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Center-of-mass tomographic approach to quantum dynamics

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ABSTRACT

In the tomography representation we propose a new approach, which describes the dynamics of quantum particles by the Kolmogorov equations for non-negative propagators. To solve the Kolmogorov equations we use a diffusive Markovian random processes described by the related nonlinear stochastic Langevin equations. As a result the dynamics of quantum particles is described by the proposed numerical scheme combining both Langevin dynamics and Monte Carlo methods. We test the developed approach by applying it to the wave packet dynamics in harmonic potentials and to particle tunneling through a barrier.

0. Introduction

In the standard formulation of quantum mechanics states of a system are described by the wave functions [1] or the density operators [2,3]. However quantum description of the system can be given in many other ways [4], for example, in the Wigner–Moyal, Feynman or Nonequlibrium Green functions representations [5–7]. Despite the unity of all formulations such objects as the wave functions, probability distributions, the Wigner functions or density operators differ in essential way from each other. Let us note that the probability distribution describing a quantum system is its fundamental characteristic. The probability representation of quantum mechanics or tomography representation was recently proposed in [8–12]. The idea of the tomography representation is to rotate and to scale the reference frame in the phase space and to work with distributions in the new frames: $X = \mu q + \nu p$, where q and p are the coordinate and momentum (μ, ν are the parameters of scaling and rotating). The probability representation is remarkable as it describes the quantum state in terms of a non-negative distribution function (the tomogram or marginal distribution), directly measurable in experiments on the state reconstruction. The tomogram is a probability distribution completely describing a quantum or classical state of the system and is very convenient for comparison results in the framework of one formalism. Sign conservation of the tomogram can be valuable in computer simulations [13,14], for example, to overcome the "sign problem" in simulation of Fermi systems [15]. An important advantage of the probability representation is that the transitions between quantum states are descried by the non-negative probabilities (propagators) instead of complex probability amplitudes.

There are two equivalent probability representations of quantum mechanics: namely 'symplectic' [22,23] and 'center-of-mass' [16–21,24,25] tomography. For example in the symplectic tomography the 1D system of N quantum particles is described by $3N$ variables namely by three N-dimensional vectors $\vec{X}$, $\vec{\mu}$ and $\vec{\nu}$. However the symplectic tomogram contains the same amount of information about the system as the density matrix does due to the fact that the symplectic tomogram is a homogeneous function and only $2N$ of its variables are independent. Sure, this increase in the number of variables is inconvenient in applications even if it implies the description of the system with non-negative distribution function. Alternatively the more convenient 'center-of-mass' tomogram depends on $2N+1$ variables—the 'center-of-mass' scalar variable $X = \sum X_i$, $\vec{X} = \{X_i\}$—and two N-dimensional vectors $\vec{\mu}$, $\vec{\nu}$. The homogeneous 'center-of-mass' tomogram depends on $2N$ independent variables and this representation is also equivalent to the other formulations of quantum mechanics due to existence of the invertible maps for connection between different representations of quantum mechanics.

In this Letter in the framework of the 'center-of-mass' tomography representation of quantum mechanics we use the Kolmogorov

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equations to describe the dynamics of quantum systems. The Kolmogorov equations for the Green functions can be solved by different regular or stochastic methods. In the simplest cases analytical methods can be used, while in general for low dimensional cases numerical schemes on grids are favorable. We have developed a new numerical stochastic approach based on solution of the generalized stochastic Langevin (GSL) equations being equivalent in stochastic sense to the Kolmogorov equations. The developed approach combines both Monte Carlo (MC) sampling and numerical solution of GSL equation for the calculation of average values of quantum operators. Normally MC methods are very effective for calculations of multidimensional integrals as these methods allow to find regions giving the main contribution to the integrals and to ignore other regions, which are not important in integral sense. The Langevin dynamics is also very effective in multidimensional case. We discuss the basic relations and the main ideas of the developed approach, compare the obtained results for average trajectories, average momentum, average energy and related variances with independent calculations for quantum oscillator and quantum particles tunneling through a barrier.

1. One-random-variable tomography

Below, following the above mentioned papers [16–21,24,25], we shortly describe the scheme for the center-of-mass tomography. Let us consider dynamics of quantum particles described by the Hamiltonian with generic potential energy $\tilde{V}$

$$\hat{H} = \frac{\hat{\tilde{p}}^2}{2m} + \tilde{V}(\vec{q}). \tag{1}$$

To consider the evolution of the quantum system let us start from the von Neumann equation

$$i\hbar \frac{\partial \hat{\rho}}{\partial \tilde{t}} = [\hat{H}, \hat{\rho}], \tag{2}$$

which determines the time evolution of the density matrix $\hat{\rho}$ (for example with matrix elements $\rho(\vec{q}', \vec{q}'', t) = \Psi(q', t)\Psi^*(q'', t)$).

The quantum mechanics in Wigner representation can be described in terms of the Wigner function defined by the invertible maps:

$$W(\vec{q}, \vec{p}, t) = \int \frac{d\vec{\xi}}{(2\pi/\alpha_1)^{\tilde{N}}} \rho\left(\vec{q} + \frac{\vec{\xi}}{2}, \vec{q} - \frac{\vec{\xi}}{2}, t\right) e^{-i\alpha_1 \langle \vec{p} | \vec{\xi} \rangle}, \tag{3}$$

$$\rho(\vec{q}', \vec{q}'', t) = \int d\vec{p}\, W\left(\frac{\vec{q}' + \vec{q}''}{2}, \vec{p}, t\right) e^{i\alpha_1 \langle \vec{p} | (\vec{q}' - \vec{q}'') \rangle}, \tag{4}$$

where $\tilde{N} = Nd$, d denotes the dimensionality of the space, N is the number of particles and dimensionless particle coordinates $\vec{q} = \tilde{q}/\sigma_0$ and momenta $\vec{p} = \tilde{p}/p_0$ are in units of σ_0 and p_0, while $\alpha_1 = p_0\sigma_0/\hbar$. Eq. (4) is the inverse map with respect to Eq. (3).

