Studying open quantum systems by means of a deterministic approach to approximate functional integration

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Representation of propagator for open quantum systems in the form of a double functional integral with respect to conditional Wiener measure is proposed. It allows one to apply the approximate formulas exact for functional polynomials of a certain power to calculation of such integrals. Within this deterministic approach the problem is reduced to evaluation of usual (Riemann) integrals of low multiplicity. The formulas are in fact the basis of a numerical method of studying time evolution of the systems. The features of the method are discussed and some examples of calculations are given.

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The development of approximate functional integration techniques promotes a wide utilization of functional integrals in contemporary physics. The Monte Carlo technique is a powerful tool and it is the most frequently used in applications. However, the problem of further development and creation of the methods which allow one to decrease computational burden for achievement of satisfactory results is always actual. Along with the Monte Carlo method there were suggested deterministic approaches [1–8]. In 1951 R. Cameron offered a formula for approximate evaluation of Wiener functional integrals, which is exact for functional polynomials of a third power [1]. The formula is similar to the quadrature rules for usual (Riemann) integrals, which are exact for algebraic polynomials of a certain power. Such an approach has later been applied to a general case of Gaussian measures [6] and to the case of functional polynomials of an arbitrary given power [7,8]. Cameron also established a connecting link between the Feynman path integral and the Wiener integral [9]. The approach was developed further by Doss, Azencott, and Haba [10–12]. Haba obtained a formula which expressed the Feynman propagator through a functional integral with respect to conditional Wiener measure [12]. That makes possible to apply the approximate formulas exact for functional polynomials of arbitrary given power to the case of Feynman path integrals. The aim of the paper is to expand the application area of the described approaches in such a way that they can be used for studying the time evolution of open quantum systems (OQS).

Dynamics of OQS is described with the help of the reduced density operator [13]. Feynman and Vernon have written the matrix elements of the operator as follows [14,15]:

$$\langle x|\hat{\rho}(t)|x'\rangle = \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dx_0' J(x,x',t;x_0,x_0',t_0)\langle x_0|\hat{\rho}(t_0)|x_0'\rangle, \tag{1}$$

where the propagator J is expressed through the double path integral

$$J = \int_{(t_0,x_0)}^{(t,x)} Dx(\tau) \int_{(t_0,x_0')}^{(t,x')} Dx'(\tau) \exp\left\{ \frac{i}{\hbar}\{S[x(\tau)] - S[x'(\tau)]\} \right\} \times F_{infl}[x(\tau),x'(\tau)], \tag{2}$$

$S[x(\tau)] = \int_{t_0}^{t} [m\dot{x}^2/2 - V(x)]d\tau$ is a classical action for the system in a potential field $V(x)$, the influence functional F_{infl} models the interaction of the system with its environment. For simplicity, we consider a one degree of freedom system. One has to represent this Feynman integral in the form of a Wiener integral in order to the approximate formulas exact for functional polynomials of a power can be employed. Omitting some simple considerations [16], we assume here heuristically that under certain conditions the following formula is valid:

$$\begin{aligned} &J(x,x',t;x_0,x_0',0) \\ &= \frac{m}{2\pi\hbar t} \exp\left\{ i\frac{m(x-x_0)^2}{2\hbar t} \right\} \exp\left\{ -i\frac{m(x'-x_0')^2}{2\hbar t} \right\} \\ &\times \int_{C^2[0,0;1,0]} \Theta\left[\sqrt{\frac{i\hbar t}{m}} x(\tau) + (x-x_0)\tau \right. \\ &\left. + x_0, \sqrt{-\frac{i\hbar t}{m}} x'(\tau) + (x'-x_0')\tau + x_0' \right] d\tilde{W}^*(x) d\tilde{W}^*(x'), \end{aligned} \tag{3}$$

$$\Theta[x,x'] = \exp\left\{ -\frac{it}{\hbar} \int_0^1 [V(x) - V(x')]d\tau \right\} F_{infl}[x,x'].$$

Here $\int_{C[0,0;1,0]} F[x(\tau)]d\tilde{W}^*(x)$ denotes the integral of functional $F[x(\tau)]$ with respect to the conditional normalized Wiener measure with integration over the set $C[0,0;1,0]$ of continuous functions $x(\tau)$ satisfying the conditions $x(0)=x(1)=0$, $C^2[0,0;1,0]=C[0,0;1,0]\times C[0,0;1,0]$. Formula (3) can be treated as a generalization of the Haba's result.

