# Simulation of tunneling in the quantum tomography approach

Yu. E. Lozovik,<sup>\*</sup> V. A. Sharapov,<sup>†</sup> and A. S. Arkhipov<sup>‡</sup>

Institute of Spectroscopy RAS, Moscow Region, u Troitsk, Russia 142190

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A method for the simulation of nonstationary quantum processes is proposed. The method is based on the tomography representation of quantum mechanics, i.e., the state of the system is described by a *nonnegative* function (quantum tomogram). In the framework of the method one uses the ensemble of trajectories in the tomographic space to represent evolution of the system (therefore direct calculation of the quantum tomogram is avoided). To illustrate the method we consider the problem of nonstationary tunneling of a wave packet. A number of characteristics of tunneling, such as tunneling time, evolution of spatial and momentum distributions, and tunneling probability are calculated within the quantum tomography approach. Tunneling of a wave packet of a composite particle, an exciton, is also considered; exciton ionization due to the scattering on the barrier is analyzed.

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## I. INTRODUCTION

Nowadays simulation of quantum systems is developed to a high extent (see, e.g., reviews [1,2]). However, the simulation methods that employ some generalization of the classical trajectory concept, for example, path integral Monte Carlo or Wigner dynamics, use nonpositively defined functions (density matrix, the Wigner function, etc.) to describe a quantum state. This leads to some difficulties in convergence of corresponding integrals, especially harmful for the simulation of Fermi systems (the sign problem, see, e.g., Refs. [3,4] and references therein). There is a hope that employing a real non-negative function, describing the quantum state, one can avoid these difficulties.

A real non-negative function in phase space, completely describing the quantum state, was proposed 60 years ago ([5], see also Refs. [1,6,7]). During the last decade another very interesting representation has been actively developed: the quantum tomography, operating with the ensemble of *scaled and rotated reference frames*, instead of the phase space [8–13]. In the framework of this formalism the state-describing function (called marginal distribution or quantum tomogram) is real and non-negative. The advantage is that the quantum tomogram is a *probability distribution* which was shown to completely describe the quantum state [14,15]. It is one of the reasons that why the quantum tomography has become so popular.

In this paper we propose a method for computer simulation of nonstationary quantum processes based on the tomography representation of quantum mechanics and illustrate the way it works considering the problem of nonstationary tunneling of a wave packet. Many simulation approaches in nonstationary quantum mechanics are based on the numerical solution of the time-dependent Schrödinger equation. There are also methods using the ensembles of classical trajectories to simulate quantum evolution. For example, the method of "Wigner trajectories," based on the Wigner representation [16], is well known (see, e.g., review [1] for details) and was recently successfully applied to investigate tunneling of a wave packet [17,18].

The quantum tomogram *w* depends on the variables  $\{X, \mu, \nu\}$ , where  $X = \mu q + \nu p$ , q, p are the coordinates and momenta of the system, respectively, and  $\mu, \nu$  are the parameters of scaling and rotation of reference frame in the phase space. The quantum tomogram is non-negative and normalized in *X* direction, therefore it can be interpreted as a distribution function of the value *X*. In our method the ensemble of trajectories in space  $\{X, \mu, \nu\}$  is introduced to describe the quantum evolution. The trajectories are governed by the dynamical equations obtained from the evolution equation for the quantum tomogram.

We demonstrate the method considering the nonstationary tunneling of a wave packet through a potential barrier. For this problem we calculated tunneling times, which are of interest now, both for fundamental science (e.g., what is the time spent by an atom to tunnel from the trap?) and for applications (electronic tunneling time is connected with the operation rate of some nanostructure-based devices). We also analyzed the evolution of the wave packet in coordinate and momentum spaces in detail. Another demonstration was designed to show that our method is not restricted to oneparticle simulations, namely, we investigated the tunneling of a wave packet of a composite quasiparticle, an exciton (coupled electron and hole in semiconductor), in a onedimensional nanostructure (quantum wire). There are two degrees of freedom in this case. For this problem, in addition to the probability density evolution, we determined the probability of ionization due to electron and hole scattering off the barrier in different directions.

In Sec. II the description of the method is presented, in Sec. III the model problem is considered and the main results for a tunneling wave packet are described. The exciton tunneling is considered in Sec. IV and the work is summarized in Sec. V.