The time evolution equation of the quantum system in terms of the Wigner function can be obtained from the von Neumann equation (2) and has the form:

$$\frac{\partial W}{\partial t} + \left\langle \frac{\vec{\tilde{p}}}{m} \middle| \frac{\partial W}{\partial \vec{\tilde{q}}} \right\rangle = \frac{i}{\hbar}\left[\tilde{V}\left(\vec{\tilde{q}} - \hbar \frac{i}{2}\frac{\partial}{\partial \vec{\tilde{p}}}\right) - \tilde{V}\left(\vec{\tilde{q}} + \hbar \frac{i}{2}\frac{\partial}{\partial \vec{\tilde{p}}}\right)\right] W. \tag{5}$$

The connection between the 'center-of-mass' tomograms and the Wigner functions is given by the following invertible maps:

$$\tilde{w}(X, \vec{\mu}, \vec{\nu}, t) = \int \frac{dk\, d\vec{q}\, d\vec{p}}{2\pi} W(\vec{q}, \vec{p}, t) e^{-ik(X - \langle \vec{\mu} | \vec{q} \rangle - \langle \vec{\nu} | \vec{p} \rangle)}, \tag{6}$$

$$W(\vec{q}, \vec{p}, t) = \int \frac{dX\, d\vec{\mu}\, d\vec{\nu}}{(2\pi)^{2\tilde{N}}} \tilde{w}(X, \vec{\mu}, \vec{\nu}, t) e^{i(X - \langle \vec{\mu} | \vec{q} \rangle - \langle \vec{\nu} | \vec{p} \rangle)}. \tag{7}$$

Consequently the evolution equation for the marginal distribution function according to the definition (3) and Eqs. (5), (6) can be obtained in the form:

$$\frac{\partial w}{\partial t} - \left\langle \vec{\mu} \middle| \frac{\partial}{\partial \vec{\nu}} w \right\rangle - i\left[V\left(-\frac{\partial}{\partial \vec{\mu}} \frac{1}{\partial/\partial X} - i\frac{\vec{\nu}}{2}\frac{\partial}{\partial X}\right) - V\left(-\frac{\partial}{\partial \vec{\mu}} \frac{1}{\partial/\partial X} + i\frac{\vec{\nu}}{2}\frac{\partial}{\partial X}\right)\right] w = 0. \tag{8}$$

Eq. (8) can be rewritten as

$$\frac{\partial w}{\partial t} + \frac{\partial w}{\partial X} G_X + \left\langle \frac{\partial w}{\partial \vec{\nu}} \middle| \vec{G}_\nu \right\rangle + \left\langle \frac{\partial w}{\partial \vec{\mu}} \middle| \vec{G}_\mu \right\rangle = 0. \tag{9}$$

An example for the functions G is given below. The evolution equation (9) has the form of a continuity equation for the quantum tomogram

$$\frac{dw}{dt} = \frac{\partial w}{\partial t} + \frac{\partial w}{\partial X}\dot{X} + \left\langle \frac{\partial w}{\partial \vec{\nu}} \middle| \dot{\vec{\nu}} \right\rangle + \left\langle \frac{\partial w}{\partial \vec{\mu}} \middle| \dot{\vec{\mu}} \right\rangle = 0, \tag{10}$$

where the equations $\dot{X}(t) = G_X$, $\dot{\vec{\nu}}(t) = \vec{G}_\nu$ and $\dot{\vec{\mu}}(t) = \vec{G}_\mu$ define trajectories in $X, \vec{\nu}, \vec{\mu}$ space. The quantum tomograms w are nonnegative and can be used as distribution functions.

2. Propagators and Kolmogorov equations

Let us now turn to the propagators (the Green functions) Π describing the time evolution of quantum systems independent of the initial state. The propagator Π obeys an evolution equation which follows from Eq. (9)

$$\frac{\partial \Pi}{\partial t} + \frac{\partial \Pi}{\partial X} G_X + \left\langle \frac{\partial \Pi}{\partial \vec{\nu}} \middle| \vec{G}_\nu \right\rangle + \left\langle \frac{\partial \Pi}{\partial \vec{\mu}} \middle| \vec{G}_\mu \right\rangle = \delta(t - t_0)\delta(X - X_0)\delta(\vec{\mu} - \vec{\mu}_0)\delta(\vec{\nu} - \vec{\nu}_0), \tag{11}$$

where δ is the Dirac delta function and with the initial condition at ($\Delta t = t - t_0 = 0$)

$$\Pi(X, \vec{\mu}, \vec{\nu}, t; X_0, \vec{\mu}_0, \vec{\nu}_0, t_0) = \delta(X - X_0)\delta(\vec{\mu} - \vec{\mu}_0)\delta(\vec{\nu} - \vec{\nu}_0). \tag{12}$$

Using the decomposition of unity $1 \equiv \sum_i [\theta(q_i - \sigma/2) - \theta(q_i + \sigma/2)] \equiv \sum_i \varphi(q_i)$ in the limit of $\sigma \to 0$ ($q_i = \sigma \times i, i = 0, \mp 1, \ldots$, $\theta(q) = 0$ for $q < 0$ and $\theta(q) = 1$ for $q > 0$) one can present a general Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(q)$ as a sum of its local harmonic approximations in the vicinity of each point q_i. Let us illustrate this for the simple example for one particle in the 1D case

$$\hat{H} = \left[\frac{\hat{p}^2}{2m} + \hat{V}(q)\right] \times 1 = \sum_i \varphi(q_i)\hat{H}_{q_i} \simeq \sum_i \varphi(q_i)\left[\frac{\hat{p}^2}{2m} + \hat{V}(q_i) + \frac{d\hat{V}(q_i)}{dq_i}(q - q_i) + \frac{1}{2}\frac{d^2\hat{V}(q_i)^2}{dq_i^2}(q - q_i)^2 + \cdots\right]. \tag{13}$$

