Transmission time of wave packets through tunneling barriers

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The transmission of wave packets through tunneling barriers is studied in detail by the method of quantum molecular dynamics. The distribution function of the times describing the arrival of a tunneling packet in front of and behind a barrier and the momentum distribution function of the packet are calculated. The behavior of the average coordinate of a packet, the average momentum, and their variances is investigated. It is found that under the barrier a part of the packet is reflected and a Gaussian barrier increases the average momentum of the transmitted packet and its variance in momentum space.

I. INTRODUCTION

The study of tunneling in nanostructures has assumed an important role in the last few years in connection with advances in nanoelectronics. The problem of tunneling of wave packets through a potential barrier arises in many cases, for example, in the study of the action of femtosecond light pulses on coupled wells. This problem is also important because of possible applications of scanning tunneling microscopes irradiated with femtosecond pulses for simultaneously high-spatial and high-temporal resolution study of nanostructures. Other interesting questions are the tunneling time in the ionization of a hydrogen atom

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by ultrashort laser pulses and the tunneling time for tunneling induced by the action of a laser pulse on low-lying nuclear energy levels. In the present paper we investigate the no less interesting question of the time duration of tunneling in nanostructures. The tunneling time is of practical interest in this case because it permits to estimate the response time of semiconductor components. In this connection we shall study the following problem: Let a laser pulse produce a wave packet of an excited electron near a tunneling barrier. The question is: When will the tunneling portion of the packet appear behind the barrier? The arrival of the wave packet can be detected by studying local variations of the optical properties using ultrashort probe pulses.

It is interesting that a number of effects which are absent in the stationary case are observed when a packet passes through a tunneling barrier. The tunneling time of a packet is determined in general not by the reciprocal of the probability of stationary tunneling, but rather it is related with quite complicated processes — a change in the shape and behavior of the packet inside the barrier. Moreover, the transmission time through a barrier depends on the measured quantities, i.e. on the type of experiment.

The investigation of the question of the presence time of a tunneling particle under a barrier started quite a long time ago, and many theoretical and experimental methods for measuring the tunneling time have been proposed. For example, there exist approaches where the peak of the packet or the average coordinate (the “centroid”) is chosen as the observed quantity while the reflection or transmission time is determined by their evolution. However, it has been shown in Refs. and subsequent works that a wave-packet peak incident on a potential barrier does not pass into the peak of the transmitted wave. In Ref. it was shown that on account of dispersion of the wave packet in momentum space the high-energy components reached the barrier before the other components. Since the tunneling probability increases with energy, these components made the main contribution to the transmitted part of the packet. The initial parameters could be chosen in a manner so that the transmitted part of the packet left the barrier long before the main peak, chosen as the observed quantity, appears. This example demonstrates the breakdown of the causality
principle, which is the basis of this method, and therefore it limits the applicability of the method. Moreover, it is difficult to conceive of an experimental method for measuring the arrival time of a packet according to its peak or “centroid.”

There also exists a class of approaches that employ an ensemble of dynamical trajectories to determine the tunneling time. These dynamical trajectories arise as a necessary apparatus of the description in the Feynman and Bohm interpretations of quantum mechanics. When Feynman trajectories were used, the transmission time through a barrier was determined as a path integral over all possible trajectories that start from a prescribed point to the left of the barrier and arrive at a certain time at a point located to the right of the barrier. The integrated function in the path integral contained the product of a classical presence time of a trajectory inside the barrier by a weighting factor \( \exp\{iS(x(t'))/\hbar\} \), where \( S(x(t')) \) is the action related with the trajectory \( x(t') \) under consideration. The calculated times possess real and imaginary parts because of the multiplication by a complex weighting factor, and the question of how these times should be associated to the physically observable quantities, which are always real, arose. To explain the complex times, which also arise in other methods (for example, in the method of “physical clocks” (see below)), Sokolovski and Connor examined so-called direct and indirect measurements. In indirect measurements as in the case of Feynman trajectories method the quantities can be complex.

