Development of the Green function method on a basis of deterministic approach to approximate functional integration

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Within the general approach which is understood as the Green function method, we develop a numerical method based on representation of the Green functions for a class of problems in the form of functional integrals with respect to Gaussian measures, and subsequent calculation of the integrals with the help of a deterministic approach. In this case the solving of the problems is reduced to evaluation of usual (Riemann) integrals of relatively low multiplicity. The method was applied to numerical solving of the Schrödinger equation and the related diffusion equation, and also to description of time evolution of some Markovian open quantum systems. The features of the method and possible area of its application are discussed.

PACS: 02.60.-x, 02.70.-c, 03.65.-w

1 Introduction

The functional integration finds a wide utilization in contemporary physics. One of the interesting directions is investigation of the connection between partial differential equations and functional integrals, which was first revealed by R. Feynman who expressed Green function (propagator) of the Schrödinger equation in the form of a path integral [1, 2]. The Feynman's work has inspired M. Kac who wrote Green function of a diffusion equation through a Wiener functional integral [3, 4]. Later I. Gelfand and A. Yaglom [5] raised a question on the relationship of partial differential equations and functional integrals in general, and certain progress has been achieved [6, 7]. Gelfand and Yaglom gave some examples when use of the functional integrals in the differential equation theory gives advantages, but they assumed that all the benefit will be understood later on. The development of approximate functional integration techniques allows us to look at the problem from a specific point of view. If Green functions of the differential equations can be expressed through the functional integrals and the last can be calculated approximately, then we have a method of solving those equations numerically. In fact, it is a kind of Green function method which has its own features and application area. The features strongly depend on chosen technique of approximate functional integration. As it will be considered below, widely used Monte Carlo method does not seem to be an appropriate choice in this case, at least for low-dimensional problems.

Along with the Monte Carlo method deterministic approaches were suggested [8]–[10]. In 1951 R. Cameron offered a formula for approximate evaluation of Wiener functional integrals, which is exact for functional polynomials of a third power [8]. 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 [9] and to the case

of functional polynomials of an arbitrary given power [10]. The method has two remarkable properties: it requires no space-time discretization, and high enough rate of convergence to values of the functional integrals with growing multiplicity of Riemann integrals which approximate functional ones. Owing to the properties the method is suitable for utilization within the Green function method. Usually the problem of numerical solution of differential equations is reduced in this case to numerical evaluation of Riemann integrals of relatively low multiplicity.

Unlike the theory of Wiener integrals, Feynman's theory of path integration was not rigorous. In 1960 Cameron also established a link connecting the Feynman path integral and the Wiener integral [13]. The approach was developed further by Doss, Azencott, and Haba [14]–[16]. Haba obtained a formula which expressed the Feynman propagator through a functional integral with respect to conditional Wiener measure [16]. That makes it possible to apply the approximate formulas exact for functional polynomials of arbitrary given power to the case of the Feynman path integrals. We generalized Haba's result to the case of propagator for open quantum systems and obtained a formula which allows one to apply the deterministic approach to the numerical studying of time evolution of open quantum systems [17].

2 Method of calculations

The equation

$$\frac{\partial Q}{\partial t} = \frac{1}{2}\frac{\partial^2 Q}{\partial x^2} - V(x)Q(x,t)\,, \tag{1}$$

$x \in R$, $t \in (t_0, +\infty)$ with the boundary condition $\lim\limits_{|x|\to\infty} Q(x,t) = 0$ serves as a convenient example for close scrutiny of the proposed numerical method. It describes the classical diffusion with a distribution of negative sources, which is determined by the function $V(x)$ [4]. For a given initial condition $Q_0(x) = Q(x,t_0)$ the solution $Q(x,t)$ can be expressed with the help of the Green function $P(x,t;x_0,t_0)$ in the following way [5]:

$$Q(x,t) = \int_{-\infty}^{+\infty} P(x,t;x_0,t_0)Q_0(x_0)\mathrm{d}x_0\,. \tag{2}$$

The Green function is regarded by Kac as a functional integral with respect to a conditional Wiener measure. If $t_0 = 0$, the Kac's result can be written as [11]

$$P(\mathrm{x},t;\mathrm{x}_0,0) = \frac{1}{\sqrt{2\pi t}}\exp\left\{-\frac{(\mathrm{x}-\mathrm{x}_0)^2}{2t}\right\}\times \tag{3}$$
$$\times \int\limits_{C[0,0;1,0]} \exp\left\{-t\int\limits_0^1 V\left(\sqrt{t}x(\tau) + (\mathrm{x}-\mathrm{x}_0)\tau + \mathrm{x}_0\right)\mathrm{d}\tau\right\}\mathrm{d}\tilde{W}^*(x)\,.$$