According to Eqs. (8)–(10) the local functions G and related trajectories for each point q_i are defined by $\dot{X}(t) = G_X = f\nu$, $\dot{\mu}(t) = G_\mu = \omega^2\nu$, $\dot{\nu}(t) = G_\nu = -\mu$ with $\omega^2 = \frac{d^2V(q_i)}{dq_i^2}$, $\beta^2 = -\omega^2$, $f = \omega^2 q_i - \frac{dV(q_i)}{dq_i}$. For small $\Delta t = t - t_0 \neq 0$ the quasiclassical Green function $\tilde{\Pi}$ in the small vicinity of point q_i can be obtained analytically in the form [8,9]

$$\tilde{\Pi}(z_1, t_1; z_2, t_2 | q_i) = \delta\left(X_2 - X_1 - f\left(\nu_1 \frac{\sinh(\beta(t_2 - t_1))}{\beta}\right.\right.$$

$$+\frac{\mu_1(\cosh(\beta(t_2-t_1))-1)}{\omega^2}\Big)\Big)$$
$$\times\delta\Big(\mu_2-\mu_1\cosh\big(\beta(t_2-t_1)\big)-\frac{\nu_1\omega^2}{\beta}\sinh\big(\beta(t_2-t_1)\big)\Big)$$
$$\times\delta\Big(\nu_2-\nu_1\cosh\big(\beta(t_2-t_1)\big)+\frac{\mu_1}{\beta}\sinh\big(\beta(t_2-t_1)\big)\Big), \qquad (14)$$

where $\Delta t = t_2 - t_1 \to 0$.

The Chapman–Kolmogorov equation (generalized Markov equation) [8,26] for Π has the form

$$\Pi(z_1,t_1;z_3,t_3)=\int \Pi(z_1,t_1;z_2,t_2)\Pi(z_2,t_2;z_3,t_3)\,dz_2, \qquad (15)$$

where $t_1 < t_2 < t_3$, vector z is defined as $|z\rangle = |z^1,\dots,z^n\rangle = \{X,\vec{\mu},\vec{\nu}\}$ and $n = 2\tilde{N}+1$. The propagator $\Pi(X_1,\vec{\mu}_1,\vec{\nu}_1,t_1;X,\vec{\mu},\vec{\nu},t) = \Pi(z_1,t_1;z,t)$ can be considered as transition probability of a Markovian random process (MP) as the following relations are satisfied

$$\Pi(z_1,t_1;z,t)\geqslant 0, \qquad \int dz\,\Pi(z_1,t_1;z,t)=1. \qquad (16)$$

Treatment of Markovian process can be strongly simplified by using the two partial differential equations proved by Kolmogorov [27] in 1931 for diffusive MP. The first and the second Kolmogorov equations with *required accuracy* have the forms

$$\frac{\partial\Pi}{\partial t_1}+\sum_{j=1}^{n}a_j(z_1,t_1)\frac{\partial\Pi}{\partial z_1^j}+\frac{1}{2}\sum_{j=1}^{n}\sum_{l=1}^{n}b_{jl}(z_1,t_1)\frac{\partial^2\Pi}{\partial z_1^j\partial z_1^l}=0,$$
$$\frac{\partial\Pi}{\partial t_2}+\sum_{j=1}^{n}\frac{\partial}{\partial z_2^j}\big(a_j(z_2,t_2)\Pi\big)-\frac{1}{2}\sum_{j=1}^{n}\sum_{l=1}^{n}\frac{\partial^2}{\partial z_2^j\partial z_2^l}\big(b(z_2,t_2)\Pi\big)=0, \qquad (17)$$

where the drift and diffusion coefficients are implicitly defined by the following relations respectively

$$a_j(z,t)=\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int \Pi(z,t;\tilde{z},t+\Delta t)\big(\tilde{z}^j-z^j\big)\,d\tilde{z},$$
$$b_{jl}(z,t)=\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int \Pi(z,t;\tilde{z},t+\Delta t)\big(\tilde{z}^j-z^j\big)\big(\tilde{z}^l-z^l\big)\,d\tilde{z}. \qquad (18)$$

Limits of small Δt relate to the quasiclassical approximation of the Green function and can be explicitly calculated using the quasiclassical propagator $\tilde{\Pi}(z,t;\tilde{z},t+\Delta t|q_i)$ (Eq. (14)). In this case the drift $a_j(z,t|q_i)$ and diffusion coefficients $b_{jl}(z,t|q_i)$ as well as the propagator $\Pi(X_1,\vec{\mu}_1,\vec{\nu}_1,t_1;X,\vec{\mu},\vec{\nu},t|q_i)$ should depend on the coordinate q_i and are correct only in its small vicinity. The second Kolmogorov equation before its rigorous derivation by Kolmogorov was used by physicists and is often called Fokker–Plank equation. Generalization to 3D Hamiltonian and N particles is trivial.

The distributions $w(X,\vec{\mu},\vec{\nu},t)$, related to different reference frames ($X = \langle\vec{\mu}|\vec{q}\rangle + \langle\vec{\nu}|\vec{p}\rangle$), have different physical meanings. For example, for the 1D case the tomogram $w(X,1,0,t_2)$ has the physical meaning of the coordinate distribution and for small Δt its time evolution can be presented in the following form as it follows from Eqs. (8)–(10), (13)

$$w(X_2,\mu_2|_{\mu_2=1},\nu_2|_{\nu_2=0},t_2)$$
$$=\sum_i w(X_2,\mu_2|_{\mu_2=1},\nu_2|_{\nu_2=0},t_2|q_i)$$
$$=\sum_i\int dX_1\,d\mu_1\,d\nu_1$$
$$\times\Pi(X_1,\vec{\mu}_1,\vec{\nu}_1,t_2;X_2,\mu_2|_{\mu_2=1},\nu_2|_{\nu_2=0},t_2-\Delta t|q_i)$$
$$\times w(X_1,\vec{\mu}_1,\vec{\nu}_1,t_2-\Delta t), \qquad (19)$$