Approaches employing physical clocks have found quite wide application. Physical clocks are various additional degrees of freedom in the system that make it possible to determine the presence time of a particle in a given region. Three types of clocks have been investigated in theoretical works. Baz’ and Rybachenko used spin precession in a weak uniform magnetic field applied inside a barrier. At first spin precession in a single plane was considered. Then Buttiker and Landauer extended the analysis to three dimensions. During the tunneling a spin of a particle acquires a component along the direction of motion and along the magnetic field. It is obvious that the intensities of the detected components with spin polarization in these two directions will be proportional to the presence time of the particle in the region with the magnetic field, i.e. in the region of the barrier. It turned
out that for a square barrier the tunneling times determined in this manner are identical to the real and imaginary parts of the complex tunneling time introduced via Feynman path integrals. The extension of this method to the case of an arbitrary potential barrier was made in Ref. Buttiker and Landauer considered as physical clocks an oscillating barrier in which the amplitude of the oscillations of the temporal component was much smaller than the barrier height. At low frequencies particles see an effective static barrier, since the transmission time through the barrier is much shorter than the period of the oscillations of the temporal component of the barrier. As the frequency increases, the delayed particles or wave-packet components see a slightly modified potential barrier. Finally, for some frequencies one or several periods of the oscillations influence the tunneling particles. The frequency at which a substantial difference from the adiabatic case corresponding to a stationary barrier appears will determine the reciprocal of the interaction time with the barrier or the transmission time through the barrier. Martin and Landauer chose as physical clocks the oscillating amplitude of the incident wave. For this, a wave function consisting of a superposition of two plane waves with different energies was chosen to the left of the barrier. It is obvious that in this case the wave function to the right of the barrier will also be a superposition of the tunneled parts of the plane waves, which, however, possess a different transmission amplitude, since the amplitude depends on the energy. The transmitted wave function will reproduce the incident wave function if the amplitudes of the tunneled plane waves differ very little; this corresponds to the adiabatic case. The energy difference between the initial plane waves for which the wave function behind the barrier does not reproduce the incident wave function makes it possible to determine the transmission time through a potential barrier. The main advantage of this method is that it is applicable for all types of potentials, but it employs two values of the energy, so that it is not clear to which energy the tunneling time obtained should be ascribed.

Do all clocks give the same measurement result? Of course, no. However, in many cases these results are close to one another or identical. The main advantage of the approaches using physical clocks is that they strive to determine the tunneling time in
terms of possible measurements in physical experiments.

The search for “time operators” and the study of their properties is no less popular. As first noted by Pauli, the main difficulty is that a measurable hermitian time operator for a system Hamiltonian with a bounded spectrum does not exist. Various attempts have been made to construct operators that would describe the necessary properties of physical times. In order that the constructed operator satisfy the correspondence principle, relations from classical mechanics were taken as the basis for the operator construction. However, it is well known that the construction of an operator expression corresponding to a classical quantity is not unique, and its relation with the measurement process requires additional analysis.

In the present work the tunneling time was determined as the difference of the average “arrival” and “presence” times of a wave packet (see Sec. 3) before and after the barrier. The method of quantum molecular dynamics was used to calculate these times and to investigate the dynamics of a tunneling wave packet.

It is well known that molecular dynamics investigates the properties of classical systems in phase space. Therefore it is natural to extend this method to quantum systems in phase space. The evolution of a system in phase space can be described, for example, on the basis of the Wigner formalism of quantum mechanics by the Wigner–Liouville equation. To solve the Wigner–Liouville equation written in integral form it is convenient to rewrite the equation in the form of an iterational series. Each term of this series can be treated as a weighted contribution of a trajectory consisting of segments of classical trajectories separated by finite disturbances of the momentum. In what follows we shall call such a trajectory a quantum trajectory. The statistical ensemble of quantum trajectories makes it possible to calculate the sum of all terms in the series. The Monte Carlo method is used to take account of only the trajectories making the main contribution. In the classical limit the quantum trajectories turn into classical trajectories, and the method of generalized molecular dynamics becomes identical to usual molecular dynamics. The principles of the method are presented in Sec. 2. The expressions for calculation of the distributions of
the arrival and presence times of a wave packet are presented in Sec. 3 on the basis of the Wigner formalism of quantum mechanics. The simulation results are discussed in Sec. 4. The one-dimensional case is considered in this paper, but the method employed makes it possible to perform similar calculations for multidimensional and multiparticle systems, where it has serious advantages from the standpoint of computer time over, for example, the solution of the nonstationary Schrödinger equation.

II. COMPUTATIONAL METHOD

To calculate the quantum-mechanical average of a quantity $A$ for a nonstationary state $|\psi\rangle$ in the Wigner formulation of quantum mechanics it is necessary to calculate an integral in phase space \[29\]

$$A(t) = \langle \psi | \hat{A}(t) | \psi \rangle = \int dq dp A(q, p) W(q, p, t),$$  \hspace{1cm} (1)

where, by definition, the Weyl symbol $A(q, p)$ is introduced for the operator $\hat{A}$ and $W(q, p, t)$ is the Wigner function, which is the Fourier transform of the off-diagonal density-matrix element:

$$A(q, p) = \int d\xi \exp \left( \frac{i p \xi}{\hbar} \right) \langle q + \frac{\xi}{2} | \hat{A} | q - \frac{\xi}{2} \rangle,$$  \hspace{1cm} (2)

$$W(q, p, t) = \frac{1}{2\pi \hbar} \int d\xi \exp \left( -\frac{i p \xi}{\hbar} \right) \psi^* \left( q - \frac{\xi}{2}, t \right) \psi \left( q + \frac{\xi}{2}, t \right).$$  \hspace{1cm} (3)

