Simulation of wave packet tunneling of interacting identical particles

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We demonstrate a different method of simulation of nonstationary quantum processes, considering the tunneling of two *interacting identical particles*, represented by wave packets. The used method of quantum molecular dynamics (WMD) is based on the Wigner representation of quantum mechanics. In the context of this method ensembles of classical trajectories are used to solve quantum Wigner-Liouville equation. These classical trajectories obey Hamiltonian-like equations, where the effective potential consists of the usual classical term and the quantum term, which depends on the Wigner function and its derivatives. The quantum term is calculated using local distribution of trajectories in phase space, therefore, classical trajectories are not independent, contrary to classical molecular dynamics. The developed WMD method takes into account the influence of exchange and interaction between particles. The role of direct and exchange interactions in tunneling is analyzed. The tunneling times for interacting particles are calculated.

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I. INTRODUCTION

A quantum molecular dynamics method (QMD) was recently successfully applied to a single wave packet tunneling [1,2]. This method is based on the Wigner representation [3,4] of quantum mechanics (further refered to as WMD—the Wigner representation based MD). In the present paper, we further develop this method and consider its application to the *many-body* problem of nonstationary tunneling of interacting identical particles. Nonstationary tunneling is a problem of great interest in particular in connection with developments of nanoelectronics. Until now role of interaction and exchange in nonstationary tunneling is not clear. To clear up this question is one of the aims of this paper. In this connection we consider the tunneling of two identical charged particles, represented by wave packets.

In the Wigner representation of quantum mechanics the state of the system is described by the Wigner function, which obeys Wigner-Liouville equation. The equation can be rewritten in the form analogous to classical Liouville equation for classical distribution function. This analogy is the basis of WMD: the ensembles of classical trajectories are used to solve numerically quantum Wigner-Liouville equation. The trajectories can be determined by equations of motion analogous to classical ones. The used modification as against classical equations of motion for the trajectories is an addition of extra quantum term in the expression for the force [1]. This quantum term is expressed through the local approximation of the Wigner function. For the approximation of the Wigner function we used multidimensional Gauss distribution with the parameters determined through the local moments of the ensemble of classical trajectories.

In the present paper, the wave packets moving in double-well potential were considered. The interparticle interactions are fully taken into account. The wave packets are initially placed in the same well on one side of the barrier. We analyze the long-time evolution of wave packets (for time scales corresponding to many oscillation periods in the well) and consider the probability to detect a particle in the first and in the second well, respectively. Besides we study the short-time evolution (characteristic times of interaction of wave packet with the barrier) and regard tunneling times.

Tunneling time is one of the most important features of nonstationary tunneling. However, the theoretical definition of this quantity is nontrivial. There exist a lot of definitions of tunneling time [5–16]. We use two common approaches to determine tunneling time, namely *presence* and *arrival* times (see Refs. [2,17] and references therein).

First, one can consider the detector that reacts to the presence of particles at some point x_0. The values measured by this detector in a set of experiments on, e.g., particles transmission through a barrier, would depend on particle density $\rho(x_0,t)$ at time t and the mean *presence time* of a particle at point x_0 would be given by

$$\langle t_p(x_0)\rangle = \int_0^\infty dt t\rho(x_0,t) \Big/ \int_0^\infty dt\rho(x_0,t). \tag{1}$$

For two points x_a and x_b one can consider the average time of transmission

$$\langle t_T(x_a,x_b)\rangle = \langle t_p(x_b)\rangle - \langle t_p(x_a)\rangle. \tag{2}$$

If the points are located on the different sides of a barrier, then expression (2) is an approximation for tunneling time.

Second, the detector that measures flux density can be used. For this set of experiments one needs to define another quantity—*arrival time*. In this case the flux density operator must be considered

$$\hat{J}(x_0) = \frac{1}{2}[\hat{p}\,\delta(\hat{q}-x_0) + \delta(\hat{q}-x_0)\hat{p}], \tag{3}$$

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$$J(x_0,t)=\frac{\langle\psi(t)|\hat{J}(x_0)|\psi(t)\rangle}{\int_0^\infty dt\langle\psi(t)|\hat{J}(x_0)|\psi(t)\rangle}, \tag{4}$$

and the *arrival time* at point x_0 can be defined as

$$\langle t_a(x_0)\rangle=\int_0^\infty dttJ(x_0,t)\Big/\int_0^\infty dtJ(x_0,t). \tag{5}$$

We stress that $J(x_0,t)$ can be negative due to the opposite flux. Therefore Eq. (4) can be used directly as a probability distribution of *arrival times* only if the opposite flux is negligible. This requirement can be fulfilled if the detector is located far from the barrier. Then Eq. (4) determines the quasidistribution of the *arrival times*. But in this case one cannot distinguish the time of transmission under the barrier and time of passing the region between the barrier and the detector—still unresolved problem of time measurement in quantum mechanics (see, e.g., Ref. [11]). We use the *presence* and *arrival* times from all variety of possible definitions of tunneling time because their measurement in the framework of WMD is relatively simple and, what is more important, the physical meaning of the Eqs. (1) and (4) is transparent and connected with the use of pointlike detectors in the set of the experiments on particles transmission.

By changing the strength of interaction between the particles, we investigate the influence of interaction on tunneling. We also consider the role of exchange. We found that the exchange is important if the interaction is weak. In this case exchange has a substantial influence on both the tunneling probability and tunneling time. With the increase of interaction initial system energy with fixed initial wave functions becomes greater. This leads to decrease of tunneling times, the role of exchange gets smaller and tunneling becomes insignificant in comparison with passing above the barrier. Our investigation had shown that WMD is an advantageous method, which can be used to solve the many-body problems without enormous computer resources, and which allows one to take into account such essentially quantum features as exchange and tunneling.