**II. THE METHOD OF SIMULATION** 

The quantum tomogram  $w(X, \mu, \nu)$  is connected with the density matrix  $\rho(q, q')$  as [19,20]

<sup>\*</sup>Electronic address: lozovik@isan.troitsk.ru

<sup>&</sup>lt;sup>†</sup>Electronic address: vladsh@e-mail.ru

<sup>&</sup>lt;sup>‡</sup>Electronic address: antoncom@id.ru

$$\rho(q,q') = \int w(X,\mu,q-q')e^{i[X-\mu(q+q')/2]}\frac{d\mu dX}{2\pi}, \quad (1)$$
$$w(X,\mu,\nu) = \int e^{-i[k(X-\mu q-\nu p)+pu]} \times \rho\left(q+\frac{u}{2},q-\frac{u}{2}\right)\frac{dp dk dq du}{2\pi^2}. \quad (2)$$

Consider the case of the particle with mass m in a onedimensional space. If the Hamiltonian of the system is

$$H = \frac{p^2}{2m} + V(q), \qquad (3)$$

then the integral transformation (2) applied to the timedependent evolution equation for the density matrix gives [8]

$$\dot{w} - \frac{\mu}{m} \frac{\partial w}{\partial \nu} - 2 \frac{\partial V(\tilde{q})}{\partial q} \left( \frac{\nu}{2} \frac{\partial}{\partial X} \right) w + 2 \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{(2n+1)!} \frac{\partial^{2n+1} V(\tilde{q})}{\partial q^{2n+1}} \left( \frac{\nu}{2} \frac{\partial}{\partial X} \right)^{2n+1} w = 0,$$
(4)

where we use  $\hbar = 1$  and  $\tilde{q}$  is given by

$$\widetilde{q} = -\left(\frac{\partial}{\partial X}\right)^{-1} \frac{\partial}{\partial \mu}.$$
(5)

Equation (4) can be rewritten as

$$\frac{\partial w}{\partial t} + \frac{\partial w}{\partial X} G_X(X,\mu,\nu) + \frac{\partial w}{\partial \mu} G_\mu(X,\mu,\nu) + \frac{\partial w}{\partial \nu} G_\nu(X,\mu,\nu)$$
  
= 0, (6)

where functions *G* depend on quantum tomogram, its derivatives, and antiderivatives [the latter corresponding to terms with  $(\partial/\partial X)^{-1}$  in Eq. (4)]. Generalization for more variables is straightforward because the form of the equations does not change. Functions *G* for the problem under investigation are given in Sec. III. The evolution equation rewritten as Eq. (6) has the form of continuity equation for the quantum tomogram

$$\frac{dw}{dt} = \frac{\partial w}{\partial t} + \frac{\partial w}{\partial X}\dot{X} + \frac{\partial w}{\partial \mu}\dot{\mu} + \frac{\partial w}{\partial \nu}\dot{\nu} = 0.$$
(7)

This equation is analogous to the continuity equation for classical distribution function and Liouville equation. As is known, the characteristics of Liouville equation are the classical trajectories in phase space and they obey Hamilton equations of motion. The quantum tomogram is non-negative and we use it as a distribution function for trajectories in the space  $\{X, \mu, \nu\}$ , obeying the equations analogous to Hamilton equations for the classical trajectories. From the comparison of Eq. (6) with Eq. (7) it is obvious that the trajectories are governed by the equations

$$\dot{X} = G_X(X,\mu,\nu), \dot{\mu} = G_\mu(X,\mu,\nu), \dot{\nu} = G_\nu(X,\mu,\nu).$$
(8)

The trajectories are used to avoid the direct calculations of the distribution function (contrary to grid methods where the wave function is calculated at each point to solve numerically Schrödinger equation). Hence it is necessary to use some approximation for the quantum tomogram and we use the local exponential approximation (as in Ref. [17] for the Wigner function)

$$w(X,\mu,\nu) = w_0 e^{-[\{y-y_a(t)\}A_a(t)\{y-y_a(t)\}+b_a(t)\{y-y_a(t)\}]},$$
(9)

where  $y = \{X, \mu, \nu\}$ , and  $y_a$  is the point under consideration. Parameters of this approximation are matrix  $A_a$  and vector  $b_a$ , and some combinations of these parameters enter the evolution equation (4), instead of the derivatives and antiderivatives of the quantum tomogram. Calculation of average  $X, \mu, \nu$  and their average products allows to obtain  $A_a$  and  $b_a$  after this functions *G* are known and dynamical equations (8) can be solved numerically.

We would like to emphasize that we use the local approximation (9) only for the calculation of right-hand side of the equations of motion (8). The use of ensemble of trajectories to represent the quantum tomogram is equivalent to the approximation of quantum tomogram as a set of  $\delta$  functions, each  $\delta$  function corresponds to one trajectory. If the number of trajectories approaches infinity, the quantum tomogram can be approximated by the set of  $\delta$  functions with arbitrary precision. This is analogous to what is conventionally done in classical statistical mechanics for the distribution function in phase space. But unlike the classical statistical mechanics now the trajectories are not independent: the approximation (9) is used to take the nonlocal character of quantummechanical evolution into account.

