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New method of quantum dynamics simulation based on the quantum tomography

A.S. Arkhipov, Yu.E. Lozovik*

Institute of Spectroscopy RAS, Troitsk 142190, Moscow region, Russia Received 16 September 2003; accepted 24 September 2003 Communicated by V.M. Agranovich

Abstract

We propose a new method to simulate the quantum dynamics, based on the tomography representation. In its framework the quantum state is described by real nonnegative distribution function. We demonstrate the method applying it to the wave packet tunneling of one and two interacting particles.

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1. Introduction

Simulation of quantum systems is popular nowadays and achieved considerable development recently (see, e.g., reviews [1-3]). However, simulation methods usually deal with the alternating-sign functions (wave function, the Wigner function, etc.) describing a quantum state. Probably, corresponding difficulties with convergence of integrals (sign problem) could be resolved if one uses real nonnegative function to describe the state.

In this Letter we propose a new method for computer simulation of nonstationary quantum processes,

E-mail addresses: antoncom@id.ru (A.S. Arkhipov), lozovik@isan.troitsk.ru (Yu.E. Lozovik).

that uses nonnegative state-describing function, the quantum tomogram. One can define a nonnegative function, completely describing the quantum state, in the phase space [1,4–6]. Quantum tomogram [7–12] is defined in the space of *scaled and rotated reference frames*, that is not so intuitively clear as the phase space. But the advantage of quantum tomogram is that this function is a *probability distribution*, completely describing the quantum state [13,14].

The quantum tomogram $w(X, \mu, \nu)$ depends on the parameters of scaling and rotation of reference frames in the phase space: $X = \mu q + \nu p$, where q, p are coordinates and momenta of the system. Function $w(X, \mu, \nu)$ is nonnegative and normalized in X direction, therefore it can be interpreted as a distribution function of value X. Our method uses $w(X, \mu, \nu)$ as a distribution function of the trajectories in space $\{X, \mu, \nu\}$, trajectories being governed by

^{*} Corresponding author.

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the dynamical equations obtained from the evolution equation for the quantum tomogram. Introduction of the trajectories possesses additional advantage: contrary to grid methods of Schrödinger equation solution, trajectory methods, such as the method of Wigner trajectories [1,15-17], do not require the storing of large arrays representing the wave function. Description of the method is presented in Section 2.

We apply the method to the tunneling of a wave packet through the potential barrier, first to the singleparticle tunneling (Section 3), and then to the collective tunneling of two attracting particles (Section 4). The latter case is represented by the exciton—composite particle consisting of electron and hole—tunneling in a nanostructure. Tunneling times, evolution of the wave packet in coordinate and momentum spaces, probability of exciton ionization due to electron and hole scattering on the barrier were analyzed in details.

2. The method

The quantum tomogram $w(X, \mu, \nu)$ is connected with the density matrix $\rho(q, q')$ as [18,19]

$$\rho(q,q') = \int w(X,\mu,q-q')e^{i(X-\mu(q+q')/2)}\frac{d\mu\,dX}{2\pi},$$
(1)

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

For the systems described by Hamiltonian

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

the integral transform (2), applied to the timedependent evolution equation for the density matrix, gives [7]

$$\dot{w} - \frac{\mu}{m} \frac{\partial w}{\partial \nu} - 2 \frac{\partial V(\tilde{q})}{\partial q} \left(\frac{\nu}{2} \frac{\partial}{\partial X} \right) w$$

$$+ 2 \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{(2n+1)!} \frac{\partial^{2n+1} V(\tilde{q})}{\partial q^{2n+1}}$$

$$\times \left(\frac{\nu}{2} \frac{\partial}{\partial X} \right)^{2n+1} w = 0, \qquad (4)$$

where we use $\hbar = 1$, consider a particle of mass *m* in one dimension (for simplicity), and \tilde{q} is given by

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

Let us rewrite Eq. (4) 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. Eq. (6) has the form of continuity equation for the quantum tomogram:

$$\frac{dw}{dt} = \frac{\partial w}{\partial t} + \frac{\partial w}{\partial X}\dot{X} + \frac{\partial w}{\partial \mu}\dot{\mu} + \frac{\partial w}{\partial \nu}\dot{\nu} = 0, \tag{7}$$

that is analogous to the continuity equation for classical distribution function and Liouville equation. As known, the characteristics of Liouville equation are the classical trajectories in phase space and they obey Hamilton equations of motion. Analogously, from Eqs. (6) and (7) we derive the motion equations in space $\{X, \mu, \nu\}$:

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

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

Generalization for the case of more variables is straightforward, the form of equations does not change. Functions G for the problem under investigation are given in Section 3.