We present here the investigation of the two-particle problem, but the generalization of WMD for the case of more particles is straightforward. The advantage of using the Wigner representation in comparison with direct numerical solution of Schrödinger equation is as follows. Using WMD, one does not need to store large data arrays as with the grid methods. The basic algorithm of WMD is very close to that of the common molecular dynamics (MD), the distinction is only in the calculation of the force and in the probability interpretation of initial conditions. During about 40 y the classical MD methods were sufficiently improved and all advantageous numerical schemes can be simply implemented in WMD. The modern MD techniques allow one to operate with thousands of particles and the same can be in principle achieved by means of WMD, but in the last case one can consider quantum particles.

We describe the simulation method and the physical model in Secs. II and III, respectively. Results are presented and discussed in Sec. IV. Main conclusions are summarized in Sec. V.

II. SIMULATION METHOD

A. Equations of motion for Wigner trajectories

The Wigner representation of quantum mechanics is one of the representations that uses quantum distribution function in phase space. The Wigner function $F^W(q,p,t)$ describes time evolution of the system and average values of physical quantities are calculated with the help of scalar functions, Weyl symbols $A^W(q,p)$,

$$\langle A\rangle=\int dp\int dqA^W(q,p)\,F^W(q,p,t). \tag{6}$$

It can be shown [3,18], that Weyl symbols are expressed through corresponding operators $A(\hat{q},\hat{p})$ as follows:

$$A^W(q,p)=\frac{\hbar}{2\pi}\int d\xi d\eta Tr[A(\hat{q},\hat{p})e^{i\xi\hat{q}+i\eta\hat{p}}]e^{-i\xi q-i\eta p}. \tag{7}$$

The Wigner function is real and satisfies the following rules:

$$\int dpF^W(q,p,t)=\langle q|\hat{\rho}|q\rangle, \tag{8}$$

$$\int dqF^W(q,p,t)=\langle p|\hat{\rho}|p\rangle, \tag{9}$$

here $\hat{\rho}$ is the density operator. The Wigner function $F^W(q,p,t)$ is also not non-negative. There are non-negative quantum distribution functions, for example Husimi function [19], but its evolution equation is usually more complicated as against the Wigner function.

If one considers the Hamiltonian $H=p^2/(2m)+V(q)$, then the evolution equation for the Wigner-function (Wigner-Liouville equation) has the form [3,18]:

$$\frac{\partial F^W}{\partial t}+\frac{p}{m}\frac{\partial F^W}{\partial q}=\sum_{n=0}^{\infty}\frac{(\hbar/2i)^{2n}}{(2n+1)!}\frac{\partial^{2n+1}V}{\partial q^{2n+1}}\frac{\partial^{2n+1}F^W}{\partial p^{2n+1}}. \tag{10}$$

If the potential does not have the terms with more than the second power of q, then Eq. (10) has the same form as for a classical distribution function f,

$$\frac{\partial f}{\partial t}+\frac{p}{m}\frac{\partial f}{\partial q}=\frac{\partial V}{\partial q}\frac{\partial f}{\partial p}. \tag{11}$$

The Wigner function must satisfy a number of conditions [18], therefore, initial function $F^W(q,p,t=0)$ cannot be chosen arbitrarily. Even if $F^W(q,p,t)$ satisfies classical equation (11) (for specific potential V) it describes quantum system adequately because all quantum corrections (all powers of $\hbar$)

are held in the initial Wigner function $F^W(q,p,t=0)$. For example, the uncertainty principle holds.

One can rewrite Eq. (10) in the form analogous to Eq. (11) as

$$\frac{\partial F^W}{\partial t}+\frac{p}{m}\frac{\partial F^W}{\partial q}=\frac{\partial V_{eff}}{\partial q}\frac{\partial F^W}{\partial p}, \tag{12}$$

where a new effective potential V_{eff} is introduced

$$\frac{\partial V_{eff}}{\partial q}\frac{\partial F^W}{\partial p}=\frac{\partial V}{\partial q}\frac{\partial F^W}{\partial p}-\frac{\hbar^2}{24}\frac{\partial^3 V}{\partial q^3}\frac{\partial^3 F^W}{\partial p^3}+\cdots. \tag{13}$$

The characteristics of Eq. (11) obey the equations coinciding with classical equations of motion

$$\frac{\partial q}{\partial t}=\frac{p}{m};\quad \frac{\partial p}{\partial t}=-\frac{\partial V(q,p,t)}{\partial q}. \tag{14}$$

From Eq. (12) one can obtain the modified equations of motion for Wigner trajectories [3]

$$\frac{\partial q}{\partial t}=\frac{p}{m};\quad \frac{\partial p}{\partial t}=-\frac{\partial V_{eff}(q,p,t)}{\partial q}. \tag{15}$$

To get information about time evolution of the system, we numerically solve Eqs. (15) for the ensemble of trajectories. To simplify our calculation of V_{eff}, Eq. (13), for the problem of interest we choose the analytical form of the external potential and the interaction between particles to contain only the 2nd and the 4th powers of coordinates. In this case only the first two terms in the right-hand side of Eq. (10) are nonzero. As a result the total force is a sum of the usual classical force and the quantum force F_k^{quant}, which is infinite series in general, but in our case contains only one term:

$$F_k^{quant}=\left(\frac{\hbar^2}{24}\right)\frac{\partial^3 V}{\partial q_i\partial q_l\partial q_k}\frac{\partial^2 F^W}{\partial p_i\partial p_l}\frac{1}{F^W}, \tag{16}$$

where index k is the kth component of the force vector (there are $N\times d$ such components, N is the number of particles and d is spatial dimensionality), repetition of indexes indicates the summation.