The validity of this approximation holds if the quantum tomogram is smooth and the trajectories are close to each other. For example, this approximation can become inappropriate when one tries to consider a plane wave with wave vector k: in this case  $w(X, \mu=0, \nu=1) = \delta(X-k)$ . Approximation (9) does not work well for unbounded motion either, because the trajectories scatter with time. If there are few trajectories in the region around a given point, then the approximation (9) will not reconstruct the quantum tomogram, due to lack of statistics.

We consider the tunneling of wave packets through a barrier. Comparing our results with exact quantum computation we see that approximation (9) is applicable for this problem (see Secs. III and IV). For example, considering the tunneling through the potential barrier from the well, we deal with the region of both bounded motion (in the well) and unbounded motion (beyond the barrier). And still the approximation gives reasonable results (Sec. III). The higher initial energy, the stronger the penetration through the barrier. Then the evolution of most trajectories corresponds to unbounded motion, and the validity of Eq. (9) becomes poorer (see the end of Sec. III), in agreement with the discussion above. But in general, the local approximation (9) works satisfactory even for quite long time intervals (see Fig. 1).



FIG. 1. The dimensionless reaction probabilities (18) for three values of initial mean coordinate of the wave packet:  $q_0 = -0.2$ , -0.3, and -0.4 a.u. Solid lines are for the simulation in the quantum tomography approach, dashed lines are for the exact numerical solution.

To obtain any information about the system, we have to calculate some averages. Consider an arbitrary operator  $A(\hat{q},\hat{p})$ . Average  $\langle A \rangle$  of corresponding physical quantity is calculated in the tomographic representation of quantum mechanics as [21]

$$\langle A \rangle = \int A(\mu, \nu) e^{iX} w(X, \mu, \nu) dX d\mu d\nu, \qquad (10)$$

where  $A(\mu, \nu)$  is the Fourier component of the Weyl symbol  $A^{W}(q,p)$  of operator  $A(\hat{q},\hat{p})$  (see, e.g., Ref. [1]):

$$A(\mu,\nu) = \int A^{W}(q,p) \exp[-i(\mu q + \nu p)] \frac{dqdp}{4\pi^2}.$$
 (11)

For the calculation of average values we use the following approximation of quantum tomogram:

$$w(X,\mu,\nu,t) = \sum_{j=1}^{J} \delta(X - X_j(t)) \delta(\mu - \mu_j(t)) \delta(\nu - \nu_j(t)),$$
(12)

where the summation is made over all *J* trajectories;  $X_j(t), \mu_j(t), \nu_j(t)$  are the coordinates of the *j*th trajectory in  $\{X, \mu, \nu\}$  space at time *t*. Such approximation corresponds to the use of the ensemble of trajectories. In the regions, where the value of  $w(X, \mu, \nu)$  is small, trajectories are rare, and where it is great, trajectories are accumulated. The more trajectories are used, the better the approximation (12) works. If during the simulation the wave function has the form of a compact wave packet, even consisting of several distinct parts, approximation (12) holds, because in this case one has the compact sets of trajectories providing good statistics. This is the case for the problems considered, and therefore the use of this approximation does not change results essentially, in comparison with the exact quantum computation (Secs. III and IV).

For the operators  $A(\hat{q})$ , depending on  $\hat{q}$  only, the expression for  $\langle A \rangle$  takes the following form:

$$\langle A \rangle = \int A(X)w(X,\mu=1,\nu=0)dX, \qquad (13)$$

where A(X) is the function corresponding to the operator  $A(\hat{q})$  in coordinate representation, A(X)=A(q=X). The method of calculation of an average  $\langle A(\hat{q}) \rangle$  at arbitrary time *t*, with the approximation (12), is quite simple. One just takes into account the trajectories with any *X* and with  $\mu(t), \nu(t)$  from the small region near  $\mu = 1, \nu = 0$  only, and performs a summation of A(X) over all such trajectories.

The developed method is similar to the well-known method of Wigner trajectories (see Ref. [1] for review), where the ensemble of trajectories is introduced in the phase space, with the Wigner function used as a quasidistribution function. The quantum tomogram is defined in the space  $\{X, \mu, \nu\}$ , which is not as simple to understand as the phase space used in the Wigner approach. On the other hand, the quantum tomogram is a positive distribution function, while the Wigner function can be both positive and negative. In spite of these differences the two approaches are quite close in general, and there are some difficulties common for both methods. The discussion (see above) of the approximation for the tomogram [such as Eq. (9)] is , in principle, applicable to the method of Wigner trajectories as well. Another important example is the discontinuity of the Wigner trajectories, due to the fact that the trajectories are not independent as in classical statistical mechanics (see Ref. [22]). Trajectories evolution depends on their local distribution. The same problem can arise in the quantum tomography approach, where the trajectories for the same reason are not independent either. A possible alternative to Wigner function was proposed in Ref. [22], namely, the authors proposed to use the Weyl transforms of some operators (the Wigner function, up to the constant, is the Weyl transform of the density operator) instead of the Wigner function to generate the ensemble of trajectories. The same approach can be introduced for the quantum tomography. Applying the transform (2) to the matrix elements of an operator A we obtain the symbol  $w_A(X,\mu,\nu)$ . This function is not non-negative in general, but in analogy with the Wigner trajectories one can use  $w_A(X,\mu,\nu)$  to develop some new ensemble of trajectories. Perhaps, as with the Wevl transforms' trajectories [22], it will be more convenient to use the trajectories corresponding to  $w_A$  in some cases. This problem needs certainly further investigation..

