}{\partial y} \right) + \left(\frac{\partial \psi^2}{\partial z} \right) - \frac{2m}{\mathcal{K}^2} (E - V(x, y, z)) \psi^2 = 0 \quad (11)$$

with $x = q_1$; $y = q_2$ and $z = q_3$. In a last step, Schrödinger obtained his famous stationary wave equation, $H\psi = E\psi$, by requiring the eigenvalues E to satisfy the variational principle³

$$\delta J = \delta \int \int \int dx dy dz \left[\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial \psi}{\partial y} \right)^2 + \left(\frac{\partial \psi}{\partial z} \right)^2 - \frac{2m}{\mathcal{K}^2} (E - V(x, y, z)) \psi^2 \right] = 0. \quad (12)$$

Using his wave equation, Schrödinger calculated the binding energies of hydrogen. In order to get the correct energy spectrum he had to identify \mathcal{K} with \hbar .

In his fourth communication[15] Schrödinger allowed the wave function to become periodic in time because he wanted to study the photoelectric effect i. e. a situation where the atom is exposed to a periodic external electric field. By writing the periodic wave function in the form

$$\Psi = \psi \exp(-iEt/\hbar), \quad (13)$$

Schrödinger arrived immediately at his time-dependent equation

$$H\Psi = i\hbar \frac{\partial}{\partial t} \Psi. \quad (14)$$

with Ψ being a time-dependent probability amplitude. Schrödinger used his result to calculate electron transition probabilities for the photo effect in perturbation theory.

We end this short contribution by coming back to the question about the nature of quantum mechanics. What is the meaning of a complex wave function Ψ . Is it an element of reality? Is it just a mirror of our knowledge about nature? Strange enough, we don't need to answer such questions. We simply follow Feynman's recipe [16]: '... everything that can be deduced from the ideas of the existence of quantum mechanical probability amplitudes, strange though they are, do work, ... one hundred percent' However, if we want to find a perhaps more satisfying answer we can pursue a Kantian-like philosophical approach by saying that Ψ produces the frame for the many different quantum mechanical histories that may take place. The experiment then generates one of the mutually exclusive histories which can be described in terms of time.

³ A differential equation can always be formulated as variational principle

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