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Functional integrals for nuclear many-particle systems

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Abstract. The new method for computation of the physical characteristics of quantum systems with many degrees of freedom is described. This method is based on the representation of the matrix element of the evolution operator in Euclidean metrics in a form of the functional integral with a certain measure in the corresponding space and on the use of approximation formulae which we constructed for this kind of integral. The method does not require preliminary discretization of space and time and allows us to use the deterministic algorithms. This approach proved to have important advantages over the other known methods, including the higher efficiency of computations. Examples of application of the method to the numerical study of some potential nuclear models as well as comparison of results with the experimental data and with the values obtained by the other authors are presented.

1. Introduction

Investigation of quantum systems consisting of many interacting particles is one of the fundamental problems in physics [1]. The convenient framework for study of the systems with many degrees of freedom is a path-integral approach [2]. Being one of the most important mathematical techniques for solution of the wide class of problems in computational physics [3], path integrals provide a useful tool for study of the variety of nuclear systems which are otherwise not amenable to definitive analysis through perturbative, variational or stationary-phase approximations, etc (see [4]). However, the existing approaches to path integrals in physics are not always correct in a mathematical sense and the usual method of their computation is Monte Carlo, which gives the results only as probabilistic averages and requires too much computer resources to obtain the good statistics. Moreover, when the nuclear many-body problem is being formulated on a lattice, the computation of characteristics of heavy nucleus would require the lattice size which is four to five orders of magnitude more than any lattice gauge calculation and which is hardly possible on any foreseeable computer [4]. First of all it concerns the ground state properties (binding energies, masses, etc). The existing results of computation of the binding energy even for the light nuclei by means of the variational or Green function Monte Carlo method, as well as by the coupled cluster and Faddeev equation methods, differ one from the other and from the experimental values more than the estimated errors of calculation (see [5, 6]), while requiring several hours on Cray–YMP and Cray-2 computers [5]. It is clear that the creation of the new methods for solution of such a complicated problem is of high importance. Increasing attention is being paid nowadays to the construction of deterministic algorithms for computation of path integrals which would be more effective than conventional Monte Carlo (see [7–9]). For instance, in [7] the authors discuss the method of path summation based on the introduction of the 'short-time' propagator in the

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range $0 < t < \varepsilon$, which is correct up to $O(\varepsilon^2)$ and on the successive iterations to the finite imaginary time t to obtain the ground-state energy of a quantum system. It should be noted that the main physical properties such as energy spectrum, wavefunctions squared, etc can be reproduced correctly only in a limit $t \to \infty$. In [8] and in extending its results to [9] the method of evaluation of discretized path integrals is developed on the basis of iteration of the short-time approximation and on the direct matrix multiplication. The authors state that this approach is more along the original lines of Feynman of integrating over all space at each intermediate time rather than accepting or rejecting paths according to a Markov process in Monte Carlo algorithms. However, their method also assumes the preliminary discretization and it can be applied to the systems with only a few quantum degrees of freedom. It is also limited by the size of the matrix that can be handled on existing computers (see [8]). It means that using this approach it is difficult to treat problems in which the system is delocalized over large distances. The method reported in [8] and [9] contains several parameters which affect the accuracy of results. The choice of these parameters is not clear and sometimes the decrease of spacing (which corresponds to approaching the continuum limit) gives worse result and requires more iterations to improve it (see [9]).

According to the recent achievements in the measure theory and in the development of functional integration methods (see, e.g. [10]) as well as in the functional methods in quantum physics [11] one can create the mathematically well-grounded methods for computation of path integrals. One of the promising approaches is the construction of approximation formulae which are exact on a given class of functionals [10]. Based on the rigorous definition of a functional integral in complete separable metric space in the framework of this approach we elaborated the new numerical method of computation of path integrals [12]. This method does not require preliminary discretization of space and time and allows us to obtain the mathematically well-grounded physical results with a guaranteed (not probabilistic) error estimate. It permits the straightforward computation of functional integrals over all space without any simplifying assumption (perturbation expansion, semiclassical or short-time approximation, etc). Our approximation formulae can be interpreted as quadratures in functional spaces. They are exact on a class of polynomial functionals of a given degree. Our method contains, therefore, all advantages of deterministic approach and is free from the limitations of other methods mentioned above. Under determined conditions we have proved the convergence of approximations to the exact value of the integral and estimated the remainder which gives upper and lower bounds of the result. We have studied in detail the functional measure of the Gaussian type and some of its important particular cases such as conditional Wiener measure in the space of continuous functions [13] in Euclidean quantum mechanics (or quantum statistical mechanics) and the functional measure in a Schwartz distribution space in two-dimensional Euclidean quantum field theory [14]. Numerical computations show [14] that our method gives significant (by an order of magnitude) economy of computer time and memory versus conventional Monte Carlo method used by other authors in the problems which we have considered. This approach is also proven to have advantages in the case of high dimensions when the other deterministic methods loose their efficiency [15]. Our deterministic algorithm of computation of functional integrals which we use in quantum statistical physics instead of traditional stochastic methods enable us to make a constructive proof of existence of continuum limit of the lattice (discretized) path integrals and to compute the physical quantities in this limit within the determined error bars. Using this method we performed the numerical investigation of the topological susceptibility and computed the θ-vacua energy in continuum for the first time [14]. Our algorithm realized in a program written in FORTRAN has been implemented on CDC-6500 and Convex C220 computers. However, it is also

possible to use personal computers since the method does not require too much computer resources. The source of the program is available from the author upon request.

In the present paper we discuss the mathematical foundations of the method and its numerical aspects. We extend it to the case of fermions (i.e. the antisymmetrized states) in continuum limit and apply it to the study of some potential nuclear models. The comparison of our numerical results with the experimental data and with the values obtained by the other authors which used both probabilistic and deterministic techniques demonstrates the advantages of our method.