### **III. SIMULATION OF TUNNELING OF A WAVE PACKET**

#### A. The model and calculated average values

We choose the same external potential as in Ref. [17]:

$$V(q) = \frac{m\omega_0^2 q^2}{2} - \frac{bq^3}{3},$$
 (14)

for further comparison of the results of simulation in quantum tomography approach with those obtained by other methods. As the potential has only the second and third powers of coordinate, all its derivatives of order more than the third vanish. Evolution equation in this case has the form ( $\hbar = 1$ ):

$$\frac{\partial w}{\partial t} - \frac{\mu}{m} \frac{\partial w}{\partial \nu} + 2 \left[ -\frac{\partial V(\tilde{q})}{\partial q} \left( \frac{\nu}{2} \frac{\partial}{\partial X} \right) + \frac{1}{6} \frac{\partial^3 V(\tilde{q})}{\partial q^3} \left( \frac{\nu}{2} \frac{\partial}{\partial X} \right)^3 \right] w$$
$$= 0. \tag{15}$$

For the potential given by Eq. (14) the evolution equation reads

$$\frac{\partial w}{\partial t} - \frac{\mu}{m} \frac{\partial w}{\partial \nu} + m \omega_0^2 \nu \frac{\partial w}{\partial \mu} - \frac{b \nu^3}{12} \frac{\partial^3 w}{\partial X^3} + b \nu \left(\frac{\partial}{\partial X}\right)^{-1} \frac{\partial^2 w}{\partial \mu^2} = 0,$$
(16)

and the dynamical equations have the form

$$\frac{\partial X}{\partial t} = \frac{b\nu^3}{12} \frac{1}{w} \frac{\partial^2 w}{\partial X^2},$$
$$\frac{\partial \mu}{\partial t} = m\omega_0^2 \nu - \frac{b\nu}{w} \left(\frac{\partial}{\partial X}\right)^{-1} \frac{\partial w}{\partial \mu},$$
$$\frac{\partial \nu}{\partial t} = -\frac{\mu}{m}.$$
(17)

We use atomic units throughout,  $\hbar = m_e = |e| = 1$ , where  $m_e$  and e is the mass and the charge of a free electron. The particle mass is taken to be m = 2000. The parameters of the potential are  $\omega_0 = 0.01$  and b = 0.2981. The potential has minimum at q = 0 [V(0) = 0] and maximum at q = 0.6709 [V(0.6709) = 0.015]. Therefore here we consider the motion of a particle in the potential well with infinite left wall and the barrier of height 0.015 at q = 0.6709. This model problem roughly describes nonstationary tunneling of an atom from the trap.

Initially the particle represented by the wave packet is located at q < 0, its mean momentum is zero. The particle can oscillate in the potential well and can tunnel or pass above the barrier. The probabilities of these processes depend on the initial energy of the wave packet. We consider the problem, where all parameters, except the initial mean coordinate  $q_0$  of the wave packet, are fixed (initial mean momentum equals zero, dispersions of the wave packet in coordinate and momentum spaces are 0.3 and 1.6, respectively).

Equations (17) are solved numerically. As in Ref. [17] we consider three values of  $q_0: -0.2, -0.3$ , and -0.4. The tunneling characteristics of most interest are reaction probability and tunneling time. The reaction probability is defined as

$$\int_{q_a}^{\infty} |\psi(x,t)|^2 dx, \qquad (18)$$

where  $q_a = 0.6709$  (the point where potential has the maximum), the maximum value of reaction probability is unity.

The reaction probability shows what part of the wave packet is currently beyond the barrier.