Differentiating the distribution function with respect to time, substituting it for the time derivative of the function $\psi$ on the right-hand side of the Schrödinger equation, and integrating by parts, we obtain the Wigner–Liouville integrodifferential equation \[30\]

$$\frac{\partial W}{\partial t} + \frac{p}{m} \frac{\partial W}{\partial q} + F(q) \frac{\partial W}{\partial p} = \int_{-\infty}^{\infty} ds W(p - s, q, t) \omega(s, q).$$  \hspace{1cm} (4)

In this equation

$$\omega(s, q) = \frac{2}{\pi \hbar^2} \int dq' V(q - q') \sin \left( \frac{2 sq'}{\hbar} \right) + F(q) \frac{d\delta(s)}{ds}$$  \hspace{1cm} (5)
takes account of the nonlocal contribution of the potential, and \( F(q) = -\partial V(q)/\partial q \) is a classical force. In the classical limit, \( \hbar \to 0 \), Eq. (4) becomes the classical Liouville equation

\[
\frac{\partial W}{\partial t} + \frac{p}{m} \frac{\partial W}{\partial q} = -F(q) \frac{\partial W}{\partial p}. \tag{6}
\]

The equation (4) can be written in an integral form. For this, one introduces the dynamical trajectories \( \{\bar{q}_{\tau}(\tau; p, q, t), \bar{p}_{\tau}(\tau; p, q, t)\} \), \( \tau \in [0, t] \), starting from the point \((p, q)\) at time \( \tau = t \):

\[
d\bar{p}/d\tau = F(\bar{p}(\tau)), \quad \bar{p}_t(t; p, q, t) = p
\]

\[
d\bar{q}/d\tau = \bar{q}(\tau)/m, \quad \bar{q}_t(t; p, q, t) = q \tag{7}
\]

An integral equation is obtained by substituting the right-hand sides of these equations into the Wigner–Liouville equation, whose left-hand side becomes a total differential, and integrating over time one have

\[
W(p, q, t) = W^0(\bar{p}_0, \bar{q}_0) + \int_0^t d\tau \int_{-\infty}^{\infty} ds W(\bar{p}_\tau - s, \bar{q}_\tau, \tau) \omega(s, \bar{q}_\tau). \tag{8}
\]

Here \( W^0(\bar{p}_0, \bar{q}_0) = W(p, q, 0) \) is the Wigner distribution function at zero time. The solution of Eq. (8) can be represented as an iterational series. For this we introduce the notation \( \tilde{W}^{\tau_1} \) for the distribution function, which evolves classically in the interval \([0, \tau_1]\), and the integral operator \( K^{\tau_{i+1}}_{\tau_i} \) describing the evolution between the times \( \tau_i \) and \( \tau_{i+1} \). Now Eq. (8) can be represented in the form

\[
W^t = \tilde{W}^t + K^t_{\tau_1} W^{\tau_1}, \tag{9}
\]

where \( \tilde{W}^t = W^0(\bar{p}_0, \bar{q}_0) \). The corresponding iterational series solving this equation can be written as

\[
W^t = \tilde{W}^t + K^t_{\tau_1} \tilde{W}^{\tau_1} + K^t_{\tau_2} K^{\tau_2}_{\tau_1} \tilde{W}^{\tau_1} + K^t_{\tau_3} K^{\tau_3}_{\tau_2} K^{\tau_2}_{\tau_1} \tilde{W}^{\tau_1} + \ldots \tag{10}
\]

Now, to calculate the quantum-mechanical average (1) it is necessary to calculate a linear functional of the Wigner distribution function

7
\[ A(t) = \int dqdpA(q,p)W(q,p,t) \]
\[ = (A|\bar{W}^t) + (A|K_{\tau_1}^t \bar{W}^{\tau_1}) + (A|K_{\tau_2}^t K_{\tau_1}^{\tau_2} \bar{W}^{\tau_1}) + ... \] (11)

Here the brackets \((... | ...)\) for the functions \(A = A(p,q)\) and \(\bar{W}^t\) or \(K_{\tau_1}^t K_{\tau_{i-1}}^{\tau_i} ... K_{\tau_1}^{\tau_2} \bar{W}^{\tau_1}\) indicate averaging over the entire phase space \(\{p,q\}\).

The first term on the right-hand side of Eq. (10) gives the classically evolving initial distribution \(W^0(\bar{p}_0, \bar{q}_0)\), i.e. the evolution of the distribution function without quantum corrections. However, even this first term of the iterational series describes not classical but rather quantum effects and can contain arbitrary powers of the Planck constant, since a quantum initial state of the system is taken as the initial data for Eq. (10). The rest of the terms in the iterational series describe quantum corrections to evolution. Each term of the iterational series (10) is a multiple integral. This multiple integral can be replaced by an integral sum, and each term of the integral sum can be represented as a contribution of trajectories of a definite topological type. These trajectories consist of segments of classical trajectories — solutions of Eqs. (7) — separated from one another by random perturbations of the momentum.