Here $\int_{C[0,0;1,0]} F[x(\tau)]\mathrm{d}\tilde{W}^*(x)$ denotes the integral of functional $F[x(\tau)]$ with respect to the conditional normalized Wiener measure with integration on the set

$C[0,0;1,0]$ of continuous functions $x(\tau)$ satisfying the conditions $x(0) = x(1) = 0$.

If we try to calculate the integral in the right hand side of the equality (2) numerically with the help of a quadrature formula, we have to replace the infinite domain of the integration by a finite one [1]). For the error of the numerical integration E_0 which include an error caused by the replacement to be negligible the initial function $Q_0(x)$ must vanish fast enough with $|x_0| \to \infty$. For instance, if the function is a narrow peak, then the narrower it the less is the error E_0. No matter how narrow the peak is, we can make an optimal choice of lattice points of the numerical integration since the location of the peak is known. As the solution $Q(x,t)$ for the moment t is obtained from the initial condition $Q_0(x)$ with no transitional states, the calculation with the use of the formula (2) gets especially efficient when the spatial domain of the numerical solution changes with time very quickly. It usually takes place just when the initial condition is a very narrow peak. It should be noted that for traditional methods of numerical solving of partial differential equations we have a reverse situation, i.e. the narrower the peak the more problems. Thus, there is a principle of complementarity in a certain sense.

However, for all the reasonings to be proved in practice, a method of evaluation of the functional integral representing the Green function should not impose too strong additional restrictions. For example, Monte Carlo method is based on discretization of a considered time interval $[0,t]$, so the solution for a moment of time is actually not obtained directly from the initial condition. Similar a discretization takes place in the widely used finite difference method of solving differential equations and the advantage of the approach with the use of functional integrals gets questionable. Alternatively, application of the used deterministic method does not imply any discretization of space of independent variables, so the initial target setting undergoes not much changes.

Here the approximate formula obtained in [10] will be employed:

$$\begin{aligned}
&\int\limits_{C[0,0;1,0]} F[x(\tau)]\,\mathrm{d}\tilde{W}^*(x) \approx \\
&\quad \approx 2^{-l}(2\pi)^{-k/2} \int\limits_{R^k} \mathrm{d}\mathbf{u} \int\limits_{-1}^{1} \mathrm{d}v_1 \ldots \int\limits_{-1}^{1} \mathrm{d}v_l \exp\left\{-\frac{1}{2}\sum_{s=1}^{k} u_s^2\right\} \times \\
&\qquad \times F[\Theta_l(\mathbf{v},\tau) - \Phi_{l,k}(\mathbf{v},\tau) + U_k(\mathbf{u},\tau)]\,,
\end{aligned} \tag{4}$$

where $\mathbf{u} = (u_1, \ldots, u_k)$, $\mathbf{v} = (v_1, \ldots, v_l)$,

$$\Theta_l(\mathbf{v},\tau) = \sum_{s=1}^{l} c_{l,s}\rho(v_s,\tau)\,, \qquad \rho(v_s\,,\tau) = \begin{cases} -\tau\,\mathrm{sign}\,(v_s)\,, & \tau \le |v_s|\,, \\ (1-\tau)\,\mathrm{sign}\,(v_s)\,, & \tau > |v_s|\,, \end{cases}$$

$$\Phi_{l,k}(\mathbf{v},\tau) = \sum_{s=1}^{k} \frac{2}{s\pi}\,\sin(s\pi\tau) \sum_{j=1}^{l} c_{l,j}\mathrm{sign}\,(v_j)\cos(s\pi v_j)\,,$$

[1]) There are techniques and quadrature formulas for evaluation of integrals with the infinite domain of integration, but they can not always be applied in a general case.

$$U_k(\mathbf{u},\tau) = \sum_{s=1}^{k} \frac{\sqrt{2}}{s\pi}\, u_s \sin(s\pi\tau)\,,$$