As functions G depend on the tomogram, and we avoid its direct calculation, it is necessary to use local approximation for the quantum tomogram:

$$w(X, \mu, \nu) = w_0 e^{-[(y - y_a(t))A_a(t)(y - y_a(t)) + b_a(t)(y - y_a(t))]},$$
(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 . Calculating the average $y - y_a$ and their average product, we obtain A_a and b_a . After that, functions *G* are known and dynamical equations (8) can be solved numerically.

The local approximation (9) is used only for the calculation of r.h.s. in the equations of motion (8). Unlike the classical statistical mechanics, the trajectories in space $\{X, \mu, \nu\}$ are not independent and approximation (9) takes the nonlocal character of quantum evolution into account. This approximation is valid for smooth quantum tomogram and dense ensemble of trajectories (if there are few trajectories in the region around the given point, then the approximation (9) will not reconstruct the quantum tomogram, due to lack of statistics). Approximation (9) also works not well for unbounded motion, because the trajectories scatter with time. Comparison with the exact numerical solution in considered cases shows that approximation (9) holds for these problems (see Sections 3, 4).

Finally, consider the calculation of average values. For an arbitrary operator $A(\hat{q}, \hat{p})$ corresponding average $\langle A \rangle$ is calculated as [20]

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

where $A(\mu, \nu)$ is the Fourier component of Weyl symbol $A^W(q, p)$ of operator $A(\hat{q}, \hat{p})$ (see, e.g., [1, 21]).

The calculation of average values is performed using the following approximation of quantum tomogram:

$$w(X, \mu, \nu, t)$$

$$= \sum_{j=1}^{J} \delta \left(X - X_j(t) \right) \delta \left(\mu - \mu_j(t) \right) \delta \left(\nu - \nu_j(t) \right),$$
(11)

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*. It was found that the use of this approximation in investigation of the wave packet tunneling did not change results essentially, in comparison with the exact quantum computation (Sections 3, 4).

3. Tunneling of a wave packet

3.1. The model

We choose the external potential to coincide with the potential used in [16], for comparison of the results of simulation in quantum tomography approach with those obtained by other methods:

$$V(q) = \frac{m\omega_0^2 q^2}{2} - \frac{bq^3}{3}.$$
 (12)

The potential has only the second and third powers of coordinate, so all its derivatives of order more than the third equal to zero. Evolution equation has the form $(\hbar = 1)$:

$$\frac{\partial w}{\partial t} - \frac{\mu}{m} \frac{\partial w}{\partial v} + 2 \left[-\frac{\partial V(\tilde{q})}{\partial q} \left(\frac{v}{2} \frac{\partial}{\partial X} \right) + \frac{1}{6} \frac{\partial^3 V(\tilde{q})}{\partial q^3} \left(\frac{v}{2} \frac{\partial}{\partial X} \right)^3 \right] w = 0,$$
(13)

or

$$\frac{\partial w}{\partial t} - \frac{\mu}{m} \frac{\partial w}{\partial v} + m\omega_0^2 v \frac{\partial w}{\partial \mu} - \frac{bv^3}{12} \frac{\partial^3 w}{\partial X^3} + bv \left(\frac{\partial}{\partial X}\right)^{-1} \frac{\partial^2 w}{\partial \mu^2} = 0, \qquad (14)$$

and dynamical equations have the form

$$\frac{\partial X}{\partial t} = \frac{bv^3}{12} \frac{1}{w} \frac{\partial^2 w}{\partial X^2},$$

$$\frac{\partial \mu}{\partial t} = m\omega_0^2 v - \frac{bv}{w} \left(\frac{\partial}{\partial X}\right)^{-1} \frac{\partial w}{\partial \mu},$$

$$\frac{\partial v}{\partial t} = -\frac{\mu}{m}.$$
(15)

We use atomic units throughout, $\hbar = m_e = |e| = 1$, where m_e and e are the mass and charge of a free electron. The particle with mass m = 2000 is regarded. Parameters of the potential are $\omega_0 = 0.01$ and b = 0.2981. This potential has the 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 situated to the left from q = 0, its mean momentum is zero. We consider the problem with all parameters fixed, except the initial mean coordinate q_0 (initial mean momentum equals zero, dispersions of the wave packet in coordinate and momentum spaces are ≈ 0.3 and ≈ 1.6 , respectively). As in [16] we consider three values of q_0 : -0.2, -0.3 and -0.4. The most interesting quantities characterizing tunneling are reaction probability and tunneling time. Reaction probability is defined as

$$\int_{q_a}^{\infty} \left| \psi(x,t) \right|^2 dx, \tag{16}$$

where $q_a = 0.6709$ (the point where potential has the maximum), the maximum value of reaction probability is unity. Reaction probability shows what part of the wave packet is currently beyond the barrier.