As one can note the quantum force depends on the Wigner function, which is unknown. To overcome this problem we use a local approximation for the Wigner function in the vicinity of phase space point x_a by Gaussian [1]:

$$F^W(q,p,t)=F_0^W\exp(-\{[x-x_a(t)]A_a(t)[x-x_a(t)] + b_a(t)[x-x_a(t)]\}), \tag{17}$$

where $x=\binom{q}{p}$ is vector of all particle coordinates and momenta, matrix A_a (in our case of dimensionality 4×4) and vector b_a (with dimensions 4×1) are obtained from the local moments of the ensemble of trajectories in the vicinity of point x_a.

B. Consideration of exchange

Exchange effects in this method can be in some cases considered simply by using special initial conditions. Consider the system with the wave function $\Psi(x,t)$. One can obtain the Wigner function as [3]

$$F^W(q,p,t)=\frac{1}{(2\pi\hbar)^N}\int d\xi e^{ip\xi/\hbar}\Psi^*\left(q+\frac{\xi}{2},t\right)\Psi\left(q-\frac{\xi}{2},t\right). \tag{18}$$

If the system consists of either bosons or fermions, wave functions must be symmetrical or antisymmetrical. If we regard the case when the Hamiltonian does not depend on spins of the particles, then we can consider only the coordinate part of wave function. Depending on the overall spin the coordinate part of wave function is either antisymmetrical or symmetrical. For example, wave function of the following form is symmetrical (antisymmetrical):

$$|\Psi(1,2)\rangle=\frac{|\phi_1(1)\rangle|\phi_2(2)\rangle\pm|\phi_1(2)\rangle|\phi_2(1)\rangle}{\sqrt{2(1\pm|\langle\phi_1|\phi_2\rangle|^2)}}, \tag{19}$$

where (i) means the dependence on variables of the ith particle. We use this wave function for the initial system state with $|\phi_k\rangle$ of the form of a Gaussian wave packet. As a result the Wigner function takes the form

$$\begin{aligned}F^W(q_1,q_2,p_1,p_2)=&\frac{1}{2(1\pm|\langle\phi_1|\phi_2\rangle|^2)(2\pi\hbar)^2}\\&\times\int dx_1dx_2e^{i/\hbar(p_1x_1+p_2x_2)}\\&\times\left[\phi_1^*\left(q_1+\frac{x_1}{2}\right)\phi_2^*\left(q_2+\frac{x_2}{2}\right)\right.\\&\left.\pm\phi_1^*\left(q_2+\frac{x_2}{2}\right)\phi_2^*\left(q_1+\frac{x_1}{2}\right)\right]\\&\times\left[\phi_1\left(q_1-\frac{x_1}{2}\right)\phi_2\left(q_2-\frac{x_2}{2}\right)\right.\\&\left.\pm\phi_1\left(q_2-\frac{x_2}{2}\right)\phi_2\left(q_1-\frac{x_1}{2}\right)\right]\end{aligned} \tag{20}$$

and can be rewritten as

$$\begin{aligned}F^W(q_1,q_2,p_1,p_2)=&\frac{1}{2(1\pm|\langle\phi_1|\phi_2\rangle|^2)}\\&\times[W_1(q_1,p_1)\,W_2(q_2,p_2)\\&+W_1(q_2,p_2)\,W_2(q_1,p_1)\\&\pm U_{12}(q_2,p_2)\,U_{21}(q_1,p_1)\\&\pm U_{12}(q_1,p_1)U_{21}(q_2,p_2)],\end{aligned} \tag{21}$$

where

$$W_k(q,p)=\frac{1}{(2\pi\hbar)}\int d\xi e^{ip\xi/\hbar}\phi_k^*\left(q+\frac{\xi}{2}\right)\phi_k\left(q-\frac{\xi}{2}\right) \tag{22}$$

and

$$U_{kj}(q,p)=\frac{1}{(2\pi\hbar)}\int dx e^{ipx/\hbar}\phi_k^*\left(q+\frac{x}{2}\right)\phi_j\left(q-\frac{x}{2}\right). \tag{23}$$

In coordinate space the initial state Eq. (19) is described by wave function of the following form:

$$\phi_k(x)=\frac{1}{(2\pi\hbar)}\exp\left(-\frac{(x-x_{k0})^2}{4\sigma_k^2}+\frac{ip_{k0}(x-x_{k0})}{\hbar}\right). \tag{24}$$

For this case,

$$W_k(q,p)=\frac{1}{\pi\hbar}\exp\left(-\frac{(q-x_{k0})^2}{2\sigma_k^2}-\frac{(p-p_{k0})^2}{2[\hbar/(2\sigma_k)]^2}\right) \tag{25}$$

and the term with U_{kj} in Eq. (21) is proportional to $\exp[-A(x_{10}-x_{20})^2]$, where A is a positive constant. If $\sigma_1=\sigma_2=\sigma$, then $A=1/(2\sigma^2)$. For $|x_{10}-x_{20}|\gg\sigma$ this term can be neglected and one gets

$$F^W(q_1,q_2,p_1,p_2)=\frac{1}{2(1\pm|\langle\phi_1|\phi_2\rangle|^2)}\times[W_1(q_1,p_1)W_2(q_2,p_2)+W_1(q_2,p_2)W_2(q_1,p_1)]. \tag{26}$$

We emphasize that this approximation is used only at the initial time moment. Further the dynamical equations are solved formally exactly.

In the considered problem two particles move in the potential

$$U(x)=\alpha(-x^2+\gamma x^4),\quad \alpha,\gamma>0. \tag{27}$$

The potential of interparticle interaction is $V_{int}=\{\text{const}-\beta r^2\}$, if $\{\text{const}-\beta r^2\}>0$, and $=0$, otherwise. If we disregard discontinuity in the interparticle potential then the distinction from harmonic oscillator is the 4th power of x and one has only one quantum term in the force Eq. (16). Using the classical trajectories and the Gaussian approximation for the Wigner function one can solve the Wigner-Liouville equation exactly. The distinction of the adopted approximation from the case of distinguishable particles is that now initial positions of two particles may be in the Gaussian centered at x_{10} or at x_{20}. In this way we regard the symmetry in exchange of particles and obtain the picture of their motion.