2. Mathematical foundations

The most important for applications are integrals with respect to a measure of the Gaussian type [11]. It contains various types of measures including the well known conditional Wiener measure. So, we consider the Lebesgue integral

$$\int_X F[x]\,\mathrm{d}\mu(x) \tag{1}$$

where $F[x]$ is an arbitrary real measurable functional on a complete separable metric space X. Gaussian measure μ on X is a normalized measure defined on Borel σ-algebra of the space X in the following way [10]. The value of this measure on an arbitrary cylinder set

$$Q_{\varphi_1\ldots\varphi_n}(A_n) = \{x \in X : [\langle\varphi_1, x\rangle, \langle\varphi_2, x\rangle, \ldots, \langle\varphi_n, x\rangle] \in A_n\}$$

where $\varphi_1 \ldots \varphi_n$ are the linear-independent elements of the space X' and A_n $(n = 1, 2, \ldots)$ are arbitrary Borel manifolds in R^n, is given by the formula

$$\mu\{Q_{\varphi_1\ldots\varphi_n}(A_n)\} = (2\pi)^{-n/2}(\det K)^{-1/2}\int_{A_n}\exp\{-\tfrac{1}{2}(K^{-1}[u - M(\varphi)], [u - M(\varphi)])\}\,\mathrm{d}u.$$

Here $K_{i,j} = K(\varphi_i, \varphi_j)$, $u = (u_1, u_2, \ldots, u_n)$,

$$M(\varphi) = \{M(\varphi_1), M(\varphi_2), \ldots, M(\varphi_n)\}$$

$$(K^{-1}[u - M(\varphi)], [u - M(\varphi)]) = \sum_{i,j=1}^{n} K^{-1}_{i,j}[u_i - M(\varphi_i)][u_j - M(\varphi_j)]$$

$K(\varphi, \psi)$ is a correlation functional of the measure, $M(\varphi)$ is a mean value [10]. Under certain conditions, functionals $K(\varphi, \psi)$ and $M(\varphi)$, $\varphi, \psi \in X'$ determine the countable-additive function of manifolds on a Borel σ-algebra of the space X.

In the particular case of conditional Wiener measure $\mathrm{d}_W x$ in the space C_0 of continuous functions $C_0 \equiv \{x(t) \in C[0, 1], x(0) = x(1) = 0\}$ we have

$$\langle\varphi, x\rangle = \int_0^1 x(t)\,\mathrm{d}\varphi(t)$$

and

$$K(\varphi, \psi) = \int_{C_0}\langle\varphi, x\rangle\langle\psi, x\rangle\,\mathrm{d}_W x = \int_0^1\int_0^1 \mathcal{K}(t, s)\,\mathrm{d}\varphi(t)\,\mathrm{d}\psi(s)$$

where

$$\mathcal{K}(t, s) = \int_{C_0} x(t)x(s)\,\mathrm{d}_W x.$$

Conditional Wiener measure is characterized by the following correlation function and mean value [10]:

$$\mathcal{K}(t, s) = \min\{t, s\} - ts \qquad M(\varphi) = 0. \tag{2}$$

According to the Feynman–Kac formula, matrix element $Z_{if}(\beta)$ of the evolution operator $\exp\{-\beta H\}$, where $H = -\frac{1}{2}\Delta + V$ is written as follows:

$$Z_{if}(\beta) = Z(x_i, x_f, \beta) \equiv \langle x_f | \mathrm{e}^{-\beta H} | x_i \rangle = \int_{C_{x_i, x_f, \beta}} \exp\left\{ - \int_0^\beta V[x(t)]\,\mathrm{d}t \right\} \mathrm{d}_W x. \tag{3}$$

The integration in (3) is performed over the manifold of continuous functions $x(t) \in C[0, \beta]$ with conditions $x(0) = x_i$, $x(\beta) = x_f$. It should be noted that as distinct from the conventional path-integral approach, integral (3) does not contain the kinetic term (the first derivative squared) since it is included now to the measure of integration, and this circumstance simplifies the numerical simulations. After the appropriate change of the functional variables we can rewrite the integral (3) with the periodic boundary conditions $x_i = x_f = x$ in the form of standard conditional Wiener integral in the space C_0:

$$Z(x, x, \beta) = (2\pi\beta)^{-1/2} \int_{C_0} \exp\left\{ - \beta \int_0^1 V[\sqrt{\beta}\; x(t) + x]\,\mathrm{d}t \right\} \mathrm{d}_W x. \tag{4}$$

Using (4) we can compute various quantities in Euclidean quantum mechanics (or in quantum statistical mechanics accordingly). Particularly, the free energy of the system is defined as follows:

$$f(\beta) = -\frac{1}{\beta} \ln Z(\beta)$$

where

$$Z(\beta) = \mathrm{Tr} \exp\{-\beta H\} = \int_{-\infty}^{\infty} Z(x, x, \beta)\,\mathrm{d}x.$$

The ground state energy can be obtained in the following way:

$$E_0 = \langle 0 | H | 0 \rangle = \lim_{\beta \to \infty} f(\beta).$$

We can also define the propagator

$$G(\tau) = \langle 0 | x(0) x(\tau) | 0 \rangle = \lim_{\beta \to \infty} \Gamma(\tau)$$

where the correlation function

$$\Gamma(\tau) = \langle x(0) x(\tau) \rangle = \frac{1}{\sqrt{2\pi\beta}} \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} \int_{C_0} \exp\left\{ - \beta \int_0^1 V[\sqrt{\beta} x(t) + x]\,\mathrm{d}t \right\} \times \left[\sqrt{\beta} x \left(\frac{\tau}{\beta} \right) + x \right] x\,\mathrm{d}_W x\,\mathrm{d}x.$$

The energy gap between the ground and the first excited states can be computed as follows:

$$\Delta E = E_1 - E_0 = - \lim_{\tau \to \infty} \frac{\mathrm{d}}{\mathrm{d}\tau} \ln G(\tau).$$

The ground state wavefunction is equal to

$$|\Psi_0(x)|^2 = \lim_{\beta \to \infty} [\exp\{E_0 \beta\} Z(x, x, \beta)].$$

The generalization of (3) to the case of higher dimensions is obvious.