For evaluation of the double Wiener integral in right-hand side (RHS) of Eq. (3) we use the approximate formula obtained in [7,8]:

$$\int_{C^l[0,0;1,0]} F[x_1(\tau),\ldots,x_l(\tau)]d\tilde{W}^*(x_1)\cdots d\tilde{W}^*(x_l)$$

$$\approx \frac{1}{2l}(2\pi)^{-N/2}\int_{R^N}\exp\left\{-\frac{1}{2}\sum_{s=1}^{l}\sum_{j=1}^{k_s}(u_j^{(s)})^2\right\}$$

$$\times\sum_{j=1}^{l}\int_{-1}^{1}F[U_{k_1}(u^{(1)}),\ldots,Q_j(\alpha(v,t)),\ldots,U_{k_l}(\mathbf{u}^{(l)})]d\mathbf{u}\,dv, \tag{4}$$

where l is the multiplicity of the functional integral,

$$\mathbf{u}=(\mathbf{u}^{(1)},\ldots,\mathbf{u}^{(l)}),\mathbf{u}^{(s)}=(u_1^{(s)},\ldots,u_{k_s}^{(s)}),N=\sum_{s=1}^{l}k_s,$$

$$U_{k_s}(\mathbf{u}^{(s)})=\sum_{j=1}^{k_s}u_j^{(s)}\frac{\sqrt{2}}{j\pi}\sin(j\pi t),$$

$$Q_j(\alpha(v,t))=\sqrt{l}[\alpha(v,t)-P_{k_s}(v,t)]+U_{k_s}(\mathbf{u}^{(s)}),$$

$$P_{k_s}(v,t)=\sum_{j=1}^{k_s}\frac{2}{j\pi}\sin(j\pi t)\cos(j\pi v)\mathrm{sgn}(v),$$

$$\alpha(v,t)=\begin{cases}-t\,\mathrm{sgn}(v), & t\leqslant|v|,\\ (1-t)\mathrm{sgn}(v), & t>|v|.\end{cases}$$

The formula is exact for functional polynomials of a third summary power. Thus, the calculation of the Wiener functional integral of multiplicity l is reduced to calculation of the approximating usual (Riemann) integral of multiplicity $N+1$. The error of formula (4) decreases with increasing N and depends on the physical parameters the functional F may contain. As we investigate a time evolution, particular attention will be given to the dependence on the parameter t. For small enough time intervals $[t_0,t]$ sufficient accuracy can often be achieved with relatively small N, in some cases with the minimum $N=l$ [17,18]. With growing t one has to increase N. However, the considerable increase of N is inexpedient due to the difficulty of evaluation of the approximating Riemann integral with an appropriate accuracy. In this case one can divide the total time interval into the parts $[t_0,t_1],[t_1,t_2],\ldots,[t_{n-1},t],t_0<t_1<t_2<\cdots<t_{n-1}<t$. Taking into account that $J(x_j,x_j',t_j;x_{j-1},x_{j-1}',t_{j-1})=J(x_j,x_j',t_j-t_{j-1};x_{j-1},x_{j-1}',0)$ and successively applying formula (1) to the subintervals $[t_{j-1},t_j]$ one can obtain

$$J(x,x',t;x_0,x_0',0)=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}J(x,x',t-t_{n-1};x_{n-1},x_{n-1}',0)$$

$$\times J(x_{n-1},x_{n-1}',t_{n-1}-t_{n-2};x_{n-2},x_{n-2}',0)\cdots J(x_1,x_1',t_1-t_0;x_0,x_0',0)dx_1dx_1'\cdots dx_{n-1}dx_{n-1}'. \tag{5}$$

The length of the subintervals should not be necessarily small. It depends on whether the arrived accuracy of formula (4) is sufficient for each subinterval.

Actually, formulas (1) and (3)–(5) are the basis of a numerical method of studying time evolution of OQS. One can outline features of this method. At first, we should note that the infinite domain of integration in RHS of Eq. (1) has to be replaced by a finite one in order to apply a quadrature or cubature formula for numerical evaluation of the integral [26]. It can be done without considerable loss of accuracy if the initial condition is a fast vanishing function. It is usual in this case that the spacial domain of the numerical solution alters with time very quickly. As the calculation of the propagator (3) with the help of formula (4) does not imply any space-time discretization or a change of a given potential, the method at most preserves the initial target setting. The solution for a moment t can then be obtained from the initial condition by formula (1) without any transitional states, so the case of fast changing solutions is especially suitable for the described approach. It is the case when application of traditional numerical methods based on different kinds of changes of initial target setting is conjugated with difficulties of different kinds. So, the possible application area of the proposed approach has a little intersection with the areas of other numerical methods.