C. Algorithm and calculation of average values

Our simulation algorithm is the following. First, the initial coordinates and momenta of every trajectory in the ensemble are distributed according to the chosen parameters of the wave packets (mean coordinate, momentum and their variances). Second, we calculate the quantum force and solve numerically equations of motion.

For the jth trajectory at time t with coordinates and momenta $\{q^{(j)}(t),\ p^{(j)}(t)\}$ one has to compute the local moments of the ensemble of trajectories in the vicinity of the point $\{q^{(j)}(t),\ p^{(j)}(t)\}$ (point x_a), using the weight function which rapidly goes to zero with the increase of distance to this point (uncertainty principle must hold) [1]. The approximation (17) is the many-dimensional Gauss distribution of the vector $x=\binom{q}{p}$. Matrix $A_a=\frac{1}{2}C_a^{-1}$, C_a^{-1} is the inverse matrix of covariance C_a, and vector $b_a=-2A_af_a$, where f_a is the vector of averages. If one calculates $\langle q_i\rangle$, $\langle p_i\rangle$, $\langle q_iq_k\rangle$, $\langle p_ip_k\rangle$, $\langle q_ip_k\rangle$, $i,k=1,\ldots,Nd$, one obtains

$$f_a=\left\langle\binom{q-q_a}{p-p_a}\right\rangle$$

and symmetrical matrix C_a with elements

$$C_a(l,m)=\langle(q_l-q_l^{(a)})(q_m-q_m^{(a)})\rangle-\langle q_l-q_l^{(a)}\rangle\langle q_m-q_m^{(a)}\rangle \tag{28}$$

for $l=1,\ldots,Nd$, $m=1,\ldots,l$,

$$C_a(l,m)=\langle(p_{l-Nd}-p_{l-Nd}^{(a)})(p_{m-Nd}-p_{m-Nd}^{(a)})\rangle-\langle(p_{l-Nd}-p_{l-Nd}^{(a)})\rangle\langle(p_{m-Nd}-p_{m-Nd}^{(a)})\rangle \tag{29}$$

for $l=Nd+1,\ldots,2Nd$, $m=Nd+1,\ldots,l$, and

$$C_a(l,m)=\langle(q_l-q_l^{(a)})(p_{m-Nd}-p_{m-Nd}^{(a)})\rangle-\langle(q_l-q_l^{(a)})\rangle\langle(p_{m-Nd}-p_{m-Nd}^{(a)})\rangle \tag{30}$$

for $l=1,\ldots,Nd$, $m=Nd+1,\ldots,2Nd$. Here q_i and p_i are the ith components of vectors of all coordinates q and momenta p; $\langle\cdots\rangle$ means the averaging over all trajectories with the weight function, which rapidly approaches zero with growing distance to x_a in phase space. After that, one can calculate the inverse matrix for C_a and get A_a and b_a.

At every time t for the jth trajectory with coordinates $q^{(j)}(t)$ and momenta $p^{(j)}(t)$ matrix $A^{(j)}(t)$ and vector $b^{(j)}(t)$ are calculated, therefore the quantum force for the jth trajectory is known. Further, one has to solve Eqs. (15), for example by Runge-Kutt and Adams methods.

To calculate average values we use the following approximation for the Wigner function:

$$F^W(q,p,t)=\frac{1}{K}\sum_{k=1}^{K}\delta\{q-q_k(t)\}\delta\{p-p_k(t)\}. \tag{31}$$

The summation is over all trajectories in the ensemble. One of the interesting values characterizing tunneling is the reaction probability:

$$R(q_a,t)=\frac{1}{N}\int_{q_a}^{\infty}\rho(x,t)dx, \tag{32}$$

where the lower limit of integration is the point of the largest height of the barrier, $\rho(x,t)$ is the particle density at point x

and N is the particle number. This quantity shows what part of wave packets are currently in the right well.

Another important value is *tunneling time*. In this paper, to determine *tunneling time* we use two methods: *presence* and *arrival* times. In the Wigner formalism these quantities are expressed through the following integrals [see Eqs. (1) and (4)]:

$$|\psi(x_0,t)|^2=\int dpF^W(x_0,p,t) \tag{33}$$

and

$$J(x_0,t)=\frac{\int dppF^W(x_0,p,t)}{\int_0^\infty dt\int dppF^W(x_0,p,t)}, \tag{34}$$

the Weyl symbol for flux operator has the form

$$J_{x_0}=\frac{\hbar}{2}\sin\left(\frac{2p(x_0-q)}{\hbar}\right)\frac{\partial}{\partial q}\delta(q-x_0).$$

III. MODEL PROBLEM

A. Hamiltonian

We consider the following model problem. Two particles move in one-dimensional space (e.g., in a quantum wire). The Hamiltonian of the system reads

$$H=\sum_{i=1}^{2}\left(\frac{p_i^2}{2m}+\alpha(-q_i^2+\gamma q_i^4)\right)+U(|q_1-q_2|), \tag{35}$$

where q_1,q_2,p_1,p_2 are particle coordinates and momenta, U is interaction energy. We use the system of units with $\{\hbar=m=\alpha=1\}$, $l_0=\hbar^{1/2}/(m\alpha)^{1/4}$ is the unit of length, $E_0=\hbar(\alpha/m)^{1/2}$ is the unit of energy, and the unit of time is $t_0=(m/\alpha)^{1/2}$.

Initially particles are placed in the left well, their wave functions have the form of the Gaussian wave packets. Initial mean momenta and coordinates of wave packets and their variance in momentum and coordinate spaces are chosen to make the transmission above the barrier as lower as possible and the overlapping of the wave packets is negligible. Particles move in the direction of the barrier. This model roughly describes nonstationary tunneling of two electrons through the potential barrier in a quantum wire or tunneling between two quantum wells. This can be realized, for example, when with the help of laser pulses one prepares the state of two electrons in the form of two wave packets in nanostructure and study the system evolution in time.