When studying the nuclear many-body problems, one needs the representation for the many-fermion evolution operator. A number of alternative functional integral representations exist for the many-fermion systems, including the many-particle

generalization of the path integral, an integral over an auxiliary field, integrals over the overcomplete sets of boson coherent states, determinants and Grassman variables (see [16]). Following the idea proposed in [16], in our present work we used the method based on insertion of a complete set of antisymmetrized many-particle states $|x_1, \dots x_A\rangle$ (A is the number of particles) at each time step of the discretized segment $[0, \beta]$. As shown in [16], for the infinitesimal time ε

$$\langle x_1^n \dots x_A^n | \mathrm{e}^{-\varepsilon H} | x_1^{n-1} \dots x_A^{n-1} \rangle = \exp\left\{ -\frac{1}{2\varepsilon} \sum_{i=1}^{A} (x_i^n - x_i^{n-1})^2 \right\}$$
$$\times \det \left| \exp\left\{ -\frac{1}{2\varepsilon} [(x_i^n - x_j^{n-1})^2 - (x_i^n - x_i^{n-1})^2] \right\} \right|$$
$$\times \exp\left\{ -\frac{\varepsilon}{4} \sum_{i,j} [V(|x_i^{n-1} - x_j^{n-1}|) + V(|x_i^n - x_j^n|)] \right\}$$

where the superscripts denote time labels and the subscripts denote particle,

$$x_i^n = x_i(t_n) \qquad t_n = \varepsilon n \qquad i = 1, \dots, A.$$

The sign of the matrix element at each step arising from the determinant is just the sign of the permutation required to bring the x^n into the same order as the x^{n-1}. Hence the cummulative sign after any number of steps is path-independent and is the sign of the permutation required to make the final order equal to the initial order [16]. It does not affect matrix elements of the evolution operator with antisymmetrized states or the trace of the evolution operator times a symmetric operator (see [16]). As reported in [4], in more than one spatial dimension, the interface between positive and negative contributions to the functional integral degrades the statistical accuracy such that the very good trial functions and exceedingly large ensembles are required to obtain useful results (it seems, however, that in our deterministic approach no such problems would arise). In one dimension the antisymmetry completely specifies the nodal points and a positive definite result may be obtained evolving the wavefunction in the ordered subspace $x_1 < x_2 < x_3 < \dots < x_A$ [4]. In this domain the determinant may be replaced by the following product in the limit $\varepsilon \to 0$ [16]:

$$\det \left| \exp\left\{ -\frac{1}{2\varepsilon} [(x_i^n - x_j^{n-1})^2 - (x_i^n - x_i^{n-1})^2] \right\} \right|$$
$$\longrightarrow \prod_{i=2}^{A} \left(1 - \exp\left\{ -\frac{1}{2\varepsilon} (x_i^n - x_{i-1}^n)(x_i^{n-1} - x_{i-1}^{n-1}) \right\} \right)$$

so that the matrix element $Z(x, x, \beta)$ can be written as follows [17, 4]:

$$Z(x, x, \beta) = \lim_{\varepsilon \to 0} Z_\varepsilon(x, x, \beta) \qquad \varepsilon = \frac{\beta}{N}$$

where

$$Z_\varepsilon(x, x, \beta) = (2\pi\varepsilon)^{-NA/2} \int P_\varepsilon(x_1^1, \dots, x_1^N, \dots, x_A^1, \dots, x_A^N)\, \mathrm{d}x_1^1 \dots \mathrm{d}x_A^N$$

$$P_\varepsilon = \exp\left\{ -\frac{1}{2\varepsilon} \sum_{i=1}^{A} \sum_{n=1}^{N} (x_i^n - x_i^{n-1})^2 \right\}$$
$$\times \exp\left\{ -\frac{\varepsilon}{2} \sum_{n=1}^{N} \sum_{i>j} [V(|x_i^n - x_j^n|) + V(|x_i^{n-1} - x_j^{n-1}|)] \right\}$$

$$\times \prod_{n=1}^{N} \prod_{i=2}^{A} \left[1 - \exp\left\{ -\frac{1}{2\varepsilon}(x_i^n - x_{i-1}^n)(x_i^{n-1} - x_{i-1}^{n-1}) \right\} \right]. \tag{5}$$

Some results on construction of the positive-definite functional integral representation for the fermions in dimensions $d \geqslant 2$ are reported in paper [18].

We can make a straightforward passage to the continuum limit in (5). Namely, we have found, that when $\varepsilon \to 0$ (or $N \to \infty$), β fixed, $Z_\varepsilon(x, x, \beta) \to Z(x, x, \beta)$, where

$$Z(x, x, \beta) = (2\pi\beta)^{-A/2} \int_{\tilde{C}_0^A} \exp\left\{ -\beta \sum_{i>j} \int_0^1 V[(\sqrt{\beta}x_i(t) + x_i) - (\sqrt{\beta}x_j(t) + x_j)]\,\mathrm{d}t \right\} \mathrm{d}_W x_1 \ldots \mathrm{d}_W x_A. \tag{6}$$

Here $\tilde{C}_0^A$ is a subset of the space C_0^A which is the direct multiplication of A copies of the space C_0 defined above. $\tilde{C}_0^A$ consists of the sequences of elements $x_1(t), x_2(t), \ldots, x_A(t)$, $x_i \in C_0$, $i = 1, 2, \ldots, A$ such that

$$\sqrt{\beta}x_{i+1}(t) + x_{i+1} > \sqrt{\beta}x_i(t) + x_i \qquad \text{for } t \in [0, \beta] \qquad i = 1, 2, \ldots, A-1.$$

This expression is obtained on the basis of the definition of conditional Wiener integral given in [19]. It is essential that the double product in (5) tends to the unity in the continuum limit $\varepsilon \to 0$.