All terms of the iterational series can be calculated in accordance with the theory of Monte Carlo methods for solving linear integral equations. For this purpose the Monte Carlo scheme was developed, which provides the essential sampling of the iteration series terms (10). This essential sampling also decreases the computer time required to calculate the rest of the integrals appearing in each term of the iterational series. Let us consider the second term of the series (10). This term can be rewritten as

\[ K_{\tau_1}^t \bar{W}^{\tau_1} = \int_0^1 d\tau_1 \int ds_1 \omega(s_1, \bar{q}_1) W^0(\bar{p}_0^1, \bar{q}_0^1) = \]
\[ = \int_0^1 d\tau_1 [B(\bar{q}_2) (1 + Q(\bar{q}_2))] \theta (1 - \tau_2) r(\tau_2) \int ds_1 P(s_1, \bar{q}) \]
\[ \times \left\{ \sigma (s_1, \bar{q}_1^2) tQ(\bar{q}_1^2) \theta (\tau_2 - \tau_1) /C(\bar{q}_1^2) r(\tau_1) \right\} \right\} W^0(\bar{p}_0^1, \bar{q}_0^1), \] (12)

where the substitution of variables \(\tau \rightarrow \tau t\) was made for all terms of the iterational series.
The quantity $r(\tau_1)$ is the probability of choosing a random time $\tau_1$ and $\theta$ is the theta function.

Once the second term of the series (10) is written in the form (12), it can be given the following probabilistic interpretation. We will take advantage of the time-reversibility of the equations of classical dynamics (7) and start the construction of a trajectory at time $\tau = 0$. At time $\tau_1$ for a trajectory representing an arbitrary term in the iterative series a perturbation of the momentum of the trajectory by an amount $s_1$ can occur with probability $C(\hat{q}_1^2)$, and the probability of rejecting a momentum perturbation is $B(\hat{q}_2)$ ($C(\hat{q}_1^2) + B(\hat{q}_2) = 1$). The probability $B$ for rejecting momentum jumps was introduced to make the algorithm more flexible, so that depending on the degree of quantization of the system a transition from quantum to classical trajectories would occur automatically.

Since we are considering a trajectory representing the second term in the iterative series, a perturbation of the momentum at the time $\tau_1$ was accepted. Now it is necessary to choose in the time interval $[\tau_1, 1]$ a random value $\tau_2$ which is the time of the next attempt to perturb the momentum. After a perturbation of the momentum by an amount $s$ we must continue the generation of the trajectory up to the time $\tau_2$ in accordance with Hamilton’s equations. At this time an attempt to perturb the momentum for the second term of the iterative series must be rejected, and we continue the generation of the trajectory up to the time $\tau = 1$. The rejected attempt of the perturbation of the momentum must be taken into account by multiplying the weighting function of the trajectory by a compensating factor, which stands in the braces on the right-hand side of the expression (12). The product of the Weyl symbol of the operator under consideration and the weighting function at different points along the trajectory gives the time dependence of the computed quantities. Averaging over a large ensemble of trajectories of this type gives the contribution of the second term of the iterative series.

Similar expressions but with a large number of intermediate times on classical trajectories when a perturbation of the momentum occurs can also be written for the other terms in the series (10). The number of the term in the iterative series (10), described by the given
trajectory, determines the number of momentum perturbations along the trajectory.

The final expression used to calculate the linear functional (11) is

\[ A(t) = M \{ \alpha (A; T_i) \} = \sum_{p,q} (\Delta p \Delta q) \sum_{i=0}^{\infty} \sum_{j=0}^{i} \sum_{s_j} \alpha (A; T_i) \times P_i \times \Omega (T_i), \]

(13)

where the functions \( P \) and \( \Omega \) are, respectively, the probability of generating a quantum trajectory \( T_i \) and the weighting function of this trajectory.

**III. MEASURED QUANTITIES**

The study of the evolution of a wave packet can be taken as the starting point for studying the temporal aspects of tunneling. The probability of observing a wave packet or particle at an arbitrary point \( X \) is determined by the squared modulus \( |\psi(X, t)|^2 \) of the wave function. In a nonstationary problem this probability depends on the time and determines the characteristic times of the wave-packet dynamics. If an ideal detector (i.e. measurement by the detector does not disturb the wave function), sensitive to the presence of particles, is used in the experiment, then the average presence time measured by the detector at the point \( X \) is

\[ \tilde{t}_X = \frac{\int_0^\infty dt \left| \psi(X, t) \right|^2}{\int_0^\infty dt \left| \psi(X, t) \right|^2}. \]

(14)

A description of these times can be found in Refs. [31]–[32]. The distribution of presence times at the point \( X \) is

\[ \tilde{P}(t_X) = \frac{\left| \psi(X, t) \right|^2}{\int_0^\infty dt \left| \psi(X, t) \right|^2}. \]

(15)

To find the squared wave function \( |\psi(X, t)|^2 \) it is sufficient to calculate a quantum-mechanical average of an operator
\[ \langle \psi(t) | \delta(\hat{q} - X) | \psi(t) \rangle = \int dq \delta(q - X) |\psi(q,t)|^2 = |\psi(X,t)|^2. \]