In the used system of units the Hamiltonian is

$$H=\sum_{i=1}^{2}\left(\frac{p_i^2}{2}-q_i^2+\gamma q_i^4\right)+U(|q_1-q_2|). \tag{36}$$

The Coulomb potential Q_1Q_2/r describes the interaction between particles. The problem becomes one dimensional if characteristic energies of the transverse quantization are much larger than the energies of the longitudinal motion. If it is valid then adiabatic approximation applies and the problem is really one dimensional. The interparticle interaction then reduces to

$$U(r)=\lambda\frac{2}{a^2}\int_0^\infty\frac{e^{-\rho^2/a^2}\rho}{\sqrt{r^2+\rho^2}}d\rho=\lambda\frac{\sqrt{\pi}}{a}e^{r^2/a^2}\left[1-erf\left(\frac{r}{a}\right)\right], \tag{37}$$

where we performed integration over the particle wave functions of transverse quantization, with a being the characteristic width of the quantum wire. The interaction parameter $\lambda=Q_1Q_2m^{3/4}/(\hbar^{3/2}\alpha^{1/4})$ is the ratio of characteristic Coulomb energy and energy of oscillator.

In our model problem we substitute the potential Eq. (37) for model quadratic one, just to avoid uncertainties related with the calculation of the quantum force, Eq. (16), and demonstrate the method for the case of exchange. Parameters of this potential are chosen to make it as close as possible to expression (37):

$$U(r)=\begin{cases}\dfrac{\lambda}{a}(\sqrt{\pi}-0.05(r/a)^2) & \text{if } r<a(20\sqrt{\pi})^{1/2}\\ 0 & \text{if } r\geqslant a(20\sqrt{\pi})^{1/2}.\end{cases} \tag{38}$$

B. Initial parameters

We analyze the system described by Hamiltonian (36) for two cases—with and without exchange, respectively. The main quantity analyzed is reaction probability (32). Its largest value is unity when both particles are entirely in the right well. The reaction probability clearly shows the distribution of particles between two wells and characterize their time evolution.

Consider two cases, we call them *zeroth order WMD* (Wigner molecular dynamics in zeroth approximation) and *nth order WMD* (further simply refered to as the *quantum case*). For *zeroth order WMD* the quantum term in force Eq. (16) is neglected and evolution of the trajectories is determined by classical Hamiltonian equations. Therefore, only passing above the barrier is taken into account. This approximation is not purely classical, because the initial distribution is the same as for the *quantum case*: $|F^W(q,p,t=0)|$ can contain arbitrary powers of $\hbar$. As a result we have a classical evolution of the quantum distribution function, therefore, we call this case *zeroth order WMD*, not the classical MD. The difference between *zeroth order* and *nth order* is that in the latter case the quantum term in the force is regarded.

The initial distribution in coordinate space has the form of two Gaussian wave packets, which practically do not overlap. In the *quantum case* one can consider two situations. First, we can consider the problem neglecting exchange (i.e., regard the distinguishable particles). Second, we can take exchange into account. In the first case the initial wave function is a product of one-particle wave functions, and the Wigner function has the form $F^W(q_1,q_2,p_1,p_2)=W_1(q_1,p_1)W_2(q_2,p_2)$ [compare with Eq. (26)]. This

means that one of the Gaussians corresponds to the first particle and another to the second one. For such initial distribution function exchange effects cannot arise and we will call this situation the *quantum case* without exchange.

In the second situation the particles are identical and the initial wave function is symmetrical (or antisymmetrical). Now the Wigner function has the form Eq. (26). Both Gaussians may correspond either to the first or to the second particle. The initial coordinates and momenta of some trajectory, $\{x_1,x_2,y_1,y_2\}$, are chosen with the probability $|F^W(q_1,q_2,p_1,p_2)|$ of the configuration $\{q_1=x_2,q_2=x_1,p_1=y_2,p_2=y_1\}$. If the wave packets are initially close to each other, the terms U_{kj} in Eq. (21) do not vanish and the procedure of setting the initial coordinates and momenta becomes more complicated.

For both *quantum cases* (without and with exchange) dynamical correlations are taken into account due to solution of the Wigner-Liouville equation. Statistical correlations are not regarded in the *quantum case* without exchange but they are allowed in the case with exchange. In this sense two situations resemble Hartree and Hartree-Fock approximations, respectively. Note that we *do not use* mean-field approximation, the similarity must be regarded only in the meaning formulated above.

For the *zeroth order* WMD both ways of setting the initial coordinates and momenta for trajectories can be applied, but it was found that the result is practically independent on it. We use the following parameters: initial coordinates and momenta for the Gaussians are $x_1(0)=-140$, $p_1(0)=45$, and $x_2(0)=-310$, $p_2(0)=90$, dispersions in coordinate space (σ_x for the Gauss function $\exp[-x^2/(2\sigma_x^2)]$) are the same for both wave packets and equal to 20, in momentum space $\sigma_p=\hbar/(2\sigma_x)=0.025$. Parameters of the external potential are $\alpha=1,\gamma=1.25\times10^{-8}$.

One of our aims is to investigate the influence of interaction on tunneling. We change the interaction parameter λ, starting with $\lambda=0$ (no interaction). Effective charge of electrons or holes in nanostructures can be controlled by changing the permittivity, but not in very wide range. Here we would like to draw the attention to the fact that due to the use of special system of units, $\hbar=m=\alpha=1$, the region of variation of the dimensionless interaction parameter can be pretty wide. Actually, in this unit system the parameters of external potential are used. Therefore, we can vary the interaction λ by changing the external potential. This change leads to scaling of the units of length, time, energy, and so on.