Tunneling time of a wave packet is also an important feature of tunneling. From the variety of theoretical methods to determine tunneling time [22–35], we choose the approach where tunneling time is calculated as a difference of *presence times* (see [35] for review) at points x_a and x_b , located on the opposite sides of the barrier:

$$t_T(x_a, x_b) = \langle t(x_b) \rangle - \langle t(x_a) \rangle.$$
(17)

The presence time at arbitrary point x_0 is

$$\langle t(x_0) \rangle = \frac{\int_0^\infty t |\psi(x_0, t)|^2 dt}{\int_0^\infty |\psi(x_0, t)|^2 dt}.$$
(18)

3.2. Reaction probability and tunneling time

The reaction probability (16) dependence on time is presented in Fig. 1. All the results obtained by means of our method are compared with the exact numerical solution of Schrödinger equation. Three values of initial mean coordinate of the wave packet $q_0 =$ -0.2, -0.3 and -0.4 are considered, and corresponding mean energies of the wave packet are $0.75V_0$, $1.25V_0$ and $2.0V_0$. Solid lines represent the results of simulation in the quantum tomography approach (QT) and dashed lines correspond to the numerical solution of Schrödinger equation (exact quantum computation). With the growth of $|q_0|$ the mean energy increases, which enhances tunneling and reaction probability becomes larger (Fig. 1). The components, that have passed through the barrier, cannot return, because for q > 0.6709 potential decreases with the growth of coordinate. Reaction probability therefore permanently grows with time, at first rapidly, due to transmission of components with the energy higher



Fig. 1. The dimensionless reaction probabilities (16) 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 quantum tomography approach, dashed lines are for the exact numerical solution.



Fig. 2. 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).

than the height of the barrier (classical solution of corresponding problem shows it), and then continues to increase due to tunneling. Due to the finite number of trajectories used in QT simulation, reaction probability for QT case is slightly higher than for the exact computation. For smaller number of trajectories (not shown) reaction probability curves resemble staircase more evidently, and quantitative deviation from exact result is stronger. Our results also agree with those presented in Ref. [16] (method of "Wigner trajectories").

In Fig. 2 we present the dependence of tunneling time on initial mean position of the wave packet. Tunneling time is determined as the difference of

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presence times (18) for points $x_a = 0.5 \times 0.6709$ and $x_b = 2.0 \times 0.6709$ (at x = 0.6709 potential has the maximum). The increase of $|q_0|$ (and corresponding increase of initial mean energy) leads to the growth of average speed both of the transmitted part and of the wave packet as a whole. The transmitted part passes the space between the points x_a and x_b faster, and we observe the decrease of tunneling time (see Fig. 2). Results of QT simulation (squares in Fig. 2) 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 (11) does not represent the quantum tomogram as exactly as for smaller $|q_0|$.

4. Exciton tunneling

The method described in Section 2 can be used to simulate the evolution of systems with more than one degree of freedom. In this section such a possibility is demonstrated. We consider the nonstationary tunneling of the composite particle, exciton in onedimensional (1D) semiconductor structure (quantum wire).

In semiconductor quasi-one-dimensional nanostructure the motion is allowed only in one direction (quantum wire). Transverse motion is restricted due to strong confining barriers. Let us consider the potential barrier in the direction of allowed motion. If an excitonic wave packet prepared, and moves to the barrier, with the help of some detectors one can investigate scattering of the exciton.

We use the constants corresponding to GaAs for reference (dielectric constant $\varepsilon = 12.5$, effective masses of electron and hole are $m_e = 0.07m_e^{(0)}$ and $m_h = 0.15m_e^{(0)}$, where $m_e^{(0)}$ is the electron mass in vacuum). 3D exciton in bulk GaAs is characterized by effective Bohr radius $a^* \approx 10$ nm and binding energy $E_C^* \approx 4$ meV. We use unit of length a^* , unit of mass m_e , and $\hbar = 1$. 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 hydrogen atom. But this is not the case for 1D exciton. First, electron-hole effective interaction potential for 1D problem 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 [36]). Second, corresponding energy spectrum and wave functions of relative motion also change in comparison with the hydrogenlike states. We choose the wave function of the exciton ground state in Gaussian form.