In the Wigner representation this is equivalent to calculation of the integral

\[ \langle \psi(t) | \delta(\hat{q} - X) | \psi(t) \rangle = \int \int dq dp \delta(q - X) W(q,p,t) = \int dp W(X,p,t). \] (16)

If the point \( X \) is chosen to the right of the barrier, then this integral makes it possible to calculate the squared wave function which has tunneled through the barrier. The distribution of the “presence” times can be rewritten, in accordance with Eq. (16), as

\[ P_X(t) = \frac{|\psi(X,t)|^2}{\int_0^\infty dt |\psi(X,t)|^2} = \frac{\int dp W(X,p,t)}{\int_0^\infty dt \int dp W(X,p,t)}. \] (17)

To determine the average time when the wave packet passes through a detector at the point \( X \) it is necessary to calculate the integral

\[ \langle t(X) \rangle = \int_0^\infty dt t P_X(t), \] (18)

and the average transition time of a packet from the point \( X_i \) to the point \( X_f \) will be

\[ \langle t_{T}(X_i,X_f) \rangle = \langle t(X_f) \rangle - \langle t(X_i) \rangle. \] (19)

If the points \( X_i \) and \( X_f \) are chosen on different sides of the potential barrier, then the expression (19) can be used to estimate the tunneling time.

The main drawback of the definition (17) is that, as a rule, detectors sensitive to a flux density and not a probability density are used in physical experiments. Therefore a different quantity must be considered in order to compare theory and experiment. For this, the distribution of arrival times of a wave packet at a prescribed point in terms of the probability flux density was introduced: \[34\]

\[ P_X(t) = \frac{\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle}{\int_0^\infty dt \langle \psi(t) | \hat{J}(X) | \psi(t) \rangle}. \] (20)

where
\[ \hat{J}(X) = \frac{1}{2} [\hat{p} \delta (\hat{q} - X) + \delta (\hat{q} - X) \hat{p}] \]. \tag{21} 

Of course, the definition (20) is not a real distribution function from probability theory, since this function can assume negative values at some points. Nonetheless the definition (20) will be a distribution function if there is no reverse flux through the point \( X \) or the flux is negligibly small. For this the point \( X \) is chosen at a sufficiently far from the barrier. Measuring the distribution of the arrival times of a packet in front of and beyond the barrier, the transition time through a region much larger than the region of the potential barrier can be calculated. This time is analogous to the asymptotic phase times and, besides the tunneling time and the packet–barrier interaction time, it also contains the transmission time through the region where the potential barrier is zero. These two times cannot be separated. Despite continuing discussions, this tunneling-time problem has still not been finally solved. \[19–24,36,37\]

Another problem concerns the physical implementation of an experiment in which simultaneous detection of a packet in front of and beyond a barrier would not lead to substantial reduction of the wave function. For this reason, ordinarily, a different quantity — the “time delay” — is measured in experiments. \[38–42\] A time delay arises because of the presence of a barrier and is defined as the difference of the average arrival times of the tunneling and free packets:

\[ \Delta \tau_{\text{arrival}}(X) = \langle t_X \rangle^\text{tun} - \langle t_X \rangle^\text{free}. \tag{22} \]

The definition (20) for calculation the average arrival times gives a reasonable estimate of the time delays measured in an experiment.

The distribution of arrival times (20) can be rewritten in the Wigner formulation of quantum mechanics as

\[
P_X(t) = \frac{\iint dqdp J_X(q,p) W(q,p,t)}{\int dt \iint dqdp J_X(q,p) W(q,p,t)}, \tag{23}
\]
where the Weyl symbol of the current operator $\hat{J}(X)$ is
\[
J_X(q,p) = \frac{\hbar}{2} \sin \left( \frac{2p(X - q)}{\hbar} \right) \frac{\partial}{\partial q} \delta(q - X). \tag{24}
\]
Substituting into Eq. (20) the expression (24) and calculating the integral over the variable $q$ by parts we obtain the expression
\[
\begin{align*}
P_X(t) &= \frac{\int dpW(X, p, t)}{\int_0^\infty dt \int dppW(X, p, t)}.
\end{align*}
\tag{25}
\]
Comparing the expressions (17) and (25), it is easy to see that they differ by the fact that the momentum $p$ appears in the numerator and denominator in Eq. (25). This momentum appeared in the last expression because the probability flux density is measured there.