The use of formula (5) means, however, a discretization of the time interval. It gives rise to the problem of determining finite limits of integration in RHS of Eq. (5), which also have to be found instead of infinite ones. The limits can be pointed out approximately for each transitional time point t_j successively from the initial condition.

Since the amount of computations by formula (4) does not grow very fast with growing l, the approach seems to be useful in case of multidimensional problems. Actually, for such problems the Monte Carlo method is the only effective technique in contemporary physics. As the Monte Carlo method has demerits, the appearance of a possible alternative is especially interesting in this case. It should be noted that increase in the number of time subintervals in formula (5) leads to considerable increase of the computation expenses with grows of the dimensionality, so one should make an optimal choice between increasing N and n.

Some examples of calculations with the help of the proposed approach are given below. Strunz has derived the expression for the influence functional F_{infl} from the most general Markovian master equation with the assump-

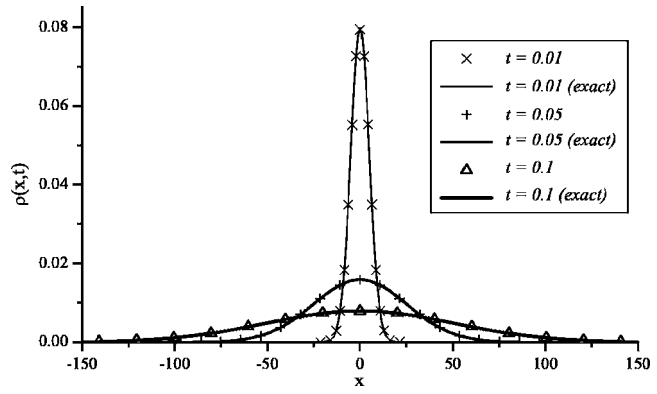

FIG. 1. The function $\rho(x,t)$ calculated for different moments of time t by formulas (1), (3), (4), (6), and (7) for potential $V(x)=-m\omega^2x^2/2$ and parameters $m=\omega=\hbar=1$, $|\gamma|^2=\bar{\omega}=\Gamma=0$, $|\beta|^2=1$, $\bar{x}(0)=\bar{p}(0)=0$, and $\xi(0)=10^{-6}$. The correspondent exact solutions obtained by formulas (8) and (9) are shown by the solid lines.

tion of momentum and position-linear environment operators [13]:

$$F_{infl}[x,x'] = \exp(\Gamma t)\exp\left\{-\frac{1}{2\hbar}D[x,x']^2\right\} \times \exp\left\{\frac{i}{\hbar}\Phi[x,x']\right\},$$

$$\Phi[x,x'] = m\Gamma\int_0^t d\tau(\dot{x}x' - x\dot{x}') - \frac{1}{2}m\Gamma^2\int_0^t d\tau(x^2 - x'^2),$$

$$D[x,x']^2 = m^2|\gamma|^2\int_0^t d\tau(\dot{x}-\dot{x}')^2 + (|\beta|^2 + m^2|\gamma|^2\Gamma^2 - 2m\bar{\omega}\Gamma)\int_0^t d\tau(x-x')^2 + 2m(\bar{\omega} - m|\gamma|^2\Gamma)\int_0^t d\tau(x-x')(\dot{x}-\dot{x}'). \quad (6)$$

Here the parameter Γ determines dissipation of energy, whereas $|\beta|^2$ and $|\gamma|^2$ are the diffusion coefficients [13,19–22].

The direct application of the approximate formula (4) for evaluation of the functional integral in the RHS of Eq. (3) with the influence functional (6) turns out to be impossible due to the presence of the term $m^2|\gamma|^2\int_0^t d\tau(\dot{x}-\dot{x}')^2$. Substitution of the functions $\dot{x}$ and $\dot{x}'$ by the approximate expressions from formula (4) leads in this case to the divergent integral of δ^2. The problem of correct approximation of derivatives and the possibility of calculation of functional integrals with such functionals remain open questions of the approach. One can equate to zero the coefficient $|\gamma|^2$, but such models are rather classical [20]. In some cases, however, they can be used for a description of quantum phenomena. In particular, the models are successfully employed in nuclear physics [23].