There are a lot of methods to determine tunneling time [23–36], another important characteristic of tunneling. We use here the approach where tunneling time is calculated as the difference of *presence times* (see Ref. [36] for a review) at point  $x_a$  and  $x_b$ , located on the opposite sides of the barrier:

$$t_T(x_a, x_b) = \langle t(x_b) \rangle - \langle t(x_a) \rangle.$$
(19)

The presence time at arbitrary point  $x_0$  is

$$\langle t(x_0) \rangle = \frac{\int_0^\infty t |\psi(x_0,t)|^2 dt}{\int_0^\infty |\psi(x_0,t)|^2 dt}.$$
 (20)

#### **B.** Reaction probability

In this section we present the results obtained within our method and compare them with the exact numerical solution of Schrödinger equation. In Fig. 1 we present the reaction probability (18) dependence on time for three values of initial mean coordinate of the wave packet  $q_0 = -0.2$ , -0.3, and -0.4, the corresponding mean energies of the wave packet are  $0.75V_0$ ,  $1.25V_0$ , and  $2.0V_0$ , respectively. Solid lines represent the results of simulation in the quantum tomography (QT) approach and dashed lines correspond to the numerical solution of Schrödinger equation (exact quantum computation). Due to the increase of initial mean energy with the increase of  $|q_0|$ , the portion of high energy components in the wave packet grows. This leads to the larger portion of components, which pass through the barrier, either because their energy is greater than the height of the barrier, or due to tunneling. Therefore, with the growth of  $|q_0|$ , reaction probability becomes larger as one can see in Fig. 1. The time evolution of reaction probability is qualitatively the same for every  $q_0$ . The components, which have passed through the barrier, cannot return, because for q > 0.6709 potential diminishes with the growth of coordinate, and consequently reaction probability cannot decrease with time. At first it grows rapidly due to transmission of components with the energy higher than the height of the barrier (comparison with the classical solution of the same problem, for which only transmission above the barrier is possible, convinces us in it). Then the reaction probability continues to grow but slowly, due to the tunneling. All these features are present for both QT simulation and exact quantum computation.

In comparison with the exact computation, reaction probability for the QT simulation is slightly higher. Note also some difference in the character of an increase of the reaction probability for QT simulation and exact solution: in the former case the curves are not so smooth. These differences stem from the finite number of trajectories used in QT simulation: for smaller number of trajectories (not shown) reaction probability curves resemble stairs more evidently (this is connected with the overestimation of the role of wave packet oscillations in the well for the finite number of trajectories),



FIG. 2. Probability density in coordinate space for QT simulation (histograms) and exact solution (smooth lines), at times t = 0 a.u. (left) and t = 200 a.u. (right). The barrier is at the point 0.6709 a.u.,  $q_0 = -0.2$  a.u.

and quantitative deviation from exact result is stronger. But in general, for quite large number of trajectories, as for the case shown in Fig. 1, QT simulation results on reaction probability are quite close to those obtained through the exact quantum computation (compare also with the method of Wigner trajectories in the work by Donoso and Martens [17]).

## C. Evolution of the wave packet and tunneling times

In addition to the reaction probability we obtained a number of new qualitative and quantitative results, describing in detail the behavior of the wave packet during tunneling. We calculated also the tunneling times using the concept of the presence time.

The following discussion concerns the tunneling of the wave packet with initial mean coordinate  $q_0 = -0.2$ . We present the normalized probability density  $|\psi(x)|^2$  in coordinate space (Figs. 2–4) and  $|\psi(p)|^2$  in momentum space (Figs. 5 and 6) for several successive time moments. In these figures smooth lines show the shape of the wave packet obtained by means of exact quantum computation. Histograms represent the result of *single QT run*. One can consider many runs with the same number of trajectories and average the probability density over all these runs to obtain smoother picture. But here we would like to show what QT simulation can give in one run, in comparison with the exact quantum computation. Therefore the histograms (QT) fit the smooth solid lines in Figs. 2–4 (exact solution) not ideally, still the resemblance is obvious.





FIG. 4. Probability density in coordinate space for QT simulation (histogram) and exact solution (smooth line), at time t= 400 a.u. The barrier is at the point 0.6709 a.u.,  $q_0 = -0.2$  a.u.

First, consider the probability density  $|\psi(x)|^2$  in coordinate space (Figs. 2-4). One can see (Fig. 2) that initially the wave packet has Gaussian form. It begins to move as a whole towards the potential minimum at x=0 (initial mean momentum is zero, but the potential inclines in that direction), passes that point, accelerates, and collides with the barrier. During the motion the wave packet broadens (due to dispersion in momentum space, compare right and left plots in Fig. 2) but the interaction with the barrier changes its form more substantially (Figs. 3 and 4). The wave packet shrinks a little, some components pass through the barrier and transmitted part can be seen beyond the barrier (x=0.6709). Since the transmitted part cannot return and accelerates (potential diminishes with the distance for x > 0.6709), the enriching of the wave packet by high-energy components must take place (see below).

All features described in the previous paragraph are common for both the exact solution and QT simulation. The histograms in Figs. 2-4 fit the smooth lines representing the exact solution better for earlier times, but even after the interaction with the barrier (Fig. 4), resemblance is quite close. This shows that approximations (9) and (12) are applicable to the problem under consideration.