3. Outline of the numerical method

3.1. Composite approximation formulae

When performing the computations for quantum systems with many degrees of freedom one has to evaluate multiple functional integrals

$$\underbrace{\int_X \ldots \int_X}_{m} F[x_1, \ldots, x_m]\,\mathrm{d}\mu(x_1) \ldots \mathrm{d}\mu(x_m) \equiv \int_{X^m} F[\boldsymbol{x}]\,\mathrm{d}\mu^{(m)}(\boldsymbol{x}). \tag{7}$$

The main problem is to reduce the integral over an abstract space X to some expression suitable for computations. It is clear that according to (7) we can consider the multiple functional integral as a single one over the multiplication of spaces X^m. For the functional integrals with an abstract Gaussian measure in complete separable metric spaces we derived some expressions which can be used for the numerical evaluation of these integrals [12]. Substituting the parameters of the measure (2) into these expressions we obtain the approximations for conditional Wiener integrals used in quantum mechanics. Particularly, the approximation formula which we call 'composite' looks as follows:

$$\int_{C_0} F[x]\,\mathrm{d}_W x = (2\pi)^{-n/2} \int_{R^n} \exp\{-\tfrac{1}{2}(u, u)\} 2^{-m} \times \underbrace{\int_{-1}^{1} \cdots \int_{-1}^{1}}_{m} F[\tilde{\rho}^{(m)}(v, \cdot) - \tilde{\rho}_n^{(m)}(v, \cdot) + \tilde{U}_n(u, \cdot)]\,\mathrm{d}v\,\mathrm{d}u + \mathcal{R}_n^{(m)}(F) \tag{8}$$

where

$$\tilde{\rho}_m(v, t) = \sum_{k=1}^{m} c_k^{(m)} \tilde{\rho}(v_k, t)$$

$$\tilde{\rho}(v,t) = \begin{cases} -t\,\mathrm{sign}(v) & t \leqslant |v| \\ (1-t)\,\mathrm{sign}(v) & t > |v| \end{cases}$$

$$\tilde{\rho}_n^{(m)}(v,t) = \sum_{k=1}^{n} \frac{2}{k\pi} \sin(k\pi t) \sum_{j=1}^{m} c_j^{(m)} \,\mathrm{sign}(v_j) \cos(k\pi v_j)$$

$$\tilde{U}_n(u,t) = \sum_{k=1}^{n} \frac{\sqrt{2}}{k\pi} u_k \sin(k\pi t)$$

$[c_k^{(m)}]^2$ are the roots of $Q_m(z) = \sum_{k=1}^{m} (-1)^k z^{m-k}/k!$, $z \in R$ and $\mathcal{R}_n^{(m)}(F)$ is the remainder term.

Formula (8) replaces the evaluation of a functional integral by the computation of an $n+m$-fold Riemann integral, where n and m are arbitrary natural parameters. This formula is exact (i.e. in this case $\mathcal{R}_n^{(m)}(F) = 0$) for any functional multinomial of degree $\leqslant 2m+1$. Note that the functional of the form

$$P_m[x] = \sum_{k=0}^{m} p_k[x]$$

where $p_k[x]$ is a homogeneous form of kth order continuous on X, is called a functional multinomial of degree m. We proved the convergence of approximations (8) to the exact value of the integral and estimated the remainder $\mathcal{R}_n^{(m)}(F)$ in dependence on n and m. It turns out that it is not necessary to approach the limits $n \to \infty$ and $m \to \infty$ simultaneously to ensure the convergence. Particularly, the order of convergence of (8) for $n \to \infty$, m fixed is $\mathrm{O}(n^{-(m+1)})$. Practical computations show (some examples will be given below) that the good accuracy (equal or better than 0.1%) can be achieved by choosing small values of n and m, even equal to unity. It allows us to use the more preferable deterministic algorithms in computations instead of stochastic (Monte Carlo) methods. Usually we employ Gaussian or Tchebyshev quadratures to evaluate low-dimensional Riemann integrals when computing functional integrals by our approximation formulae.

3.2. Approximation formulae with the weight

Since the functionals of the type $F[x] = \exp\{\int_0^\beta V[x(t)]\,\mathrm{d}t\}$ often appear in applications, in many cases it is convenient to use the approximation formulae with exponential weight. For conditional Wiener integrals

$$I = \int_{C_0} P[x]F[x]\,\mathrm{d}_W x$$

with the weight functional

$$P[x] = \exp\left\{\int_0^1 [p(t)x^2(t) + q(t)x(t)]\,\mathrm{d}t\right\} \qquad p(t), q(t) \in C[0,1]$$

we obtained the approximation formula of the $2m+1$ order of accuracy (i.e. exact for every functional multinomial of degree $\leqslant 2m+1$). This formula (we call it 'elementary') replaces the functional integral by the m-fold Riemann one. More precise approximations for the large class of functionals can be achieved by the use of the 'composite' formulae containing the $(n+m)$-fold Riemann integrals (even for $n = 1$). Combining these two approaches, we derived the composite approximation formula for the conditional Wiener integrals with the

considered weight:

$$I = (2\pi)^{-n/2}[W(1)]^{-1/2}\exp\left\{\int_0^1 L^2(t)\,\mathrm{d}t\right\}\int_{R^n}\exp\{-\tfrac{1}{2}(u,u)\}2^{-m}$$
$$\times\underbrace{\int_{-1}^{1}\cdots\int_{-1}^{1}}_{m}\Phi[\tilde{\rho}^{(m)}(v,\cdot)-\tilde{\rho}_n^{(m)}(v,\cdot)+\tilde{U}_n(u,\cdot)]\,\mathrm{d}v\,\mathrm{d}u+\mathcal{R}_n^{(m)}(F). \qquad (9)$$

This formula is exact for every polynomial functional of degree $\leqslant 2m+1$. Here

$$\Phi[x] = F[\hat{A}x + a]$$
$$\hat{A}x(t) = x(t) - \frac{1-t}{W(t)}\int_0^1 B(s)W(s)x(s)\,\mathrm{d}s$$
$$W(t) = \exp\left\{\int_0^1 (1-s)B(s)\,\mathrm{d}s\right\}$$
$$a(t) = \int_0^t L(s)\,\mathrm{d}s - \frac{1-t}{W(t)}\int_0^t B(s)W(s)\left[\int_0^s L(u)\,\mathrm{d}u\right]\mathrm{d}s$$
$$L(t) = \int_0^t [B(s)\,W(s)\,H(s) - q(s)]\,\mathrm{d}s \qquad H(t) = \int_t^1 q(s)\frac{1-s}{W(s)}\,\mathrm{d}s$$

and $B(s)$ is the solution of differential equation

$$(1-s)B'(s) - (1-s)B(s) - 3B(s) = 2p(s) \qquad s \in [0,1] \qquad (10)$$

with initial condition

$$B(1) = -\tfrac{2}{3}\,p(1).$$

Note that in particular case $p(t) \equiv p = \text{constant}$, $q(t) \equiv q = \text{constant}$ the Riccati equation (10) can be solved explicitly and the approximation formula (9) aquires the significant simplification.