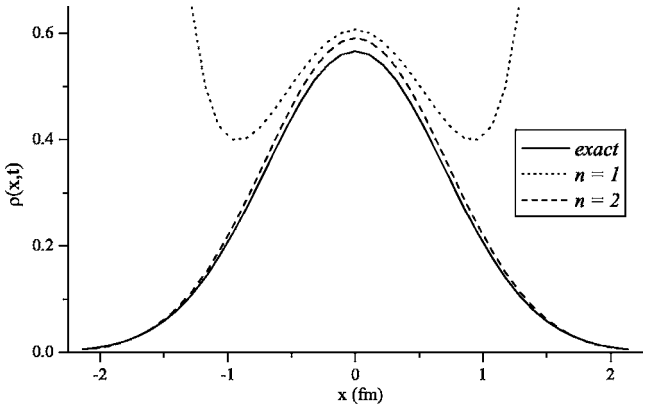

FIG. 2. The function $\rho(x,t)$ calculated for $t=6.6\times10^{-22}$ sec by formulas (1), (3), (4), (6), and (7) for potential $V(x)=m\omega^2x^2/2$ and parameters $m=53m_0$, m_0 is the mass of nucleon, $|\gamma|^2=\bar{\omega}=0$, $\hbar\Gamma=1$ MeV, $\hbar\omega=2$ MeV, $|\beta|^2=\Gamma m\omega$ [19–22], $\bar{x}(0)=\bar{p}(0)=0$, $\xi(0)=0.01$ fm^2. Propagator (3) also was calculated with the use of formula (5) for $n=2$ with the transitional point $t_1=2.64\times10^{-22}$ sec. The correspondent exact solution obtained by formulas (8) and (9), where ω has been replaced by $i\omega$, is shown by the solid line.

Starting from the Strunz's results, Adamian, Antonenko, and Scheid [19] have obtained an explicit expression for the diagonal elements of the reduced density matrix for a system with the initial state

$$\Psi(x) = [2\pi\xi(0)]^{-1/4}\exp\left\{-\frac{[x-\bar{x}(0)]^2}{4\xi(0)} + \frac{i}{\hbar}\bar{p}(0)x\right\} \quad (7)$$

and the potential $V(x)=-m\omega^2x^2/2$:

$$\rho(x,t) = \langle x|\hat{\rho}(t)|x\rangle = [2\pi\xi(t)]^{-1/2}\exp\left\{-\frac{[x-\bar{x}(t)]^2}{2\xi(t)}\right\}. \quad (8)$$

If $\bar{x}(0)=\bar{p}(0)=0$, $\bar{x}(t)$ also equals zero and the dispersion in this Gaussian depends on time for $|\gamma|^2=\bar{\omega}=0$ in the following way [27]:

$$\xi(t) = \frac{\hbar|\beta|^2}{4m^2\Gamma(\Gamma^2-\omega^2)} + \frac{1}{2}e^{-2\Gamma t}\left\{\frac{\hbar|\beta|^2}{2m^2\omega^2\Gamma} + \xi(0) - \frac{\hbar^2}{4m^2\omega^2\xi(0)} - \frac{\hbar|\beta|^2}{2m^2\omega(\Gamma^2-\omega^2)}\sinh(2\omega t) + \left(\xi(0) + \frac{\hbar^2}{4m^2\omega^2\xi(0)} - \frac{\hbar|\beta|^2\Gamma}{2m^2\omega^2(\Gamma^2-\omega^2)}\right)\cosh(2\omega t)\right\}. \quad (9)$$

Thus, one can compare the outcomes of numerical computations with the exact solutions. Figure 1 demonstrates the evolution of the density matrix for three fixed moments of time. One can see from the figure that the method gives a high accuracy for the considered time interval even with the use of formula (4) with the minimum value $N=2$. It is interesting to note that in this example we use the potential unbounded from below, whereas Haba considered the potentials bounded from below only [12]. In the next example represented in Figure 2 a fixed moment of time was chosen so that the

approximate formula (4) with $N=2$ gives an unsatisfactorily crude result. So far formula (5) was not employed, what actually corresponds to the case $n=1$. The use of formula (5) with one transitional time point ($n=2$) considerably improves accuracy of the solution. In this example the chosen values of physical parameters are used in real problems from heavy ion physics.

In the given examples the multiplicity of approximating Riemann integrals does not exceed 3. Thus, for calculation of the density matrix we estimated the Riemann integral of multiplicity 5 without dividing of the total time interval and 7 with the one division. The multiplicity may considerably increase in some cases. Now there are different effective deterministic numerical methods for evaluation of Riemann integrals of multiplicity up to 20 [24,25]. If needed, one can also use a Monte Carlo technique. Many questions concerned both mathematical and physical aspects arise in connection with the proposed approach. We hope that it will be useful in practice application, which stimulates development of a correspondent rigorous theory.

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