Now we proceed to the evolution of the wave packet in momentum space. To confirm our analysis concerning the acceleration of transmitted part of the wave packet, we present the probability density  $|\psi(p)|^2$  in momentum space in Figs. 5 and 6, at times t=0 and t=400, respectively. As the wave function is initially the Gaussian wave packet, the initial distributions are Gaussian both in coordinate and momentum space (compare Figs. 2 and 5). But after the wave packet has interacted with the barrier, the distribution in mo-



FIG. 5. Initial probability density in momentum space for QT simulation (histogram) and exact solution (smooth line). t=0 a.u.



FIG. 6. Probability density in momentum space for QT simulation (histogram) and exact solution (smooth line) at t = 400 a.u.

mentum space changes substantially (Fig. 6). The higher the energy of incident particle, the greater the tunneling probability. Therefore the barrier transmits mainly the wave packet components with relatively high energy, serving as an energy selector. Transmitted part of the wave packet is accelerated in the region of lowering potential beyond the barrier. Due to this reason the components with high momentum arise, and the enriching of the wave packet by high-energy components is observed.

Resemblance between the histograms (OT simulation) and smooth solid lines (exact solution) is somewhat poorer for momentum distribution at large times (t = 400, Fig. 6) than for coordinate distribution (Fig. 4). This is due to the fact that one deals with finite number of trajectories and has to sample quite large interval in momentum space, because the transmitted part is permanently accelerated. Therefore, with time, momentum distribution spreads and there are not many trajectories with  $\mu$ ,  $\nu$  close enough to  $\mu = 0, \nu = 1$  for given momentum p (see Sec. III). As for the considered value of initial mean coordinate  $q_0 = -0.2$  the initial energy is not very large ( $\approx 0.75V_0$ , where  $V_0$  is the height of the barrier), the wave packet stays mainly in the well (for the time considered t = 400 only  $\approx 20\%$  of the wave packet is transmitted, see Fig. 1) and the distribution in coordinate space is more compact.

In Fig. 7 we present the dependence of tunneling time on initial mean position of the wave packet. Tunneling time is determined as the difference of presence times (20) for points  $x_a = 0.5(0.6709)$  and  $x_b = 2.0(0.6709)$  (at x = 0.6709) potential has the maximum). Tunneling is usually stronger for the higher energy. Therefore, the increase of  $|q_0|$  (and corresponding increase of initial mean energy) leads to the growth of the average speed of both the transmitted part and the wave packet as a whole. Transmitted part passes the region of the barrier (space between the points  $x_a$  and  $x_b$ ) faster, and so one expects that the increase in  $|q_0|$  causes the decrease in tunneling time. Indeed, the value of tunneling time drops with increasing  $|q_0|$ . Results of QT simulation (squares in Fig. 7) deviate from those of exact computation (circles) within the range of errors. The deviation is maximal for large  $|q_0|$ . Probably, this is because for large  $|q_0|$  the wave packet leaves the well almost entirely (see Fig. 1), and the evolution of most trajectories corresponds to the unbounded accelerated motion. In such situation trajectories scatter and approximation (12) does not represent the quantum tomogram as exactly as for smaller  $|q_0|$ .



FIG. 7. Tunneling times with errors for several values of initial mean coordinate of the wave packet  $q_0$ . Results of the QT simulation (squares) are compared with exact quantum computation (circles).

#### IV. SIMULATION OF THE EXCITON TUNNELING

The method described in Sec. II can be used to simulate the evolution of systems with more than one degree of freedom. In this section we demonstrate this possibility, considering nonstationary tunneling of the composite particle, exciton, through the potential barrier in one-dimensional (1D) semiconductor structure (quantum wire). Exciton is a bound state of electron and hole in semiconductor, therefore we deal with two degrees of freedom in contrast to Sec. III.

Possible experimental realization is as follows. Consider quasi-one-dimensional semiconductor nanostructure where the motion is allowed only in one direction (quantum wire). Transverse motion is restricted due to strong confining barriers. Potential barrier in the direction of allowed motion can be located at some point of the quantum wire either using semiconductor heterojunction or by gate. Using femtosecond laser pulses, we can form an excitonic wave packet, either by the quasiresonance pumping, or exciting an electron from valence band with the formation of a hole and subsequent binding of two particles into exciton. Then the excitonic wave packet can move to the barrier and with the help of some detectors one can investigate scattering of the exciton.

Keeping this in mind let us construct the model for the simulation. We use the parameters corresponding to GaAs for reference (the dielectric constant  $\varepsilon = 12.5$ , the effective masses of electron and hole are  $m_e = 0.07 m_e^{(0)}$  and  $m_h = 0.15 m_e^{(0)}$ , respectively, here  $m_e^{(0)}$  is the electron mass in vacuum). Three-dimensional exciton in bulk GaAs is characterized by effective Bohr radius  $a^* \approx 10$  nm and binding energy  $E_C^* \approx 4$  meV. We use the unit of length  $a^*$ , the unit of mass  $m_e$ , and  $\hbar = 1$ . The corresponding units of energy and time are  $E_0 = \hbar^2/(m_e a^{*2}) \approx 10$  meV and  $t_0 = m_e a^*/\hbar \approx 100$  fs.