where the propagator Π can be obtained as solution of Kolmogorov equations or the equivalent system of Langevin equations (see below). Here each term in sum is the contribution of a dynamic trajectory (defined by q_i) in $X,\vec{\nu},\vec{\mu}$ space. The main contribution to this sum can be calculated for example by Monte Carlo methods sampling q_i from tomogram $w(X,\mu|_{\mu=1},\nu|_{\nu=0},t_2)$. The contribution of each trajectory is correct for small enough $\Delta t = t_2 - t_1$. A possible criterion for the correctness is the smallness of the difference along the average trajectory $\langle q(t_2-\Delta t)\rangle$ between the exact potential $V(\langle q(t_2-\Delta t)\rangle)$ and its harmonic approximation $V_{\langle q(t_2)\rangle}(\langle q(t_2-\Delta t)\rangle)$ taken at point $\langle q(t_2)\rangle$ (for example, less than 0.001 percent). If this difference becomes larger then the next local piece of solution (from $t_2-\Delta t$ to $t_2-2\Delta t$) can be obtained by recurrent application of Eq. (19) replacing $w(X,\mu,\nu,t_2)$ by $w(X,\mu,\nu,t_2-\Delta t)$ and $w(X,\mu,\nu,t_2-\Delta t)$ by $w(X,\mu,\nu,t_2-2\Delta t)$. An analogous solution can be obtained for the momentum distribution $w(X,0,1,t_2)$.

To be able to obtain the different distributions simultaneously we assume that the product of the Green functions $\Pi(U_1,t_2;U_2,t_1|q_i) = \prod_{k=1}^{s}\Pi(X_k^1,\vec{\mu}_k^1,\vec{\nu}_k^1,t_2;X_k^2,\vec{\mu}_k^2,\vec{\nu}_k^2,t_1|q_i)$ defines s Markovian random processes of $|U(t)\rangle = \{X_k,\vec{\mu}_k,\vec{\nu}_k,(k=1,\dots,s)\}$ with s different initial conditions $|U_k(t_2)\rangle = \{X_k(t_2),\vec{\mu}_k(t_2),\vec{\nu}_k(t_2)\}$ at $t=t_2$. Let us define the initial function w as the product $w(U,t_1) = \prod_{k=1}^{s} w(X_k^1,\vec{\mu}_k^1,\vec{\nu}_k^1,t_1)$ in direct sum of $\{X,\vec{\mu},\vec{\nu}\}$ spaces. So vector $|U(t)\rangle$ is defined by the expression $|U\rangle = \{z^1,\dots,z^n\} = \{X_1,\vec{\mu}_1,\vec{\nu}_1,\dots,X_s,\vec{\mu}_s,\vec{\nu}_s\}$, $n = (2\tilde{N}+1)*s$ and all multidimensional distributions of the Markovian random processes $|U(t)\rangle$ are defined by the initial distribution $w(U,t_1)$ and transition probability $\Pi(U_1,t_2;U_2,t_1|q_i)$. Let us assume that $s=1$ always relates to initial conditions defining coordinate distributions.

3. Stochastic differential equations

Quantum dynamics of the system is defined by the time evolution of the initial tomogram according to Eqs. (8), (17). To obtain the time evolution Eq. (17) can be replaced by the system of nonlinear GSL equations of the form [26,27]

$$\frac{dU_j(t)}{dt}=\psi_j\big(\vec{U}(t),t|q_i\big)+\sum_{l=1}^{n}g_{jl}(q_i)\xi_l(t) \quad (j=1,n), \qquad (20)$$

where ψ_j and g_{jl} are given deterministic functions of their arguments, while $\xi_l(t)$ are independent delta correlated random processes of white noise with zero expectation value. These equations allow to solve equations Eqs. (8), (17) if the drift and diffusion coefficients in Eq. (17) are connected with functions ψ_j and matrix g_{jl} in Eq. (20) by the following expressions [26,27]

$$b_{jl}(U,t|q_i)=\sum_{k=1}^{n}g_{jk}g_{lk},$$
$$a_j(U,t|q_i)=\psi_j(U,t|q_i)+\frac{1}{2}\sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial g_{jl}}{\partial z_k}g_{kl}. \qquad (21)$$

So the time evolution of any initial tomogram (Eq. (19)) can be calculated as the average over an ensemble of random Markovian processes described by the systems of nonlinear GSL (Eq. (20)).

To finish this discussion, let us note that the expression

$$\frac{1}{2}\sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial g_{jl}(U,t|q_i)}{\partial U^k}g_{kl}(U,t|q_i)$$
$$=\lim_{\Delta t\to 0}\frac{1}{\Delta t}M\left\{\sum_{l=1}^{n}g_{jl}\left[U+\frac{\Delta U(t)}{2},t|q_i\right]\Delta\eta_l(t)\right\} \qquad (22)$$

can be calculated according to the definition of g from the relation

$$b\left[U+\frac{\Delta U(t)}{2}\middle|q_i\right]=g\left[U+\frac{\Delta U(t)}{2},t|q_i\right]g'\left[U+\frac{\Delta U(t)}{2},t|q_i\right], \quad (23)$$

where ΔU and $\Delta\eta_l$ denote the increments of related random processes, while M means expectation value for averaging over the before mentioned normal Wiener processes $\eta_l(t)$.

4. Numerical scheme

For a numerical solution the symbolic equation (20) should be rewritten in finite-difference form

$$dU_j(t)=\psi_j\big(U(t),t|q_i\big)\,dt+\sum_{l=1}^{n}g_{jl}\,d\eta_l(t) \quad (j=1,n), \quad (24)$$

where $d\eta_l(t)$ is an increment of a normal Wiener random process [26]. For the solution of last Eq. (24) we use the 'predictor-corrector' scheme developed for numerical simulation of gas and plasma dynamics by particle-in-cell method [28]:

$$\begin{aligned}U_j^{k+0.5}&=U_j^k+\frac{\tau}{2}\psi_j\big(U^k,t^k|q_i\big)+\sum_{l=1}^{n}g_{jl}\big(U^k,t^k|q_i\big)[\Delta\eta_l]_{1/2},\\ U_j^{k+1}&=U_j^k+\tau\psi_j\big(U^{k+0.5},t^{k+0.5}|q_i\big)\\ &\quad+\sum_{l=1}^{n}g_{jl}\big(U^{k+0.5},t^{k+0.5}|q_i\big)\Delta\eta_l,\end{aligned} \quad (25)$$

where τ is the small time step for numerical integration of these equations, U_j^k relates to time $t^k=t_2+k*\tau$, $\Delta\eta_l=\tilde{\gamma}_l^k\sqrt{|\tau|}$ and $[\Delta\eta_l]_{1/2}=0.5\gamma_l^k\sqrt{|\tau|}$, while $\tilde{\gamma}_l^k$ and γ_l^k are normal Gaussian random values. This scheme is written for given q_i and relates to the symmetrized form of solution of stochastic differential equation (Stratonovich integration).