$[c_{l,s}]^2$ are roots of the polynomial

$$Q_l(r) = \sum_{s=0}^{l} (-1)^s \frac{r^{l-s}}{s!}\,, \qquad s = 1, 2, \ldots, l\,, \quad r \in R\,.$$

The formula is exact for functional polynomials of the power $\leq 2l+1$. For the functionals not belonging to the class and satisfying certain conditions the error E_{for} of the formula is estimated as $O(k^{-l-1})$ [10]. Thus, the approximate evaluation of a Wiener functional integral is reduced to calculation of a usual (Riemann) integral of multiplicity $k+l$ with integration along the auxiliary variables $u_1, \ldots, u_k$, $v_1, \ldots, v_l$. The variables x and t as well as other physical values are contained in this approximating Riemann integral as parameters. The error $E_{\rm for}$ and therefore the accuracy of solution to the differential equation may crucially depend on those parameters. As the solution describes a time evolution, the main attention will be devoted to the dependence on the time variable t.

If a satisfactory result cannot be obtained for a required time interval $[0, t]$, one can try to increase the value of k or l. However, increasing the multiplicity $k+l$ gives rise to increasing the error $E_{\rm int}$ of calculation of the approximating Riemann integral, which for large enough $k+l$ can become a main contribution to the total error $E = E_0 + E_{\rm for} + E_{\rm int}$. Tables 1, 2 demonstrate a dependence of $E_{\rm for}$ and $E_n = E_{\rm for} + E_{\rm int}$ on k and l in case of calculation of the functional integral having the explicit expression:

$$I = \int\limits_{C[0,0;1,0]} \exp\left\{\int_0^1 p x^2(\tau) \mathrm{d}\tau\right\} \mathrm{d}\tilde{W}^* x = \left(\frac{\sqrt{-2p}}{\sinh\sqrt{-2p}}\right)^{1/2},$$

$-\infty < p \leq 0$. For the selected value $p = -30$ the exact value of the integral is 0.08185356. In case of such a functional the approximating integral along the variables $u_1, \ldots, u_k$ can be taken explicitly. If l is small enough, the integral along the rest variables $v_1, \ldots, v_l$ can be evaluated with a high accuracy, so that the error $E_{\rm int}$ is negligible and we can obtain the value $E_{\rm for}$ with a sufficient accuracy. In the tables the corresponding approximate value of the functional integral is denoted through I_f. On the other hand, the result of direct numerical calculation of the approximating integral along all the variables $u_1, \ldots, u_k$, $v_1, \ldots, v_l$ is denoted through I_n, the corresponding error is E_n which includes the error $E_{\rm for}$. In the last case the computer calculation time T is also given. The tables 1 and 2 represent the results obtained accordingly for $l = 1$ and $l = 2$.

Although the results depend on used computers and numerical integration methods, the obtained data show a regularity. Decreasing the error $E_{\rm for}$ has a sense until the condition $E_{\rm int} \ll E_{\rm for}$ is satisfied. As seen from the tables, it can be easily achieved for not large $l + k$. Now there are different numerical integration

methods which give a high accuracy and a relatively small computation time in case of Riemann integrals of low multiplicity [18, 19]. Further increasing $l + k$ is inexpedient.

It should be noted that direct computation of the approximating integral requires a limitation of the infinite domain of the integration along the variables $u_1, \ldots, u_k$. Thus, the error E_{int} includes also an error arising from such a limitation. One should heed that the neglected part of the integral be small enough for any values of parameters contained in the functional $F[x(\tau)]$. As it will be shown below, the decrease rate of the integrand with growing $|u_1|, \ldots, |u_k|$ may crucially depend on the function $V(x)$.

Table 1.

k	I_f	E_{for}, %	I_n	E_n, %	T, sec.
1	0.062104	24.1	0.062103	24.1	0.02
2	0.074310	9.2	0.074307	9.2	0.03
3	0.078450	4.2	0.078445	4.2	0.47
4	0.080085	2.2	0.080083	2.2	7.6
5	0.080832	1.2	0.080829	1.3	45.9
6	0.081215	0.8	0.081124	0.9	52.7
7	0.081430	0.5	0.085440	4.4	60.5
8	0.081558	0.4	0.126745	55	68.1
9	0.081640	0.3	0.125091	53	75.3
10	0.081694	0.2	0.351862	330	83.1

Table 2.