The energy spectrum and wave functions of relative electron and hole motion in 3D exciton are analogous to those of the hydrogen atom. But this is not the case for 1D exciton. First, electron-hole effective interaction potential in quasi-1D structure is not Coulomb. Indeed, if the exciton size in the direction of allowed motion is much greater than the width of the quantum wire (in the transverse direction), then the adiabatic approximation is applicable and 3D interaction potential must be averaged over the transverse degrees of freedom. Resulting 1D effective potential substantially differs from Coulomb (see Ref. [37] for the discussion of similar model). Second, corresponding energy spectrum and wave functions of electron and hole relative motion also change in comparison with the hydrogenlike states. We choose the wave function of the exciton ground state in Gaussian form.

The excitonic wave packet can be represented as a Gaussian wave packet in the following center-of-mass coordinates:

$$\Psi(x_e, x_h, t=0) = \frac{e^{-r^2/(2\sigma)}}{(\pi\sigma)^{1/4}} \frac{e^{-(R-x_0)^2/(2S)+iRp_0}}{(\pi S)^{1/4}}, \quad (21)$$

where  $R = (m_e x_e + m_h x_h)/(m_e + m_h)$ ,  $r = |x_e - x_h|$ ,  $x_e$  and  $x_h$  are electron and hole coordinates,  $x_0, p_0$  and *S* are parameters; for them we used the following values:  $x_0 = -10$ ,  $p_0 = 3$ , S = 2, and  $\sigma = 1$ .

The external potential is assumed to be zero everywhere except the region of barrier; we use the barrier of thickness 5 nm, or 0.5 in accepted units. For simplicity we set the barriers for an electron and a hole to be the same and use both external and interaction potentials in quadratic form, cut at some distance. Then external potential is given by

$$V_{ext}(x) = \begin{cases} C - Dx^2 & \text{if } |x| < \sqrt{\frac{C}{D}}, \\ 0 & \text{if } |x| \ge \sqrt{\frac{C}{D}}, \end{cases}$$
(22)

C is the height of the barrier, its width is  $\sqrt{C/D} = 0.5$ .

Interaction potential  $V_{int}$  is also assumed to be quadratic:

$$V_{int}(r) = \begin{cases} Br^2 - A & \text{if } r < \sqrt{\frac{A}{B}}, \\ 0 & \text{if } r \ge \sqrt{\frac{A}{B}}, \end{cases}$$
(23)

where  $r = |x_e - x_h|$ . The potential (23) can describe, e.g., electron-hole interaction in spatially indirect exciton, for example in coupled quantum wires with a large interwire separation [38]. The initial wave function of relative motion, chosen to be Gaussian with unity dispersion, is negligible within one percent accuracy at r=3. Thus we choose the radius of electron-hole interaction to be  $\sqrt{A/B}=3$ .

We assume that we deal with a quasi-1D exciton with binding energy  $E_C = 1/8$ . In fact, for an exciton in quantum wire, the wave function, binding energy, etc., are essentially influenced by the properties of quantum wire. We also neglect the possibility of electron and hole recombination at the time scales studied.

Here we consider just an example and therefore use a relatively simple model. Still this model contains the main features of exciton tunneling, such as the possibility of ionization, a barrier and an interaction with realistic strength and size, the fact that a composite particle is the bounded state of two particles.



FIG. 8. Probability density distributions in coordinate space for electron  $[\rho_e(x)]$  and hole  $[\rho_h(x)]$  at times t=0 and t=10. QT simulation (solid lines) is compared with the exact numerical solution (dashed lines). All values are in units  $\hbar = m_e^* = E_C = 1$ ,  $m_e^*$  is the electron effective mass and  $E_C$  is the binding energy of the exciton. The height of the barrier C=1, width  $\sqrt{C/D} = 0.5$ .

For a stationary state the binding energy is  $-E_C = \int \Psi_{int}^*(r) H_{int}(r) \Psi_{int}(r) dr$ , where  $\Psi_{int}(r)$  is the wave function of relative motion. Then, from Eq. (23) and condition  $\sqrt{A/B} = 3$  we have  $A \approx 18E_C/17$ .

We do not use the variables of relative and center-of-mass motion, for QT simulation it is easier to deal with the initial conditions and evolution equation in coordinates of electron and hole  $x_e$  and  $x_h$ . The potentials (22) and (23) are quadratic, that makes tomographic consideration of the problem easier (see Sec. III), discontinuity is neglected. On the other hand, in coordinates  $x_e$  and  $x_h$  the evolution equations depend on trajectory distribution (see Sec. II). Therefore the problem considered allows to employ all techniques developed for one degree of freedom, in the case of two degrees of freedom.