However as was mentioned before the global solution of Eq. (17) can be obtained as the sequence of matched local solutions by recurrent application of Eq. (19). So for the global solution we need a series of particle coordinates $q^k=q(t^k)$ sampled from of the marginal distribution functions $w(U_1(t^k)|q(t^k))$ related to times t^k and random process $U_1=\{X_1,\mu_1,\nu_1\}$ (with initial condition $\{X=0,\mu=1,\nu=0\}$ at $t=t_2$). So the full algorithm for numerical solution of generalized Langevin equation can be written in the form:

Calculate $q^{k+0.5}=\langle q(t^{k+0.5})\rangle$ from $w\big(U_1(t^k-\tau/2),t^k-\tau/2|q(t^k)\big)$

$$\begin{aligned}U_j^{k+0.5}&=U_j^k+\frac{\tau}{2}\psi_j\big(U^k,t^k|q^{k+0.5}\big)+\sum_{l=1}^{n}g_{jl}\big(U^k,t^k|q^{k+0.5}\big)[\Delta\eta_l]_{0.5},\\ U_j^{k+1}&=U_j^k+\tau\psi_j\big(U^{k+0.5},t^{k+0.5}|q^{k+0.5}\big)\\ &\quad+\sum_{l=1}^{n}g_{jl}\big(U^{k+0.5},t^{k+0.5}|q^{k+0.5}\big)\Delta\eta_l.\end{aligned}$$

If the parabolic approximation becomes wrong sample $q^{k+0.5+m}$ from

$$w\big(U_1(t^{k+m}-\tau/2),t^{k+m}-\tau/2|q(t^{k+m})\big), \quad (26)$$

where $m\sim 1\backsim 100$. Sampling is taken only if the error of the parabolic approximation of potential along the average trajectory is larger than a given small value. Sure the presented algorithm is only one of the possible numerical schemes to solve system of Langevin equation and we are working on an improvement of the numerical accuracy of our calculations.

5. Initial conditions and average values

In presented calculations for 1D case the initial wave functions $\psi(q)$ were chosen in Gaussian form describing, for example, the ground state of the harmonic oscillator

$$\psi_0(q)=(A/\pi)^{1/4}\exp\left(-\frac{A}{2}(q-q_0)^2+ipp_0\right). \quad (27)$$

From (Eq. (3)) the corresponding Wigner function looks like

$$W_0(q,p)=\exp\big(-A(q-q_0)^2\big)\exp\big(-B(p-p_0)^2\big)(A*B)^{1/2}/\pi, \quad (28)$$

where $B=1/A$. The tomogram of Gaussian states as it follows from Eq. (6) has the form

$$\begin{aligned}w_0(X,\mu,\nu)&=\frac{\exp(-(X-\mu q_0-\nu p_0)^2/C)}{\sqrt{\pi C}},\\ C&=\left(\frac{\mu^2}{A}+\frac{\nu^2}{B}\right).\end{aligned} \quad (29)$$

The average values of quantum operators $\hat{A}$ defined in terms of density matrix read

$$\langle\hat{A}(t)\rangle=\mathrm{Tr}\big(\hat{\rho}(t)\hat{A}\big) \quad (30)$$

where $\mathrm{Tr}\,\hat{\rho}=1$. In the Wigner–Moyal formulation of quantum mechanics $\langle\hat{A}\rangle$ can be rewritten as

$$\langle\hat{A}(t)\rangle=\int A^W(\vec{q},\vec{p})W(\vec{q},\vec{p},t)\,d\vec{q}\,d\vec{p}, \quad (31)$$

where the Weil symbol of the operator is given by

$$A^W(\vec{q},\vec{p})=\int A\left(\vec{q}-\frac{\vec{\xi}}{2},\vec{q}+\frac{\vec{\xi}}{2},t\right)\mathrm{e}^{\mathrm{i}\alpha_1\langle\vec{p}|\vec{\xi}\rangle}\,d\vec{\xi}. \quad (32)$$

The expression for the average values in the center-of-mass tomography formulation is obtained using the relation between w and the Wigner function

$$\begin{aligned}\langle\hat{A}(t)\rangle&=\int\exp(iX)w(X,\vec{\mu},\vec{\nu},t)A(\vec{\mu},\vec{\nu})\,dX\,d\vec{\mu}\,d\vec{\nu},\\ A(\vec{\mu},\vec{\nu})&=\int A^W(\vec{q},\vec{p})\exp\big(-i\big(\langle\vec{\mu}|\vec{q}\rangle+\langle\vec{\nu}|\vec{p}\rangle\big)\big)\frac{d\vec{q}\,d\vec{p}}{(2\pi)^{2\tilde{N}}}.\end{aligned} \quad (33)$$