The remainder of the formula can be estimated as follows:

$$|\mathcal{R}_n^{(m)}(F)| \leqslant D\alpha^{m+1}[\xi_m + (2m)^{m+1}\eta_m]\frac{1}{n^{m+1}}$$

where

$$D = [W(1)]^{-1/2}\exp\left\{\tfrac{1}{2}\int_0^1 L^2(t)\,\mathrm{d}t\right\}$$
$$\alpha = 1 + w + 2\sqrt{w} \qquad w = \frac{1}{\sin^4\sqrt{2p}}\left(\sqrt{2p}\cos\sqrt{2p} - \sin\sqrt{2p}\right)^2\left(1 - \frac{\sin 2\sqrt{2p}}{2\sqrt{2p}}\right)$$

ξ_m and η_m are positive constants dependent on m and on the functional F [13]. Particularly, it follows from this estimate that the convergence of approximations obtained according to (9) for $n \to \infty$, m fixed has the order $\mathrm{O}(n^{-(m+1)})$.

3.3. Approximations with the total order of accuracy

It turns out that it is more economical to use approximation formulae possessing a given total order of accuracy on X^m to calculate the m-fold functional integral [20]. In the case

of conditional Wiener measure the composite formula of the third-order accuracy has the form

$$\int_{C_0^m} F[\boldsymbol{x}]\,\mathrm{d}_W\boldsymbol{x} = (2\pi)^{-N/2}\int_{R^N}\exp\left\{-\tfrac{1}{2}\sum_{i=1}^{m}(\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)})\right\}$$
$$\times\frac{1}{m}\sum_{i=1}^{m}\int_R F(\tilde{U}_{n_1}(\boldsymbol{u}^{(1)}),\ldots,\underbrace{\sqrt{m}\,\tilde{\Sigma}_i(\rho(v,\cdot),\boldsymbol{u}^{(i)})}_{i},$$
$$\ldots,\tilde{U}_{n_m}(\boldsymbol{u}^{(m)}))\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}v + \mathcal{R}_N(F) \tag{11}$$

where

$$\rho(v,t) = \begin{cases} -t\,\mathrm{sign}(v) & t \leqslant |v| \\ (1-t)\,\mathrm{sign}(v) & t > |v| \end{cases} \qquad N = \sum_{i=1}^{m} n_i$$
$$\tilde{\Sigma}_i(\rho(v,t),\boldsymbol{u}^{(i)}) = \rho(v,t) - S_{n_i}(\rho(v,t)) + \tilde{U}_{n_i}(\boldsymbol{u}^{(i)})$$
$$S_{n_i}(\rho(v,t)) = 2\sum_{j=1}^{n_i}\frac{1}{j\pi}\sin(j\pi t)\,\mathrm{sign}(v)\cos(j\pi v)$$
$$\tilde{U}_{n_i}(\boldsymbol{u}^{(i)}) = \sqrt{2}\sum_{j=1}^{n_i}u_j^{(i)}\frac{1}{j\pi}\sin(j\pi t) \qquad \text{for all } i = 1,2,\ldots,m.$$

We compute the multidimensional Riemann integrals which appear in (11), using the Korobov method.

For the m-fold conditional Wiener integrals with the weight functional

$$P[x_1,\ldots,x_m] = \exp\left\{\sum_{i=1}^{m}\int_0^1 [p_i(t)\,x_i^2(t) + q_i(t)\,x_i(t)]\,\mathrm{d}t\right\}$$

we derived the following approximation formula:

$$\int_{C_0^m} P[x_1,\ldots,x_m]F[x_1,\ldots,x_m]\,\mathrm{d}_W^{(m)}x = \exp\left\{-\tfrac{1}{2}\sum_{i=1}^{m}\int_0^1(1-s)B_i(s)\,\mathrm{d}s\right\}(2m)^{-1}$$
$$\times\exp\left\{\tfrac{1}{2}\sum_{i=1}^{m}\int_0^1 L_i^2(t)\,\mathrm{d}t\right\}\sum_{i=1}^{m}\int_{-1}^{1}F[a_1(\cdot),\ldots,a_{i-1}(\cdot),\sqrt{m}\Psi_i(v,\cdot)$$
$$+a_i(\cdot),a_{i+1}(\cdot),\ldots,a_m(\cdot)]\,\mathrm{d}v + \mathcal{R}_m(F) \tag{12}$$

where $B_i(s)$ is the solution of the differential equation

$$(1-s)\,B_i'(s) - (1-s)^2B_i^2(s) - 3B_i(s) - 2p_i(s) = 0 \qquad s\in[0,1]$$
$$B_i(1) = -\tfrac{2}{3}p_i(1) \tag{13}$$

and

$$\Psi_i(v,\cdot) = f_i(v,\cdot) - \sigma(v,\cdot) \qquad W_i(t) = \exp\left\{\int_0^1(1-s)B_i(s)\,\mathrm{d}s\right\}$$
$$f_i(v,t) = \mathrm{sign}(v)\frac{1-t}{W_i(t)}\left[1 + \int_0^{\min\{|v|,t\}} B_i(s)W_i(s)\,\mathrm{d}s\right.$$
$$bigg]$$
$$a_i(t) = \int_0^t L_i(s)\,\mathrm{d}s - \frac{1-t}{W_i(t)}\int_0^t B_i(s)W_i(s)\int_0^s L_i(u)\,\mathrm{d}u\,\mathrm{d}s$$

$$L_i(t) = \int_0^t [B_i(s)W_i(s)K_i(s) - q_i(s)]\,\mathrm{d}s + c_i$$

$$K_i(s) = \int_s^1 q_i(u)\frac{1-u}{W_i(u)}\,\mathrm{d}u \qquad \sigma(v,t) = \begin{cases} \operatorname{sign}(v) & t \leqslant |v| \\ 0 & t > |v| \end{cases}$$

and the constants c_i are determined by the condition $\int_0^1 L_i(s)\,\mathrm{d}s = 0$.