**IV. SIMULATION RESULTS**

We shall examine a series of experiments on the tunneling of an electron with the wave function
\[
\psi(x,0) = \frac{1}{(2\pi\sigma_x)^{1/4}} \exp \left[ -\left( \frac{x-x_0}{2\sigma_x} \right)^2 + ik_0x \right] \tag{26}
\]
through a Gaussian potential barrier
\[
V(x) = V_0 \exp \left[ -\frac{(x-d)^2}{\sigma^2} \right].
\]
The Wigner distribution function (3) corresponding to the initial wave function of the electron can be written as
\[
W(p,q,0) = 2 \exp \left[ -\frac{(p-x_0)^2}{2\sigma^2} \right] \exp \left[ -\frac{2\sigma^2(p-\hbar k_0)^2}{\hbar^2} \right]. \tag{27}
\]
The center $x_0 = \langle \psi(x,0)|\hat{x}|\psi(x,0) \rangle$ of the wave packet at zero time was chosen far enough from the left-hand boundary of the barrier so that the probability density beyond the barrier would be negligibly small compared with the transmission probability $|T|^2$ through the
barrier. Tunneling occurred through a “wide” (σ = 2.5 nm — this parameter of the barrier is characteristic for Al$_x$Ga$_{1-x}$As structures) and a “narrow” (σ = 0.5 nm) Gaussian barrier of height $V_0 = 0.3$ eV centered at $d = 0$. The electron kinetic energy was $E_0 = \hbar^2k_0^2/2m = V_0/2 = 0.15$ eV. We used the system of units where $\hbar = m = V_0 = 1$. Distances were measured in units of the reduced de Broglie wavelength $\lambda = 1/k_0$. In this system of units the parameters of the wave packet and barrier are: $E_0 = 0.5$, $\Delta k = 0.04$ (0.125), $\sigma_x = 1/2\Delta k = 12.5$ (4), $x_0 = -92.5$ (−43), $\sigma = 5$ (2.5 nm), and $\sigma = 1$ (0.5 nm).

A. Evolution of the wave packet

The interaction of a wave packet ($\hbar\Delta k = 0.125$) with a narrow potential barrier ($\sigma = 1$ (0.5 nm)) is shown in Figs. 1a and b. These figures show the probability density $|\psi(x,t)|^2$ (curves 1–5) of reflected (Fig. 1a) and tunneled (Fig. 1b) wave packets at successive times $t = 114 – 239$ fs. The probability density was calculated using Eq. (16), i.e. in terms of the Wigner distribution function. This integral was calculated along quantum and classical trajectories. In the calculation over classical trajectories only the high-energy components of a packet could pass classically above the barrier. This calculation corresponds to the curve 1 in Fig. 1c, and the evolution of the Wigner function can be described only by the first term of the series (10). In the formalism of quantum trajectories the passage of the components of a packet beyond the barrier is associated with random perturbations of the momentum, i.e. with a virtual change in energy. The results of this calculation correspond to the curve 2 in Fig. 1c. Now the quantum corrections introduced by all terms in the series (10) are taken into account in the evolution of the Wigner function.

Of course, the calculation over quantum trajectories also takes account of the high-energy components that pass above the barrier, since they describe the contribution of the first term in the series (10). However, comparing the curves 1 and 2 in Fig. 1c shows that their role is negligible for a narrow barrier and most of the packet passes above the barrier on account of the virtual change in energy, described as random perturbations of the momentum of the
quantum trajectories. A study of tunneling through a wide barrier leads to the opposite conclusion. The curves 1 and 2 in Fig. 1d approximately coincide. This means that most of the packet has passed above the barrier, and the contribution of all terms in the series (10), except for the first term, is negligibly small. To avoid such a situation and to restore the importance of quantum effects, it is necessary to decrease the uncertainty of the momentum of the initial wave packet. In what follows all calculations for a wide barrier are presented for momentum uncertainty $\hbar \Delta k = 0.04$.

B. Average coordinate, average momentum, and their variances

Figure 2a shows the evolution of the average coordinate $\langle \psi(t) | \hat{X} | \psi(t) \rangle$ of the wave packet for calculation according to classical (curve 1) and quantum (curve 2) trajectories. In these two methods for calculation the average coordinate $\bar{X}$ no differences are observed before interaction with the barrier (curves 1 and 2 are coincident). This result can be explained as follows. In the method under discussion the quantum-mechanical properties appear at two points: in the properties of the initial state of a wave packet and in the evolution of the packet. Since the same initial data were chosen for the quantum and classical trajectories, the fact that $\bar{X}$ is the same must be explained by the evolution of the wave packet. Specifically, while the packet moves freely in front of the barrier, it is correctly described by classical trajectories also. In this case the first term in the series (10) is sufficient to describe the evolution of the Wigner function. This result can also be obtained analytically, estimating the right-hand side of the Wigner–Liouville equation (4). For the initial Wigner function (27) and Gaussian barrier which we have chosen it is easy to show that the integral on the right-hand side of Eq. (4) decays exponentially with increasing distance from the barrier. In this case Eq. (4) becomes the classical Liouville equation, whose characteristics are ordinary classical trajectories.

A difference in the behavior of the curves 1 and 2 appears after the packet interacts with a barrier. Now the classical trajectories are no longer characteristics and do not describe
the evolution of the wave packet correctly. In Figs. 2a and b the average coordinate and the momentum of the calculation over quantum trajectories (curve 2) are greater than for classical trajectories (curve 1). This is due to the following circumstances. In the first place, since most of the packet is reflected, as one can see from Fig. 2b the average momentum changes sign after being scattered by the barrier. In the second place, the classical trajectories (curve 1) do not take account of tunneling; they only take account of the negligible above-barrier transmission, arising because of the uncertainty in the momentum of a Gaussian wave packet. At the same time it is obvious that the tunneling part of the packet has positive momentum and moves in the opposite direction relative to the reflected part. Therefore its contribution to \( \bar{X} \) and \( \bar{P} \) has a different sign. This is the explanation of the difference between the curves 1 and 2.