If the considered operators depend only on coordinates or momenta then formula Eq. (33) can be transformed to

$$\begin{aligned}\langle\hat{A}_q(t)\rangle&=\int A_q(X)w(X,\mu_1=1,\vec{\tilde{\mu}}=0,\vec{\nu}=0,t)\,dX,\\ \langle\hat{A}_p(t)\rangle&=\int A_p(X)w(X,\vec{\mu}=0,\nu_1=1,\vec{\tilde{\nu}}=0,t)\,dX,\end{aligned} \quad (34)$$

where $A_q(X)\equiv A^W(q)$ $(A_p(X)\equiv A^W(p))$, $\vec{\tilde{\mu}}(\vec{\tilde{\nu}})$ designates all $\mu_j(\nu_j)$ except for the specified $\mu_j=1$ $(\nu_j=1)$ at time t. As discussed before, the calculation of average values according to Eq. (34) can be done simultaneously for a proper choice of random Markovian processes with proper initial conditions $\{X_k,\mu_k,\nu_k,k=1,\ldots,s\}$. In this Letter in 1D case we choose $s=2$ and take for coordinates $(k=1)$ $\{X_1=0,\mu_1=1,\nu_1=0\}$, while for momentum $(k=2)$ $\{X_2=0,\mu_2=0,\nu_2=1\}$. This set of initial values allows us to calculate average energy $\langle E(t)\rangle=\langle\hat{H}(t)\rangle$ according to the expression

$$\begin{aligned}\langle\hat{H}(t)\rangle&=\int K_p^W(X)w(X,\vec{\mu}=0,\nu_1=1,\vec{\tilde{\nu}}=0,t)\,dX\\ &\quad+\int V_q^W(X)w(X,\mu_1=1,\vec{\tilde{\mu}}=0,\vec{\nu}=0,t)\,dX,\end{aligned} \quad (35)$$

where $K_p^W(X)=p^2/2|_{p=X}$ and $V_q^W(X)=V(q)|_{q=X}$.

For a pure state $\rho(q,q') = \psi(q)\psi^*(q)$ and the tomograms w are connected with the density matrix ρ by relation [16–18]

$$w(X,\mu,\nu,t) = \begin{cases} \frac{1}{2\pi|\nu|}\left|\int \psi(y)\exp(-i\frac{\mu}{2|\nu|}y^2 - i\frac{X}{\nu}y)\,dy\right|^2, & \nu \neq 0, \\ \frac{1}{2\pi|\mu|}\left|\int \tilde{\psi}(p)\exp(-i\frac{\nu}{2|\mu|}p^2 + i\frac{X}{\mu}p)\,dp\right|^2, & \mu \neq 0, \end{cases}$$

$$\tilde{\psi}(p) = \frac{1}{2\pi}\int \psi(y)\exp(-ipy)\,dy. \tag{36}$$

So for the before mentioned set of initial conditions the tomograms are equal to the wave functions $|\psi(q)|^2$ or $|\psi(p)|^2$. For both $\mu = \nu = 0$ we get $w(X,0,0) = \delta(X)$.

6. Wigner–Moyal approach

The integral form of the Wigner–Liouville (WL) equation can be derived by adding the classical force term to both parts of Eq. (5). Then we can rewrite the evolution equation as

$$\frac{\partial W}{\partial t} + \left\langle \frac{p}{m} \middle| \frac{\partial W}{\partial \vec{q}} \right\rangle + \left\langle F(\vec{q}) \middle| \frac{\partial W}{\partial \vec{p}} \right\rangle = \int_{-\infty}^{\infty} d\vec{s}\, W(\vec{p}-\vec{s},\vec{q},t)\omega(\vec{s},\vec{q}), \tag{37}$$

with $\omega(\vec{s},\vec{q}) = \frac{2}{(2\pi)^N}\int d\vec{q}'\, V(\vec{q}-\vec{q}')\sin(\frac{2(\vec{s}|\vec{q}')}{\hbar}) + \vec{F}(\vec{q})\frac{d\delta(\vec{s})}{d\vec{s}}$. Using Hamiltonian equations let us introduce the dynamic trajectories $\{\bar{q}_t(t;p_{\tau'},q_{\tau'},\tau'), \bar{p}_t(t;p_{\tau'},q_{\tau'},\tau')\}$ starting from point $p_{\tau'}, q_{\tau'}$ at time τ' and evolving according to

$$d\bar{p}/d\tau = F(\bar{q}(t)), \quad \bar{q}_{\tau'}(\tau';p_{\tau'},q_{\tau'},\tau') = q_{\tau'},$$

$$d\bar{q}/d\tau = \bar{p}(t)/m, \quad \bar{p}_{\tau'}(\tau';p_{\tau'},q_{\tau'},\tau') = p_{\tau'}$$

and the Green function $\Pi^W(p,q,t;p_{\tau'},q_{\tau'},\tau') = \delta(p-\bar{p}_t(t;p_{\tau'},q_{\tau'},\tau'))\delta(q-\bar{q}_t(t;p_{\tau'},q_{\tau'},\tau'))$. Then the integral form of the Wigner–Liouville equation (37) can be written as [29–32]:

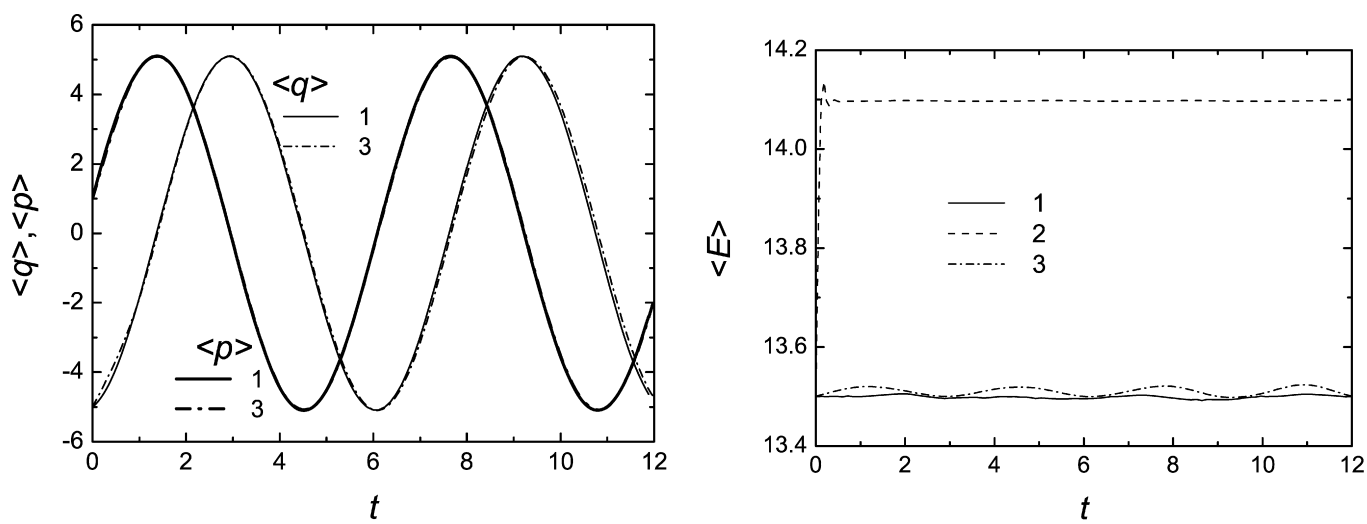

Fig. 1. (a) Average coordinate $\langle q(t)\rangle$ and momentum $\langle p(t)\rangle$ for oscillator, (b) Average energy for oscillator. Solid lines (1) tomography approach, dashed lines (2) the first iteration in Wigner approach, dash-dotted lines (3) finite–difference solution of the Schrödinger equation. The occouring oscillation in energy is a finite-size effect which vanishes for higher grid resolution.

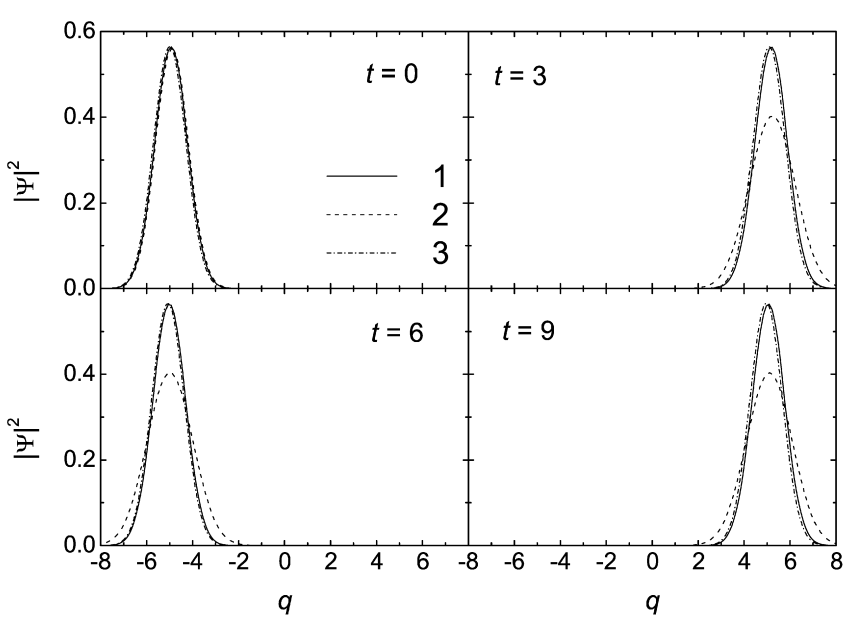

Fig. 2. Square of the wave function modulus for harmonic oscillator at different times. Notations are the same as in Fig. 1.

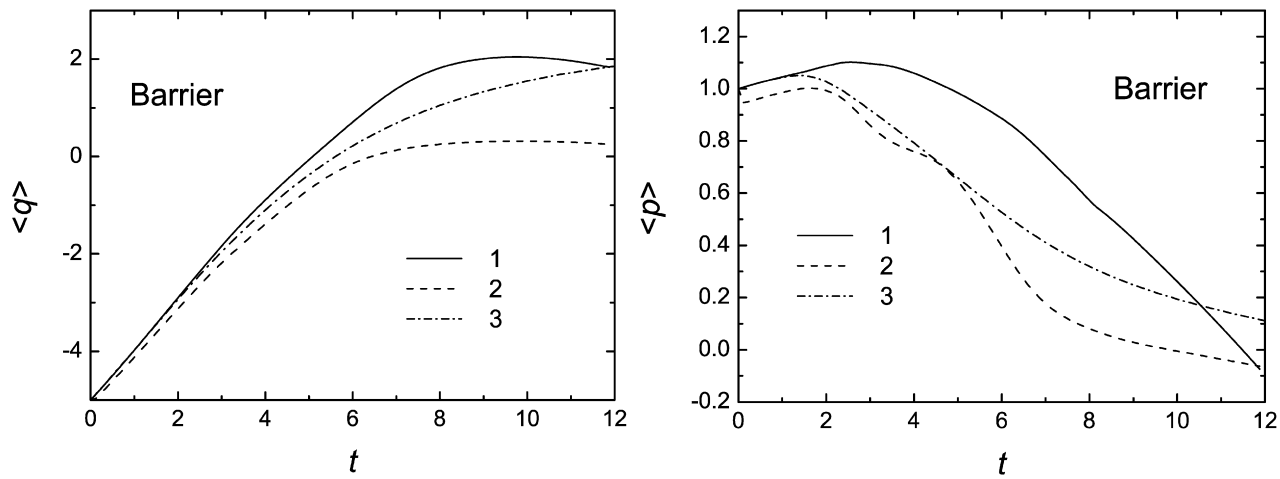

Fig. 3. Average coordinate $\langle q(t)\rangle$ (left) and momentum $\langle p(t)\rangle$ (right) for a wave packet tunneling through the barrier. Notations are the same as in Fig. 1.