IV. RESULTS AND DISCUSSION

The definition of tunneling is usually given for one particle. We analyze the motion of two particles and as the *under barrier transmission* is of interest for us, the *total* initial energy of the system is set about 0.99 of the height of the barrier. So even if one of particles borrows all the energy the latter is still lower than the height of the barrier. We deal with the wave packets, therefore, though the mean energy per particle is lower than the barrier height, the transmission above the barrier is still possible due to the dispersion in the momentum space. The comparison between *zeroth* and *nth order* WMD allows us to estimate the transmission under the barrier. The state of the particles is considered as an entangled unified whole and the ''transmission under the barrier'' means the transmission of at least one of the particles.

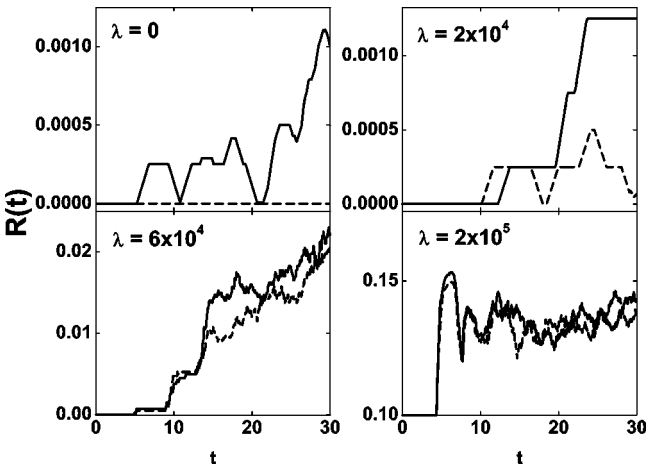

FIG. 1. Time dependence of the reaction probability $R(t)$, for the *zeroth order* WMD (dashed lines) and *quantum case* (solid lines). Interaction strengths are $\lambda=0,2\times10^4,6\times10^4,2\times10^5$. Maximum value of the reaction probability $R(t)=1$, time t is in the units $t_0=(m/\alpha)^{1/2}$, α is the potential parameter, Eq. (35).

A. Reaction probabilities

In Fig. 1 we show the reaction probability for the interaction $\lambda=0,2\times10^4,6\times10^4$, and 2×10^5. The *quantum case* (with exchange) and *zeroth order* WMD are compared. One can see that for weak interaction there is a large difference between these two cases. Under barrier transmission takes place only for the *quantum case*, in the *zeroth order* only wave packet components with the energy above the height of the barrier can pass to the right well.

With the increase of the interaction the reaction probability grows for both cases. The reason is that the initial energy becomes larger with the increase of λ and there are more wave packet components with the energy above the barrier height. For the *quantum case* it is also important that there are some high-energy components which pass under the barrier. For very large values $\lambda\geqslant6\times10^4$ reaction probabilities of the *zeroth order* and the *quantum case* are almost the same. It means that for strong interaction the role of tunneling is negligible, wave packets include too many components, which can pass above the barrier.

In Fig. 2 we present reaction probabilities for the *quantum case* with and without exchange. For large λ classical transmission above the barrier prevails and the influence of exchange on tunneling is considerably small. For small λ one can see a large difference in the reaction probabilities. If the particles are distinguishable, the reaction probability is larger, but the sign of the effect depends on the initial parameters of the wave packets, they can be fitted to make reaction probability greater for the case with exchange. Initially the distribution of the particles in coordinate space has the form of two separated Gaussians. We found that, for the used parameters, these two peaks quickly merge, forming a single

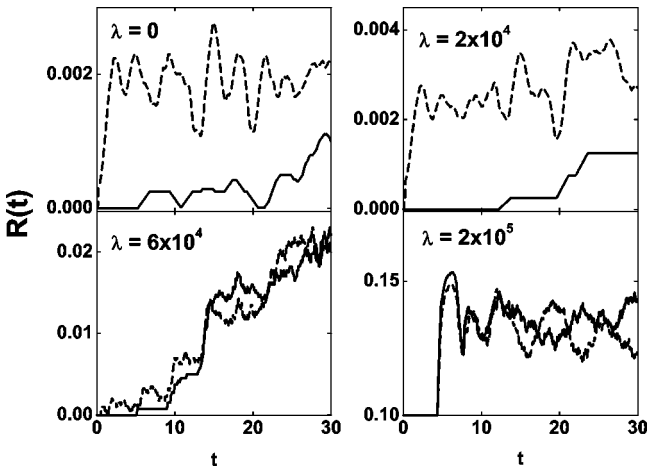

FIG. 2. Time dependence of the reaction probability $R(t)$ for the *quantum case* with exchange (solid lines) and without exchange (dashed lines). Interaction strengths are $\lambda = 0, 2\times10^4, 6\times10^4, 2\times10^5$.

peak, and very seldom they can be seen as two separated wave packets. It means that particles are close to each other during most of the time of simulation and exchange effects must be substantial. From Fig. 2 one can see that exchange almost does not influence the reaction probability for large λ. In this situation the contribution of transmission above the barrier to the reaction probability is very high (in comparison with tunneling, compare with the *zeroth order* WMD in Fig. 1). So it is difficult to notice exchange effects against this background. It is possible that the observed effect of the increase of transmission above the barrier with the growth of the interaction parameter masks the effect of the increase of dynamical correlations between electrons, which also suppress exchange effects.

The reaction probabilities presented in Figs. 1 and 2 were measured with the finite precision, connected with the finite time step and finite number of the used trajectories. Therefore, the regions of constant reaction probability for small λ arise—the subtle noise was smoothed over the errors. The substantial features (differences) of *zeroth order* and *nth order* WMD in cases *with* and *without exchange* become apparent on much larger scales and they are easily taken into account. Probably, the observed noise is due to the additional oscillations of high-energy parts of the wave packets. It will be the subject of detailed investigations in the next work.