In addition, the motion of the tunneling and reflected packets on different sides of the barrier also explains the more rapid increase of the coordinate variance in the quantum calculation (curve 2, Fig. 2c) as compared with the classical calculation (curve 1), which takes into account only the spreading of the wave packet. The behavior of the packet width on scattering by a barrier is shown in greater detail in the upper left-hand part of Fig. 2c.

The interaction of a packet with the barrier also leads to an interesting behavior of the momentum variance in Fig. 2d. The constant values (curve 1) on the initial and final sections show the momentum variance in the incident and reflected wave packets, i.e. before and after interaction with the barrier. The observed peak is due to the change in the sign of the momentum of the packet and to the fact that different components reach the barrier and are reflected from it at different times. The increase in the momentum variance (curve 2) on the final section is explained by the appearance of a tunneling packet with positive momentum in the quantum computational method, while the total average momentum is negative.
C. Distribution of arrival and presence times. Momentum distribution function

The results of the calculation of the unnormalized presence time distribution (17) at different points in front of the barrier, inside the barrier, and beyond barrier are presented in Figs. 3a and b (curves 1–5). Figures 3a and b show the analogous results for the unnormalized distribution (20) of the arrival times. The curves 1 in Figs. 3a and 4a show the behavior of the probability density and flux, corresponding to the fact that the incident and reflected wave packets pass through the detector at different times. Curve 2 in Fig. 4a shows the behavior of the flux measured at a certain point to the left of barrier center. The tunneling and high-energy components present in the initial packet can classically reach this point. An interesting result is obtained for the probability flux density in Fig. 4b (curves 3–5). The flux measured at barrier center (curve 3) is much less than the flux on the right-hand boundary of the barrier (curve 4) and far to the right of the barrier (curve 5). This means that interference of the tunneling components of the wave packet which move in opposite directions occurs inside the barrier. Some of these components pass completely through the barrier, while others are reflected inside the barrier and do not reach its right-hand boundary. Interference of the reflected and transmitted components leads to the observed decrease in the flux amplitude at barrier center (curve 3) and at the right-hand boundary (compare curves 4 and 5). It is interesting that the investigation of tunneling using classical trajectories in complex time also reveals the similar effect. It was found that transition through a barrier occurs as a series of attempts, many of which are unsuccessful because of reflections in different regions under the barrier.

The comparison of the presence and arrival times distributions in Figs. 3b and 4b shows that they are almost identical. The computed average presence and arrival times (18) are also identical (the difference is less than 1 fs). As we have already stated, the distribution of the arrival times (20) is not a true distribution function and, as one can see from Fig. 4a (curve 2), it is not suitable for calculation of the average arrival time of a packet in front of the barrier. This makes it impossible to calculate the tunneling time as the difference (19)
of the average arrival times of the packet in front of and beyond the barrier. Nonetheless the expression (19) can be used to estimate the tunneling time, if the average presence time (14) is used instead of the average arrival time in front of the barrier. Then the tunneling time through the potential barrier is \( \tau_T (-0.67\sigma, +0.67\sigma) = 12 \) fs, i.e. it is almost equal to the transmission time of a free packet through a similar region \( \tau_T^{\text{class}} (-0.67\sigma, +0.67\sigma) = 13.5 \) fs.

The time delays were measured at the points \( x_4 = 0.67\sigma \) (1.6 nm) and \( x_5 = 5\sigma \) (12 nm) and were found to be \( \Delta \tau_{\text{arrival}} (x_4) = 8 \) fs and \( \Delta \tau_{\text{arrival}} (x_5) \leq 0.5 \) fs. If these measurements were performed even farther to the right of the barrier, then \( \Delta \tau_{\text{arrival}} (x) \) would become negative. Thus an interesting behavior is discerned: Even though the tunneling wave packet is delayed by the barrier \( \Delta \tau_{\text{arrival}} (x_4) = 8 \) fs and passes through the barrier approximately in the same time as a free packet, it appears earlier at a definite distance to the right of the barrier. This effect can be explained by the fact that the transmission probability through a Gaussian barrier increases with energy, so that packet components with a larger momentum have a higher probability of ending up beyond the barrier. These components move more rapidly than a free packet and eventually overtake a free packet. Then the time delays can only be negative. This confirms the momentum distribution function

\[
\frac{\langle \psi (t) | \delta (\hat{p} - p) | \psi (t) \rangle}{\langle \psi (t) | \psi (t) \rangle}, \tag{28}
\]

calculated for narrow (Fig. 5a) and wide (Fig. 5b) barriers, respectively, at times \( t = 218 \) and 385 fs. At these characteristic times the distribution function no longer changes, since the interaction with the barrier has finished. It is evident from Fig. 5 that the average momentum of the tunneled wave packet (curve 2) is greater than the average momentum of the wave packet initially (curve 1). The peak observed in the momentum distribution function (curve 2 in Fig. 5a) is due to the packet components that had a quite large momentum and passed above the barrier. It is evident that tunneling through a narrow potential barrier leads to a larger variance of the distribution function, while tunneling through a wide barrier substantially shifts the center of the distribution in the direction of large momenta (curve 2 in Fig. 5b).
V. CONCLUSIONS