Approximation formula (12) is exact when $F[x]$ is arbitrary polynomial functional of the third total degree on C_0^m. We compute the Riemann integral in (12) using Gaussian or Tchebyshev quadratures with the relative accuracy 0.01.

In the particular case $p_i(t) \equiv p_i = \text{constant}$ the solution of the Riccati equation (13) is the following:

$$B_i(s) = \frac{1}{1-s}\left\{\sqrt{2p_i}\operatorname{ctg}\left[\sqrt{2p_i}(1-s)\right] - \frac{1}{1-s}\right\}.$$

If we set also $q_i(t) \equiv q_i = \text{constant}$, then $a_i(t)$ can be expressed explicitly

$$a_i(t) = q_i\left[p_i\cos\sqrt{\tfrac{1}{2}p_i}\right]^{-1}\sin\left(\sqrt{\tfrac{1}{2}p_i}\,t\right)\sin\left(\sqrt{\tfrac{1}{2}p_i}(1-t)\right)$$

and the approximation formula (12) acquires the form

$$\begin{aligned}\int_{C_0^m} P[x_1,\ldots,x_m]F[x_1,\ldots,x_m]\,\mathrm{d}_W^{(m)}x = (2m)^{-1}\prod_{i=1}^m\left(\frac{\sqrt{2p_i}}{\sin\sqrt{2p_i}}\right)^{\frac{1}{2}} \\ \times\exp\left\{\frac{q_i^2}{(2p_i)^{3/2}}\left[\tan\sqrt{\tfrac{1}{2}p_i} - \sqrt{\tfrac{1}{2}p_i}\right]\right\} \\ \times\sum_{i=1}^m\int_{-1}^1 F[a_1(\cdot),\ldots,a_{i-1}(\cdot),\sqrt{m}\Psi_i(v,\cdot) \\ +a_i(\cdot),a_{i+1}(\cdot),\ldots,a_m(\cdot)]\,\mathrm{d}v + \mathcal{R}_m(F). \qquad (14)\end{aligned}$$

For the functional integrals without weight, formula (14) can be applied by setting $p_i = q_i = 0$ for all $i = 1,\ldots,m$. Other approximation formulae and theorems on the error estimate are given in [12, 13, 20].

3.4. Numerical examples

Let us consider the approximate calculation of the two-fold functional integral with conditional Wiener measure

$$I = \int_{C_0^2}\exp\left\{\int_0^1 (px^2(t) + qx(t) + py^2(t) + qy(t))\,\mathrm{d}t\right\}\mathrm{d}_W x\,\mathrm{d}_W y$$

using (11). The results for $q = 5$ and various p, n_1 and n_2 are given in tables 1 and 2. The (n_1+n_2)-fold Riemann integral in (11) can be evaluated explicitly in this case. We compute the remaining single integral using the Thebyshev quadrature. The computations took about 1 s on CDC-6500 computer. We use I^* to denote the exact value of the functional integral. We found it by the substitution of functional variables given by the linear transformation mapping the space C_0 onto itself in one-to-one correspondence [13]. It is seen that the good approximations are obtained with the small dimensions n_1 and n_2 and that the results converge to exact value as $n_1, n_2 \to \infty$.

Table 1. Values of the two-fold functional integral for $p = 0.5$. $I^* = 12.033\,906\,88$.

$n_1; n_2$	1	2	3	5	10
1	12.033 2950				
2	12.034 2440	12.033 8116			
3	12.039 5110	12.035 6295	12.033 9518		
5	12.042 3562	12.037 4153	12.034 2150	12.033 9122	
10	12.044 7756	12.039 0693	12.034 7689	12.034 0572	12.033 9069

Table 2. Values of the two-fold functional integral for $p = -0.5$. $I^* = 5.655\,919\,950$.

$n_1; n_2$	1	2	3	5	10
1	5.653 388 31				
2	5.654 722 54	5.655 150 20			
3	5.654 654 95	5.655 575 58	5.655 732 96		
5	5.654 876 46	5.655 542 52	5.655 838 32	5.655 872 19	
10	5.655 136 82	5.655 532 13	5.655 975 14	5.655 932 99	5.655 912 93

Let us now consider the computation of functional integrals characterizing the quantum system described by the Hamiltonian operator $H = -\frac{1}{2}\Delta + V$ with the potential

$$V(x) = \tfrac{1}{2}(x^2 - x_0^2)^2 \qquad x \in (-\infty, \infty)$$

which has minima at $\pm x_0$. This double-well system is of interest because it provides the convenient framework for studying the tunnelling and instanton effects. The properties of this system are used in studying ferroelectrics, semiconductors, and so on. Owing to tunnelling, the ground-state wavefunction is an even superposition of the wavefunctions of each well. The main effect is the splitting of the energy levels (which are doubly degenerate if tunnelling is neglected). The method of functional integrals is a convenient technique for studying tunnelling effects [22]. Our results of computation of the ground state E_0 obtained using the approximation formula (8) are presented in table 3 for the different values of the strength of potential barrier x_0 and for various parameters n and m. The computations took few seconds per point x_0. E_0^* are exact results taken from [23]. For comparison we cite the results E_0^{st} of [7] obtained by the use of 'short-time' propagator with dimension N and k iterations. The CPU time in this work is reported to be rather large although less than in Monte Carlo computations. E_0^{it} denotes the result of [9] obtained by an iterative matrix multiplication method. Since the results of other authors are given in a graphic form, we compare them with our results of computation of E_0 and of the splitting of levels $\triangle E$ obtained with $n = m = 1$ in figure 1. In [24] the ground-state energy has been obtained by evaluation of the lattice (discretized) path integral via Monte Carlo simulations. The results of [25] are reported to be obtained evaluating the N-fold integral via averaging over 10 Monte Carlo iterations on the lattice with $N = 303$ points and spacing $\varepsilon = 0.25$. It is seen that our functional deterministic method gives better results while requiring essentially less computer time and memory versus other numerical methods, both stochastic and deterministic, used by the other authors.

Table 3. Comparison of results for the system with a double-well potential.