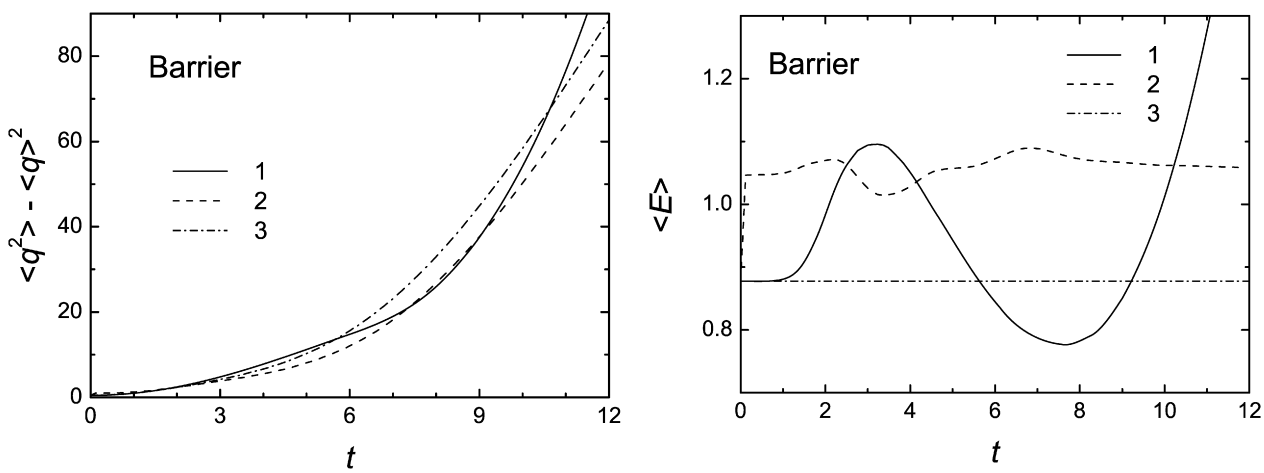

Fig. 4. Variance of coordinate $\langle q(t)\rangle$ for a quantum particle tunneling through the barrier (left). Average energy for a wave packet tunneling through the barrier (right). Notations are the same as in Fig. 1.

$$W(\vec{p},\vec{q},t) = \int \Pi^W(\vec{p},\vec{q},t;\vec{p}_0,\vec{q}_0,0) \times W_0(\vec{p}_0,\vec{q}_0)\,d\vec{p}_0\,d\vec{q}_0 + \int_0^t d\tau' \iint d\vec{p}_{\tau'}\,d\vec{q}_{\tau'}\,\Pi^W(\vec{p},\vec{q},t;\vec{p}_{\tau'},\vec{q}_{\tau'},\tau') \times \int_{-\infty}^{\infty} d\vec{s}\,W(\vec{p}_{\tau'}-\vec{s},\vec{q}_{\tau'},\tau')\omega(\vec{s},\vec{q}_{\tau'}), \tag{38}$$

where $\tau' \in [0,t]$. The first term in Eq. (38) gives the classically evolving initial distribution $W^0(\bar{p}_0,\bar{q}_0)$ which may correspond to a pure quantum state (for example, the ground state). Thus this term describes not classical but rather quantum effects and may contain arbitrary high degrees of Planck's constant. Presenting the solution of Eq. (38) as iteration series, we can take into account all corrections to classical dynamics of the quantum distribution [29–33]. In this Letter for comparison of results in tomography and Wigner representation of quantum dynamics we are going to use only the first term of the iteration series, namely the first term in Eq. (38). In this approximation we can also calculate the averaged values of quantum operators in Wigner representation (using Eq. (31)).

7. Numerical results

In this section we are going to test the developed approach. We compare results obtained by tomography approach (TA) with independent finite difference solutions of the Schrödinger equation (SE) and results obtained by using the first term of iteration series in Wigner approach (WA) for a 1D harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2} + \frac{q^2}{2}$ and a quantum particle tunneling through the barrier ($V_1(q) = \exp(-q)$) in a very broad harmonic trap $V_2(q) = 0.01\frac{q^2}{2}$. The broad harmonic trap $V_2(q)$ is introduced to prevent a fast decay of the wave packet after the barrier in infinite space.

Results for harmonic oscillator are presented by Figs. 1 and 2. Fig. 1(a) presents average trajectories $\langle q(t)\rangle$ and $\langle p(t)\rangle$ (Eq. (34)). All average trajectories practically coincide with each other. Fig. 1(b) shows average energies. Here average energies in TA and SE practically coincide, while the average energy from WA deviates by 4% from exact values (SE).

Fig. 2 presents $|\psi(q,t)|^2$ (Eq. (36)) from TA, WA and SE. Agreement between TA and SE wave packets is good, but WA results deviate from exact wave functions.

As it follows from previous consideration the developed approach is exact for harmonic potential and that is the reason of excellent agreement of the presented TA and SE results.

Now let us consider analogous results for particle tunneling through a barrier. Fig. 3 presents average $\langle q(t)\rangle$ and $\langle p(t)\rangle$ trajectories. Here the tunneling time (time of crossing barrier) is of order 1. Now agreement between TA, WA and SE is worse. The physical reason for this disagreement is that for large times t the tomograms are widely spread and very flat if the particle can move

to infinity after interaction with the barrier. So the main contributions to $\langle q(t)\rangle$ and $\langle p(t)\rangle$ come from large values of coordinate and momentum $(q * w(\vec{U}_1(t)), p * w(\vec{U}_2(t)))$. Now average trajectories are small in comparison with positive and negative contributions (from $q > 0$ ($p > 0$) and $q < 0$ ($p < 0$)). To improve the accuracy of our calculations we should develop a more sophisticated numerical scheme for the solution of the system of stochastic Langevin equations. This is our task for future activity.

Results for the squares of probable deviations from the average $\langle q(t)\rangle$ trajectories in TA, WA and SE are presented by Fig. 4. Now as in the previous case we have moderate disagreement between TA, WA and SE approach. Physical reasons of this difference is the same and have been discussed before.

Results for average energy in TA, WA and SE are shown in Fig. 4. Deviations of TA and WA from the exact values is of order 15%.

8. Conclusion

In the framework of the center-of mass tomography representation of quantum mechanics the tomograms defined by the time evolution equations are positive and are associated with probability distributions of random variables. In this Letter we present an approach which describes the dynamics of quantum particles by the Kolmogorov equations for the Green functions. To solve Kolmogorov equations we use diffusive Markovian random processes described by the nonlinear stochastic Langevin equations related to Kolmogorov equations. As a result, the quantum dynamics can be described by Markovian random processes, which can be generated by the proposed numerical scheme combining finite-difference time steps and random sampling. The developed approach is exact for harmonic potentials and that is the reason of the excellent agreement of the presented results with an independent finite-difference solution of the Schrödinger equation. Preliminary results for particles tunneling through a barrier show that the numerical scheme used in this Letter for the solution of the stochastic equations has moderate accuracy and should be modified to reduce systematical errors in calculations for long calculation times.

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