The quantum generalization of classical molecular dynamics was used to solve the Wigner–Liouville integral equation in the Wigner formulation of quantum mechanics. The method discussed for solving this equation does not require a large increase of computer time and makes it possible to avoid the computational difficulties that arise when solving the nonstationary Schrödinger equation.

This approach was used to solve the nonstationary problem of tunneling of a finite wave packet, i.e. a problem in which it is important to take account of exponentially small quantum effects. The evolution of a wave packet, the behavior of the average and the variances of the coordinate and momentum and the distributions of the presence and arrival times for the wave packet at different positions of an ideal detector were analyzed. The following results were obtained: 1) The tunneling time through a potential barrier is approximately of the same order of magnitude as the transmission time of a free wave packet over a similar distance; 2) the tunneling wave packet is delayed by the potential barrier, so that after the barrier the time delay should be positive; 3) measurement of negative time delays is possible only at sufficiently large distances from the barrier and is associated with a shift of the momentum distribution function; 4) a Gaussian barrier transmits mainly the high-energy components of a packet, interaction with the barrier shifts the center of the momentum distribution function so that the average momentum of the transmitted packet is larger than the initial average momentum of the entire packet; 5) tunneling through a narrow potential barrier leads to a larger variance of the momenta of the tunneled components, while tunneling through a wide barrier leads to an appreciable increase in the average momentum; and, 6) the computational results for the probability flux density showed that the tunneling wave packet does not pass completely through the barrier, a portion of the packet under the barrier is reflected and does not reach its right boundary.

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FIG. 1. Probability density $|\psi_{ref}(x,t)|^2$ (a) of the reflected wave packet (a) and probability density $|\psi_{tr}(x,t)|^2$ (b) of the tunneled wave packet (b) at successive times $t_i = 144 - 239$ fs (curves 1–5) with $\Delta k = 0.125$ and barrier “thickness” $\sigma = 1$ (0.5 nm); $|\psi_{tr}(x,t)|^2$ (c, d) at time $t = 187$ fs, $\Delta k = 0.125$ with barrier thickness $\sigma = 1$ (0.5 nm) (c) and $\sigma = 5$ (2.5 nm) (d): curve 1 — calculation using classical trajectories, curve 2 — calculation using quantum trajectories.

FIG. 2. Average coordinate $\bar{X}$ (a), average momentum $\bar{P}$ (b), coordinate variance $\langle (X - \bar{X})^2 \rangle$ (c) and momentum variance $\langle (P - \bar{P})^2 \rangle$ (d): 1 — calculation using classical trajectories; 2 — calculation using quantum trajectories.

FIG. 3. Probability density or unnormalized distributions of the presence times (17): a — $|\psi(x_i, t)|^2$ at the point $x_1 = -5\sigma$ (curve 1); b — $|\psi(x_i, t)|^2$ at the point $x_2 = -0.67\sigma$ (curve 2), at $x_4 = 0.67\sigma$ (curve 4), and $x_5 = 5\sigma$ (curve 5); the center of the barrier is located at $x_3 = 0$, the barrier “thickness” $\sigma = 5$ (2.5 nm).

FIG. 4. Flux of probability density or unnormalized distributions of the arrival times (20): a — $J(x_i, t)$ at the points $x_1 = -5\sigma$ (curve 1) and point $x_2 = -0.67\sigma$ (curve 2); b — $J(x_i, t)$ at $x_3 = 0$ (curve 3), $x_4 = 0.67\sigma$ (curve 4), and $x_5 = 5\sigma$ (curve 5); the center of the barrier is located at $x_3 = 0$, the barrier “thickness” $\sigma = 5$ (2.5 nm).

FIG. 5. Momentum distribution in a packet at $t = 0$ (curve 1) and in a packet transmitted through a potential barrier (curve 2): a — $\Delta k = 0.125$, barrier “thickness” $\sigma = 1$ (0.5 nm), $t = 218$ fs; b — $\Delta k = 0.04$, barrier “thickness” $\sigma = 5$ (2.5 nm), $t = 385$ fs.
\[ 10^{-2} \psi_{\text{ref}}^2(x,t) \]

\[ 10^{-4} \psi_{\text{tr}}^2(x,t) \]

\[ 10^{-5} \psi^2(x,t) \]

\[ 10^{-4} \psi^2(x,t) \]
$10^{-4} F(p,t)$