	E_0/E_0^* (this work)			E_0^{st}/E_0^* [7]			
x_0^2	$n=m=1$	$n=1,\ m=2$	$n=2,\ m=1$	k	$N=17$	$N=33$	E_0^{it}/E_0^* [9]
0	1.0008	1.0002	1.0001		—	—	—
				5	0.9852	0.9725	
1	1.0016	1.0004	1.0003	10	0.9949	0.9996	—
				15	0.9949	0.9996	
				5	0.9158	0.8399	
2	0.9982	1.0007	0.9994	10	0.9537	0.9919	0.9856
				15	0.9550	0.9967	

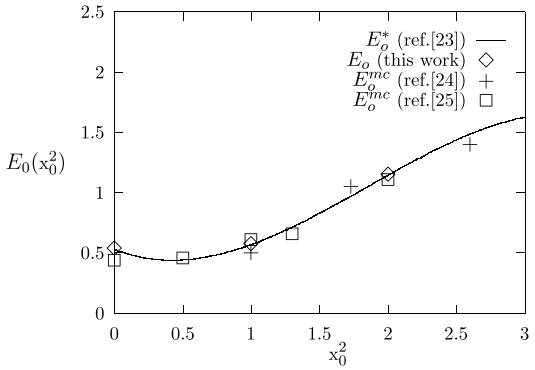

Figure 1. Ground-state energy of the double well.

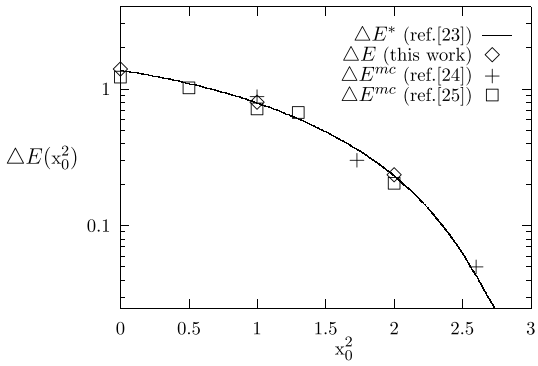

Figure 2. Difference of energies of the ground and the first excited states of the double well.

4. Application to the quantum many-body systems

4.1. Many-body Calogero model

Let us consider first some pedagogical example for which the exact solution is known, namely the Calogero model which is characterized by the following Hamiltonian operator

$$H = -\sum_{k=1}^{n} \frac{\partial^2}{\partial x_k^2} + \tfrac{1}{2}\omega^2 \sum_{i<j}^{n} (x_i - x_j)^2 + g \sum_{i<j}^{n} (x_i - x_j)^{-2}. \tag{15}$$

Table 4. Ground-state energy of the Calogero model for $n = 3$, $g = 1.5$.

ω	E_0 (this work)	E_0^{mc} [26]	E_0^*
0.10	1.346	—	1.3472
0.20	2.700	—	2.6944
0.25	3.366	3.35 ± 0.004	3.3680
0.50	6.738	—	6.7361

Table 5. Ground-state energy of the Calogero model for $\omega = 0.25$, $g = 1.5$.

n	E_0 (this work)	E_0^{mc} [26]	E_0^*
5	13.447	13.37 ± 0.04	13.4397
7	32.249	32.34 ± 0.09	32.2718
9	61.473	61.31 ± 0.10	61.5183
11	102.865	102.31 ± 0.14	102.6028

This model corresponds to the system of n particles which interact via centrifugal repulsion and linear attraction forces with the coupling constants g and ω respectively. It was studied by many authors (see, e.g. [26]), which used the Monte Carlo method. We computed the statistical sum (partition function) Z and the ground-state energy E_0 for this model using our approximation method for functional integrals. The results for three particles and various values of the constant ω are listed in table 4, whereas those for the fixed ω and various numbers of particles n are given in table 5. The CPU time of computation of E_0 was 11 s per point ω for $n = 3$. For comparison we cite the results E_0^{mc} obtained by the Monte Carlo method [26] using 1000 points of time discretization and 100 iterations. The exact values are denoted by E_0^*. The CPU time of our computation of E_0 for $n = 11$ was about 3 min on CDC-6500, whereas the computation of E_0^{mc} required as long as 15 min on the same computer [26]. It is seen from the tables that our deterministic method gives better results than those obtained by the Monte Carlo algorithm which did not even provide the agreement of E_0^{mc} with E_0^* in the framework of the presented error estimates. So, as distinct from the other deterministic techniques of computation of path integrals, our functional method works well also in a study of quantum systems with many degrees of freedom, i.e. in a multidimensional case, and ensures the higher efficiency of computations versus traditional stochastic methods.

4.2. Nuclear potential models

4.2.1. The triton problem. Let us now consider the numerical investigation of interaction of particles (nucleons) in the nucleus of tritium. This three-body problem is of the real interest in physics (see [6, 27]). The Hamiltonian describing this system is the following:

$$H = \sum_{i=1}^{3} \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial \boldsymbol{x}_i^2} + \sum_{i<j} V(|r_{ij}|). \tag{16}$$

Here $\boldsymbol{x}_i = (x_i^{(1)}, x_i^{(2)}, x_i^{(3)})$, $i = 1, 2, 3$ denote the coordinates of the particle with the mass m_i and

$$r_{ij} = \boldsymbol{x}_i - \boldsymbol{x}_j.$$

As shown in [27], various types of interaction potentials yield different values of the binding energy and even for the same potential the different methods of calculation give different binding energies.

We have studied the following model of triton used by the various authors:

$$V(r) = -51.5 \exp\left\{-\frac{r^2}{b^2}\right\} \text{ MeV} \qquad b = 1.6F \tag{17}$$

$m_1 = m_2 = m_3 = m_p$, where $m_p = 938.279$ MeV is the proton mass. The following values of the ground-state energy have been obtained in this model by means of variational E_v and Monte Carlo E_{mc} methods (see [6, 26] and the references therein):

$$\begin{aligned}
&E_{mc} = -9.77 \pm 0.06 \text{ MeV}\\
&E_v = -9.42 \text{ MeV}\\
&E_v = -9.47 \pm 0.4 \text{ MeV}\\
&-9.99 \pm 0.05 \text{ MeV} < E_v < -9.75 \pm 0.04 \text{ MeV}\\
&E_v = -9.78 \text{ MeV}.
\end{aligned}$$

It is seen, that the difference between these results is larger than the presented error estimates. Therefore, the solution of this problem by some other method is of interest for obtaining a more precise result.