k	I_f	E_{for}, %	I_n	E_n, %	T, sec.
1	0.097060	18.6	0.097067	18.6	5.6
2	0.084371	3.1	0.084380	3.1	9.4
3	0.082498	0.8	0.082490	0.8	28
4	0.082070	0.3	0.082070	0.3	34
5	0.081941	0.1	0.082171	0.4	41
6	0.081894	0.05	0.083983	2.6	120
7	0.081874	0.03	0.082839	1.2	138
8	0.081865	0.014	0.075436	7.8	156
9	0.081860	0.008	0.109991	34	174
10	0.081858	0.005	0.104792	28	182

In case of $V(x) = \frac{1}{2}\,x^2$ and the initial condition in the form of Gaussian

$$Q_0(x) = \frac{1}{\sqrt{2\pi\xi^2}}\,\exp\left\{-\frac{x^2}{2\xi^2}\right\}$$

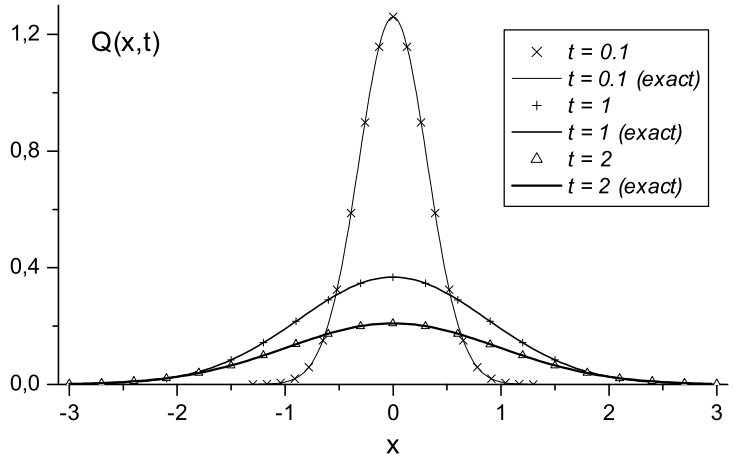

Fig. 1. The function $Q(x,t)$ calculated by the formulas (2) and (3) for $\xi^2 = 10^{-300}$ and different moments of time t. The Green function (3) was computed by the formula (4) with $l = k = 1$. Corresponding exact solutions obtained by the formula (5) are presented by the solid lines.

the solution of the equation (1) can be expressed explicitly:

$$Q(x,t) = \frac{1}{\sqrt{2\pi(\xi^2\cosh t + \sinh t)}} \times \\ \times \exp\left\{-\frac{x^2}{2}\left(\coth t - \frac{\xi^2}{(\xi^2\cosh t + \sinh t)\sinh t}\right)\right\}. \tag{5}$$

It allows one to compare the outcomes of the numerical calculations with the exact solution. Fig. 1 shows a time evolution of the initial Gaussian distribution function with extremely small dispersion ξ. Thus, we can examine the efficiency of the method when the initial condition is a very narrow peak. As appears from the figure, the high accuracy has been achieved for considered time intervals with the minimum multiplicity of the approximating integral. It is also interesting to test the method in a reverse situation when ξ is comparatively large. The results corresponding to the case are shown on the fig. 2. The upper value of ξ was chosen in such a way that within the range of variation of the dispersion, which is marked by the two values of ξ, the computation time changes relatively slowly.

It may turns out in some cases that for large enough time interval $[0,t]$ no satisfactory accuracy can be achieved for a reasonable computation time. In such a situation one can divide the interval into the parts $[0,t_1]$, $[t_1,t_2]$, $\ldots$, $[t_{n-1},t]$, $t_0 < t_1 < t_2 < \cdots < t_{n-1} < t$, so that the condition $E_{\rm int} \ll E_{\rm for}$ be easily accomplished for each of the subintervals. According to the formula (2), one can