Excitonic wave packet can be represented as a Gaussian wave packet in center-of-mass coordinates

$$\Psi(x_e, x_h, t=0) = \frac{e^{-r^2/(2\sigma)}}{(\pi\sigma)^{1/4}} \frac{e^{-(R-x_0)^2/(2S)+iRp_0}}{(\pi S)^{1/4}},$$
(19)

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: we choose $x_0 = -10$, $p_0 = 3$, S = 2and $\sigma = 1$.

External potential is assumed to be zero everywhere except the region of barrier; we use the barrier of thickness equal to 5 nm, or 0.5 in accepted units. For simplicity we set the barriers for electron and 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

$$V_{\text{ext}}(x) = \begin{cases} C - Dx^2, & \text{if } |x| < \sqrt{C/D}, \\ 0, & \text{if } |x| \ge \sqrt{C/D}, \end{cases}$$
(20)

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:

$$V_{\text{int}}(r) = \begin{cases} Br^2 - A, & \text{if } r < \sqrt{A/B}, \\ 0, & \text{if } r \ge \sqrt{A/B}, \end{cases}$$
(21)

where $r = |x_e - x_h|$. Potential (21) can describe, e.g., e-h interaction in spatially indirect exciton, for example in coupled quantum wires with large interwire separation [37]. Initial wave function of relative motion, chosen to be Gaussian with unity dispersion, is negligible within one percent accuracy at r = 3.



Fig. 3. 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 exact numerical solution (dashed lines). All values are in units $\hbar = m_e^* = E_C = 1$, m_e^* is electron effective mass and E_C is binding energy of the exciton. The height of the barrier C = 1, width $\sqrt{C/D} = 0.5$.

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. For 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. (21) and condition $\sqrt{A/B} = 3$ we have $A \approx 18E_C/17$.

In coordinates x_e and x_h the evolution equations depend on trajectory distribution (see Section 2), potentials are quadratic, therefore the problem considered allows to employ all techniques, developed for one degree of freedom (see Section 3).

Results of exciton tunneling simulation are presented in Figs. 3–5. In Figs. 3 and 4 we show the probability density for electron and hole in successive time moments, barrier height C = 1. Solid lines in Figs. 3, 4 and circles in Fig. 5 correspond to QT simulation, while dashed lines and squares represent the exact numerical computation. Coincidence of QT and exact computation results, initially very good, be-



Fig. 4. 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. 3 are used.



Fig. 5. Probability of exciton ionization P_{Ion} 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. 3.

comes poorer with time (Figs. 3 and 4), but QT simulation reproduces main properties of exciton tunneling: wave packets broadening with time and due to interaction with the barrier, shrinking near the barrier, dividing into two parts (reflected and transmitted). Integral values (in Fig. 5) obtained in QT approach also agree with the exact results.

The electron and hole wave packets begin the motion from the point x = -10 and, shrinking near

the barrier, are partially reflected and transmitted. For the case presented in Figs. 3, 4 about the half of wave packets is transmitted. Interesting is the question about the ionization probability of exciton, induced by interaction with the barrier. If 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 exciton is not ionized after such scattering, because one of the particles can be 'pulled' beyond the barrier, to 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. Denote the probability of ionization due to electron and hole scattering in different directions as P_{Ion} . Then, the probability to find electron and 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 $t \to \infty$.

The probability of ionization due to electron and hole scattering in different directions on the barrier P_{Ion} is presented in Fig. 5. The dependence on barrier height *C* is investigated. 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. 5, and P_{Ion} is maximal 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.

5. Conclusion

We presented the new method for quantum nonstationary processes simulation and applied it to tunneling of one-particle and two-particles wave packets through the potential barriers. The method is based on tomographic representation of quantum mechanics, and uses real nonnegative distribution function to describe the quantum state.

Our method gave the results in agreement with those obtained by the method of "Wigner trajectories" and by exact quantum computation for tunneling of both single-particle wave packet and two particles. We could calculate different characteristics of tunneling: reaction probability, probability densities, tunneling times and ionization probability for composite particle.

Proposed method operates with the ensemble of trajectories generated by the nonnegative state-describing distribution function. The similar approach (in the framework of "Wigner trajectories"), but with the alternating-sign state-describing function, has been already successfully applied for the investigation of tunneling of two identical particles [36]. Many-body problem for fermionic and bosonic systems should be analyzed by means of the quantum tomography method to check if it is useful for extensive manyparticles calculations, particularly to overcome "sign problem" in the simulation of many-fermion system.

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