The results of exciton tunneling simulation are presented in Figs. 8-10. All parameters are fixed (see above), except the barrier height C in Fig. 10. In Figs. 8 and 9 we depict the evolution of probability density for an electron and a hole, the barrier height C=1. The solid lines in Figs. 8-9 and the circles in Fig. 10 correspond to the simulation in quantum tomography approach, while the dashed lines and the squares represent the exact numerical computation. Unlike in Figs. 2-6, here we show the results of several combined QT simulation runs, therefore corresponding lines are relatively smooth. Coincidence of QT and exact computation results, initially very good, becomes poorer with time (Figs. 8 and 9). But OT simulation reproduces the main features of exciton tunneling: wave packets broadening with time, shrinking near the barrier, dividing of the wave packets into two parts (reflected and transmitted). Note that OT results are quite close to the exact ones even for long times (t=30), despite the fact that the motion is unbounded (see Sec. II). Integral values (in Fig. 10) obtained in QT approach also agree with the exact results. Larger discrepancies correspond to higher barriers, which is probably due to larger inaccuracies, introduced by neglecting the potential discontinuity in the case of



FIG. 9. Probability density distributions in coordinate space for electron  $[\rho_e(x)]$  and hole  $[\rho_h(x)]$  at times t=20 and t=30. QT simulation (solid lines) is compared with exact numerical solution (dashed lines). The same units and barrier parameters as in Fig. 8 are used.

stronger interaction with the external potential.

The electron and hole wave packets begin their motion from the point x = -10 and, shrinking near the barrier, are partially reflected and transmitted. For the case presented in Figs. 8–9, about the half of wave packets is transmitted. An interesting question is the ionization probability of exciton, induced by interaction with the barrier. If the electron and hole are scattered in different directions on the barrier, the distance between them can become quite large, but, in principle, there is a possibility that the exciton is not ionized after this scattering, because one of the particles can be "pulled" beyond the barrier, toward the other particle, due to electron-hole attraction. On the other hand, the electron-hole interaction is cut at the distance  $\sqrt{A/B}$  in our model. After the interaction with the barrier the wave packet divides into reflected and transmitted parts moving in opposite directions. For the time large enough, these two parts are well separated, the separation between them grows and the leakage through the barrier in both directions is negligible.  $P_{1on}$  denote the probability of ionization due to electron and hole scattering in different directions. Then, the probability to find an electron and a hole in different directions in respect to the barrier, with e-h distance being larger than  $\sqrt{A/B}$ , approaches  $P_{Ion}$ in the limit  $t \rightarrow \infty$ .

The probability of ionization due to electron and hole scattering on the barrier in different directions  $P_{Ion}$  is presented in Fig. 10, depending on the barrier height *C*. For very high and very low barriers  $P_{Ion}$  must approach zero, because in former case both particles are reflected and in the latter they both are transmitted. This trend is seen in Fig. 10, and  $P_{Ion}$  depending on *C* is maximal (other parameters are fixed, see above) at  $C \approx 1$ . Note that these features are obvious for curves representing both QT simulation (circles) and exact computation (squares), and in general two curves are quite close to each other.



FIG. 10. Probability of exciton ionization  $P_{lon}$  due to electron and hole scattering on the barrier in opposite directions versus barrier height *C*. Circles and squares represent QT simulation and exact solution, respectively. Considered is the barrier of thickness 0.5. The units are the same as in Fig. 8.

#### V. CONCLUSION

We have developed a method of numerical simulation of quantum nonstationary processes based on tomographic representation of quantum mechanics and applied it to the problem of tunneling of the wave packet through the potential barrier. The quantum tomogram is used in a sense as the distribution function for the ensemble of trajectories in space  $X, \mu, \nu$ , where  $X = \mu q + \nu p$  is the coordinate measured in rotated and scaled reference frame, q, p are coordinate and momentum of the system, respectively. The trajectories are governed by the equations, resembling the Hamilton equations of motion, therefore, some analog of molecular dynamics can be used. The Gaussian approximation allows to avoid the direct calculation of the quantum tomogram. Instead of the quantum tomogram, the parameters of the approximation are used in the equations of motion. Those parameters can be obtained if one calculates the local moments of the ensemble of trajectories.

To demonstrate the method we considered the problems of nonstationary tunneling of one- and two-particle wave packets. Our method gave the results in agreement with those obtained by the method of Wigner trajectories and by exact quantum computation.

Of course, we made only the first step toward development of this simulation method. The fact that the quantum tomogram is non-negative may lead to additional advantage of more rapid convergence, which may help to overcome the sign problem for fermionic systems. In the next work we intend to consider the many-body problem for fermionic and bosonic systems by means of the QT method.

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