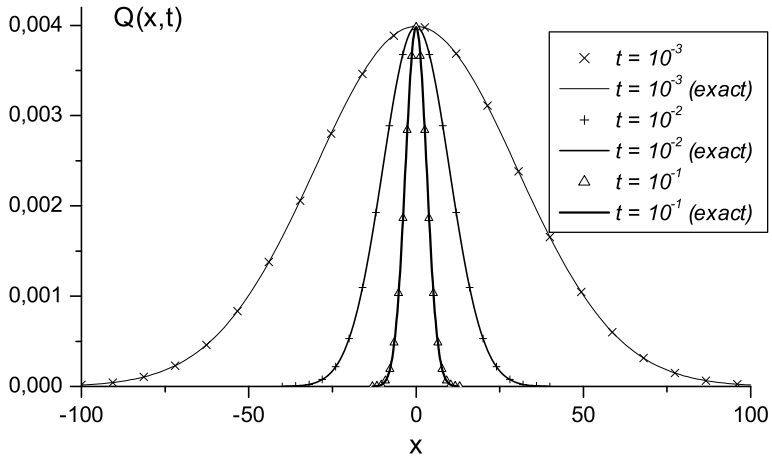

Fig. 2. The function $Q(x,t)$ calculated by the formulas (2) and (3) for $\xi^2 = 100$ and different moments of time t. The Green function (3) was computed by the formula (4) with $l = k = 1$. Corresponding exact solutions obtained by the formula (5) are presented by the solid lines.

write:

$$Q(x_j,t_j) = \int_{-\infty}^{+\infty} P(x_j,t_j;x_{j-1},t_{j-1})Q(x_{j-1},t_{j-1})\mathrm{d}x_{j-1}\,, \tag{6}$$

$j = 1,\ldots,n$, $t_n = t$, $x_n = x$. Thus, there is an iteration procedure when the solution for the moment of time t_j is expressed through solution for the previous moment t_{j-1} only. The propagator $P(x_j,t_j;x_{j-1},t_{j-1})$ depends actually on the difference $t_j - t_{j-1}$, i.e. $P(x_j,t_j;x_{j-1},t_{j-1}) = P(x_j,t_j - t_{j-1};x_{j-1},0)$ [5]. The using of the formula (6) means serial computation of n one-dimensional integrals along the variables $x_0,\ldots,x_{n-1}$, which is equivalent to calculation of the function $Q(x,t)$ by the formula (2) where the propagator is expressed through the integral of multiplicity $n-1$:

$$\begin{aligned} P(x,t;x_0,0) = \int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} P(x,t-t_{n-1};x_{n-1},0)\times \\ \times P(x_{n-1},t_{n-1}-t_{n-2};x_{n-2},0)\times\ldots\times P(x_1,t_1;x_0,0)\,\mathrm{d}x_1\ldots\mathrm{d}x_{n-1}. \end{aligned} \tag{7}$$

The equality is a consequence from the well known Kolmogorov–Chepmen–Smoluchovski formula [4]. If the integration along x_0, ..., x_{n-1} is considered as calculation of a n-dimensional integral and it is performed by a cubature formula, then the described procedure is not actually iterative. The using of the formula (7) allows one to expand the total interval $[0,t]$ for which the propagator $P(x,t;x_0,0)$ can be evaluated with a satisfactory accuracy. On the other hand, the increase of n results in the growing volume of calculations related to the multiple numerical integration

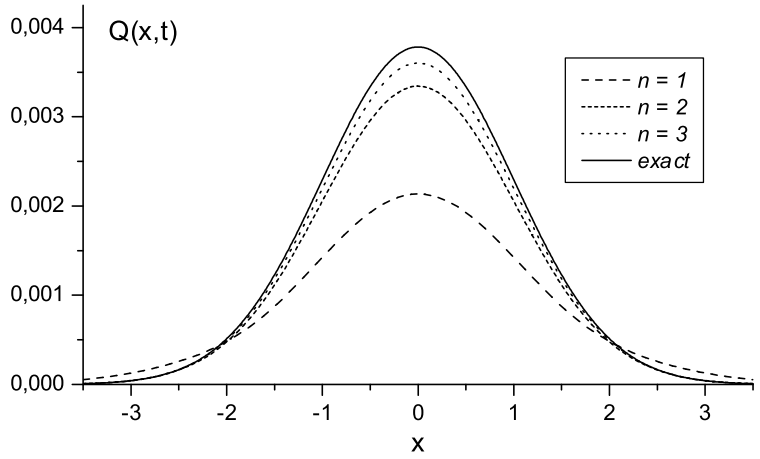

Fig. 3. The function $Q(x,t)$ calculated by the formulas (2) and (3) for $\xi^2 = 0.01$ and $t = 10$. The Green function (3) was computed by the formulas (4) with $l = k = 1$ and (7) for $n = 2$ with intermediate point $t_1 = 5$ and for $n = 3$ with intermediate points $t_1 = 3$, $t_2 = 6$. The exact solution obtained by the formula (5) is presented by the solid line.

along the variables $x_1, \ldots, x_{n-1}$. Besides, one has to replace the infinite limits of integration in the formula (7) by finite ones. It is necessary to take into account the changing of the spatial domain of the numerical solution with time in order to determine the limits correctly. Within the iteration procedure the domain for variable x_k corresponding to the moment t_k can be estimated using a solution for the previous moment t_{k-1}, which is considered as an initial condition.