Another common feature of Figs. 1 and 2 is the behavior of the reaction probability for $\lambda = 2\times10^5$. At the end of considered time interval, $0 \leqslant t \leqslant 30$, the reaction probabilities settle around the value ≈ 0.15. It seems that in the limit of infinite λ the equilibrium corresponds to the situation when both the wells are occupied with the equal probability, because in this case the total initial energy is much greater than the height of the barrier. Then the reaction probability must settle around 0.5. Probably, $\lambda = 2\times10^5$ is not large enough and the value of initial total energy is sufficient only to push a small part of the wave packet through the barrier. It is possible that then the leakage to the right well is balanced by the opposite transmission to the left well and that is why the reaction probability $R(t)$ stays near the value 0.15. On the other hand, there can be another explanation: after the transmission of some part of the wave packets to the right well, the repulsion between this part and the part in the left well prevents further penetration of particles to the right well, as a result the reaction probability settles at ≈ 0.15 (i.e., mechanism analogous to Coulomb blockade). Whether this second mechanism realizes is unclear, perhaps, these two processes take place simultaneously. As for the first scenario, the kinetic equilibrium, there are no doubts it can exist: the reaction probability also settles around some value for $\lambda = 0$ (the *quantum case* without exchange, Fig. 2). For this case there is no interaction, therefore, the only explanation can be the equality of transmissions through the barrier in both directions. In fact, there are no reasons to believe that the reaction probability will always stay near, say, 0.15 (for $\lambda = 2\times10^5$), possibly here we observe only the intermediate equilibrium and later the system can come to the state when the reaction probability is about 0.5. But such extra-long-time evolution must be the subject of special investigation.

B. Hartree description of the tunneling

Both Fig. 1 and Fig. 2 demonstrate oscillations of the reaction probability, with the growth of interaction parameter λ their period decreases and the picture becomes less regular. This is due to the behavior of the transmitted part of wave packets: to the right from the barrier there is the wall of the right well, transmitted part is reflected from it and moves to the left. Then it is partially transmitted back to the left well, making some modulation of the reaction probability curve. Transmission takes place mainly when the wave packets come to the barrier, therefore, reaction probability changes step by step with some period. When the interaction is weak, the particles move almost independently and this period coincides approximately with that of oscillations of one particle in the well ($T \approx 4$, see Figs. 1 and 2, the curves for $\lambda = 0$). But with the increase of λ this period is changed accordingly to the influence of one particle on the motion of the other particle. This influence can be illustrated more transparently in the picture of effective one-particle barriers (see below).

In terms of Hartree approximation it means that each particle moves effectively in the double-barrier potential. The first barrier is the stationary barrier between the wells and the second one is the effective time-dependent barrier due to the interaction of particles. Each particle either falls on two barriers, or moves between them. In the latter case a particle is inside the potential well. As the other particle moves closely, the well becomes more narrow and the energy levels in it higher. Therefore, the energy of the particle in the well becomes greater and the probability of transmission increases. Another mechanism is that due to the nonadiabatic narrowing of the well the particle can jump on the higher-energy levels, which also results in the increase of transmission probability.

The effective potential for the first particle in Hartree approximation can be defined as

$$V_{eff}(x_1,t) = V_{ext}(x_1) + \int U(x_1,x_2)\,|\psi(x_2,t)|^2 dx_2, \quad (39)$$

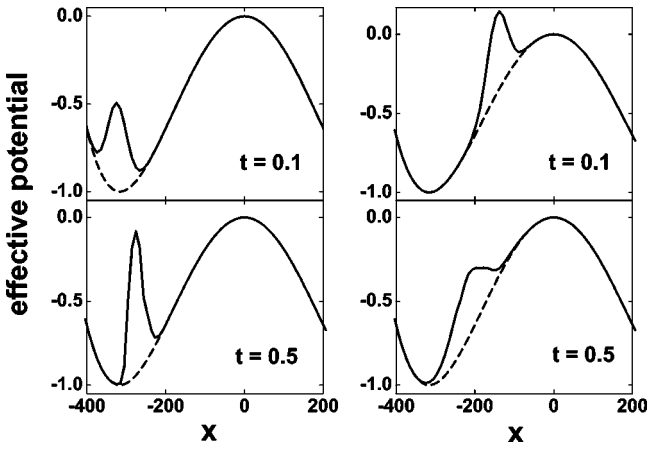

FIG. 3. Effective potentials (39) (solid lines), compared with the stationary external potential (dashed lines), in units of the height of the barrier. Two times, $t=0.1$ and $t=0.5$, are considered. Two left (right) plots are the effective potentials for the particle, which is initially closer (farther) to (from) the barrier. We consider the *quantum case* without exchange, $\lambda=2\times10^5$, x is in units $l_0=\hbar^{1/2}(m\alpha)^{-1/4}$, α is the potential parameter, Eq. (35).

where V_{ext} is the external potential, U is the interaction between particles, and $|\psi(x_2,t)|^2$ is the probability density for the second particle. The effective potential for the second electron is given by the analogous equation. Of course, this can be applied only to the case when the particles are distinguishable. If the particles are identical, one can use the Hartree-Fock approximation, and the potential becomes nonlocal. *We use neither Hartree nor Hartree-Fock approximation* in our method, they are just very convenient tools of visualizing the behavior of quantum particles, which interact with the barrier and between each other.

In Fig. 3 we plot the effective potentials, Eq. (39), $\lambda=2\times10^5$. The dotted line is the shape of external potential. The *quantum case* without exchange is considered, the particles are not identical, therefore, *Hartree approximation* can be used. The case with exchange is more interesting but if particles are identical, one can regard the effective potential, which is the same for all particles. Here we just illustrate the possible mechanisms of transmission and the case of distinguishable particles is more representative. In this case one can differ two situations. First, the barrier, which arises due to interparticle interaction, is close to the stationary barrier (effective broadening of the stationary barrier in the two right plots in Fig. 3). Second, this effective barrier is closer to the left wall of the well (the two left plots in Fig. 3). For identical particles, these situations take place simultaneously and the effective potential is the same for every particle.