The outcomes of calculation of the function $Q(x,t)$ with different n and fixed moment of time and values of l, k are presented in fig. 3. For comparison the results obtained with fixed n and different k are shown in fig. 4. It follows from the figures that the iteration procedure can be even more efficient than increasing the multiplicity of the approximating Riemann integral. If necessary, one can also combine those two techniques.

Quite similar consideration is given in the paper [11] for the case of Schrödinger equation, and also in [17] where such an approach was employed for numerical description of time evolution of open quantum systems. In the last case an approximate formula for evaluation of multiple functional integrals, which is exact for functional polynomials of third summary power was used.

3 Summary and conclusions

In the frame of the paper it is only possible to outline the conditions the proposed approach can be efficiently used. A complete determination of its "compu-

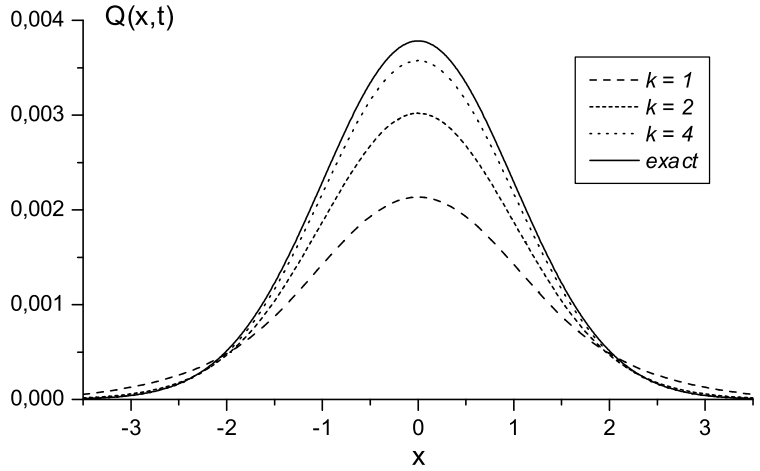

Fig. 4. The function $Q(x,t)$ calculated by the formulas (2) and (3) for $\xi^2 = 0.01$ and $t = 10$. The Green function (3) was computed by the formulas (4) with $l = 1$ and different values of k. The exact solution obtained by the formula (5) is presented by the solid line.

tational niche" can be fulfilled in process of wide practical use.

In many respects the method preserves initial target setting, which is important when the spatial domain of the numerical solution changes with time quickly enough. It usually takes place if the initial condition is a rapidly vanishing function.

The numerical solving of the equations is reduced in the method to evaluation of Riemann integrals of low multiplicity. It does not exceed 5 in the given examples. Now there are different deterministic methods of calculating integrals of multiplicity up to 20. If needed, one can also use a Monte Carlo technique.

When applying the numerical methods, the problems of convergence and stability of obtained approximations with respect to a parameter appear. In the used deterministic technique of functional integration such a parameter is the multiplicity of the approximating Riemann integral. In this case convergence and stability follow from the estimation of error for the formula (4) (or similar formulas exact for functional polynomials of a power). For one's part the problem of stability is not urgent for the numerical calculation of Riemann integrals. Along with simplicity of target setting it makes the method relatively simple in use.

As shown in [10], multiple functional integrals can also be approximated satisfactorily by Riemann integrals of low multiplicity. It points out that the method can be successfully employed for multidimensional problems.

The difficulties concerned with definition of a countably additive measure in the space of paths in case of Feynman integral show that practical application of the proposed approach may require development of the functional integration theory related to specific partial differential equations. Besides, the corresponding methods

of approximate calculation of the functional integrals should also be developed.

We wish to thank Dr. Adamian, Dr. Antonenko, and Dr. Palchikov, who have proposed the physical target setting, for fruitful discussions, Prof. Zhidkov for helpful remarks and Prof. Puzynin for support. The work was supported in part by RFBR Grant 04-01-81011.

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