The right plots in Fig. 3 show that the interaction makes the barrier wider and it prevents the transmission. But in the left plots, the well becomes not so deep, the energy levels in it grow and low-energy components of the wave packet can be reflected from the effective barrier in the direction of the stationary barrier. The tunneling and transmission above the barrier from the higher-energy levels are stronger. The oscillations of the low-energy components between the stationary and effective barriers make the tunneling probability larger.

TABLE I. Tunneling times for the spatial interval $[-45,45]$. (The system of units is $\hbar=m=\alpha=1$.)

	$\lambda=0$	$\lambda=6\times10^4$	$\lambda=2\times10^5$
Presence time (no exchange)	$0.8(\pm0.1)$	$0.72(\pm0.09)$	$0.38(\pm0.05)$
Arrival time (no exchange)	$0.9(\pm0.1)$	$0.86(\pm0.09)$	$0.80(\pm0.08)$
Presence time (exchange)	$0.8(\pm0.1)$	$0.78(\pm0.08)$	$0.36(\pm0.04)$
Arrival time (exchange)	$1.2(\pm0.1)$	$1.06(\pm0.09)$	$0.72(\pm0.07)$

C. Tunneling times

Consider now Table I, where we present tunneling times for the spatial interval $[-45,45]$ determined by two methods: *presence* (1) and *arrival* times (4). The interaction strengths are $\lambda=0,6\times10^4,2\times10^5$. We consider two situations: the *quantum case* with and without exchange. At the edge points of this spatial interval the value of the external potential approximately coincides with the initial energy of the system. Two methods give close results, *tunneling time* calculated with the help of Eq. (4) is in general greater than that with use of Eq. (1), but the trend connected with changes in tunneling time with change of the interaction parameter is the same for both methods. Tunneling time is greater for the case with exchange, because for our parameters there are fewer high-energy components in wave packets and tunneling is weaker for this case. With the increase of λ the tunneling time gets smaller, this can also be connected with the fact that for strong interaction there are more high-energy components in the wave packets. Those components make the main contribution to the transmission because the more the energy the greater the transmission probability. Because the components with higher-energy move faster the time of passing some interval becomes smaller. We do not list in Table I transmission times for the case of free motion. These times are all about 2.0 and are almost independent on λ, exchange and method of their calculation. One can see that the presence of the barrier makes the transmission (tunneling) time smaller. It is due to enriching of the transmitted part of the wave packet by high-energy components, which has greater probability to go through the barrier and move faster. Therefore, on average transmitted part arrives to detector *earlier* than the whole wave packet in the case of free motion.

V. CONCLUSION

We analyzed the nonstationary tunneling of two interacting identical particles by quantum molecular dynamics method based on the Wigner representation. The WMD method allows one to calculate different features characterizing quantum evolution and influence of particle interaction and exchange on tunneling. We found that the strong interaction in this problem leads to decrease of the role of tunneling in the transmission. If the interaction is not very strong ($\lambda<6\times10^4$) then exchange effects are substantial

and affect tunneling. The developed WMD method allowed us to analyze some interesting features of tunneling and proved to be a powerful tool for study of nonstationary quantum processes. Of course, the numerical solution of Schrödinger equation would not be too difficult for the problem under consideration, but in this work we just demonstrate the method, regarding relatively simple system of two identical particles in the double-well potential. We made only the first step in the development of WMD for the many-body problems and we intend to report the results of investigation of many-particles system in the next paper.

ACKNOWLEDGMENTS

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[1] A. Donoso and C.C. Martens, Phys. Rev. Lett. **87**, 223202 (2001).
[2] Yu.E. Lozovik and A.V. Filinov, Zh. Éksp. Teor. Fiz. **115**, 5, 1872 (1999) [JETP **88**, 1026 (1999)].
[3] H.W. Lee, Phys. Rep. **259**, 147 (1995).
[4] E. Wigner, Phys. Rev. **40**, 749 (1932).
[5] R. Landauer and Th. Martin, Solid State Commun. **84**, 115 (1992).
[6] D. Sokolovski and J.N.L. Connor, Phys. Rev. A **47**, 4677 (1993).
[7] A.J. Baz', Sov. J. Nucl. Phys. **5**, 161 (1967).
[8] V.F. Rybachenko, Sov. J. Nucl. Phys. **5**, 635 (1967).
[9] M. Buttiker and R. Landauer, Phys. Rev. Lett. **49**, 1739 (1982).
[10] M. Buttiker, Phys. Rev. B **27**, 6178 (1983).
[11] E.H. Hauge and J.A. Stovneng, Rev. Mod. Phys. **61**, 917 (1989).
[12] M. Buttiker and R. Landauer, IBM J. Res. Dev. **30**, 451 (1986).
[13] Y. Aharonov and D. Bohm, Phys. Rev. **122**, 1649 (1961).
[14] J.J. Włodarz, Phys. Rev. A **65**, 044103 (2002).
[15] A.D. Baute, I.L. Egusquiza, and J.G. Muga, Phys. Rev. A **65**, 032114 (2002).
[16] S. Longhi, P. Laporta, M. Belmonte, and E. Recami, Phys. Rev. E **65**, 046610 (2002).
[17] V. Delgado and J.G. Muga, Phys. Rev. A **56**, 3425 (1997).
[18] V.I. Tatarsky, Sov. Phys. Usp. **139**, 587 (1983).
[19] K. Husimi, Prog. Phys. Math. Soc. Jpn. **22**, 264 (1940).