We consider the problem (16)–(17) in the framework of the functional integral approach. We compute the partition function (the nine-fold functional integral) using our numerical technique. The computations have been performed with the relative accuracy $\varepsilon = 0.01$. Our result $E = -9.7$ MeV agrees well with the data of other authors. The CPU time was about 15 min, which is less than the times reported in the other known works. It is desirable, however, to take into account the three-nucleon force as well as the more realistic potentials like Argonne v_{14} and the Paris ones [27] which would make a subject of our future work.

4.2.2. One-dimensional nuclear model. We have studied the one-dimensional nuclear model proposed in [16] with the parameters chosen so that to conform to the three-dimensional case:

$$\begin{aligned}
&V(x) = \sum_{k=1}^{2} \frac{V_k}{\sigma_k\sqrt{\pi}} \exp\left\{-\frac{x^2}{\sigma_k^2}\right\}\\
&V_1 = 12 \qquad V_2 = -12 \qquad \sigma_1 = 0.2 \qquad \sigma_2 = 0.8 \qquad \hbar = m = 1
\end{aligned} \tag{18}$$

in units of length $l_0 = 1.89$ Fm and energy $E_0 = \hbar^2/(ml_0^2) = 11.6$ MeV. Applying our numerical method in the case of antisymmetrized states in accordance with (6) and using the approximation formula of the third total degree of accuracy for the multiple functional integrals, we have:

$$\begin{aligned}
Z(\boldsymbol{x}, \boldsymbol{x}, \beta) \simeq (2\pi\beta)^{-A/2} \frac{1}{2n} \sum_{i=1}^{A} \int_{-1}^{1} \exp\Bigg\{ &- \beta \int_0^1 F\Big[x_1, x_2, \ldots, x_{i-1}, \sqrt{A\beta}\rho(v,t)\\
&+ x_i, x_{i+1}, \ldots, x_A\Big]\,\mathrm{d}t\Bigg\}\\
&\times \Omega\Big[x_1, x_2, \ldots, x_{i-1}, \sqrt{A\beta}\rho(v,\cdot) + x_i, x_{i+1}, \ldots, x_A\Big]\,\mathrm{d}v
\end{aligned} \tag{19}$$

where

$$F[x_1,\ldots,x_A]=\sum_{i>j}V(|x_i-x_j|)\qquad \rho(v,t)=\begin{cases}-t\,\mathrm{sign}(v) & t\leqslant|v|\\ (1-t)\,\mathrm{sign}(v) & t>|v|\end{cases}$$

$$\Omega[x_1,\ldots,x_A]=\begin{cases}1 & x_1(t)<x_2(t)<\ldots<x_A(t),\ t\in[0,1]\\ 0 & \text{otherwise.}\end{cases}$$

Functional $\Omega[x_1,\ldots,x_A]$ is introduced to define the integration domain in the space C_0^A. It imposes the conditions on the minimal and maximal values of the integration variable v in dependence on the given set of $x_1, x_2, \ldots, x_A$. We compute the Riemannian integrals using the Gaussian quadrature with the relative accuracy 0.01.

4.2.3. The 2N system. For the system of two nucleons (deuteron) our result of computation of the binding energy is $E_d = 2.24$ MeV which can be compared with the experimental data $E_{ex} = 2.2$ MeV, with the prediction of the semi-empirical formula [28] $E_{se} = 3.5$ MeV and with the value $E = 2.243$ MeV obtained in [7]. Our results can be considered as satisfactory and it provides the basis for study of the more realistic types of interaction.

4.2.4. The 4N system. For the system of four nucleons (α-particle) we computed the binding energy with result $E_F = 27.6$ MeV which is close to the experimental value $E_{ex} = 28.3$ MeV [5]. The prediction of the semi-empirical formula is $E_{se} = 18.8$ MeV. We compare our results with those obtained in [16] by means of the lattice Monte Carlo simulations in the framework of the same model. Since the results of [16] are given in a graphical form, we reproduce them in figure 3. It shows the binding energy of four particles in the dimensionless units E/E_0, where $E_0 = \hbar^2/(ml_0^2) = 11.6$ MeV, as a function of the lattice spacing ε, obtained in [16] by simulation of 10^4 events. E_T and E_N denote the trial energy and the normalization energy respectively, and E_M are the values obtained by the Metropolis algorithm [16]. The problem of extrapolation of results to the continuum limit ($\varepsilon \to 0$) has been discussed in [16] and [17] and found to be not simple enough. In contrast, in our approach we do not have such problems since we do not introduce the lattice discretization and consider the quantities directly in continuum limit. Our functional-integral result E_F/E_0 is shown in figure 3 at the point $\varepsilon = 0$.

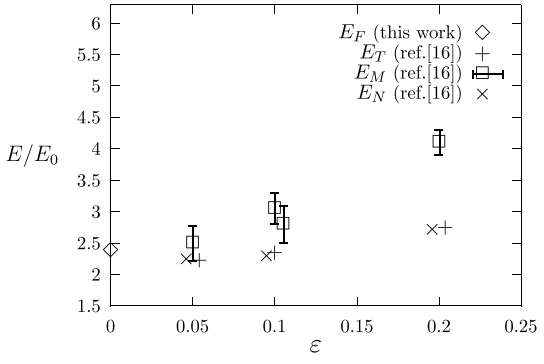

Figure 3. Binding energy of the four-particle bound state.

5. Conclusion

The described method of computation of functional integrals based on a rigorous definition of measure in metric spaces has important advantages over conventional Monte Carlo simulation method. The employment of this approach replaces the evaluation of functional integrals by computation of the ordinary ones of a low dimension thus allowing us to use the more preferable deterministic algorithms and provides significant economy of computer time and memory. This approach is very useful when other methods (perturbative, semiclassical approximation, etc) cannot be applied. Our method works effectively also in a case of high dimensions where other deterministic methods of numerical path integration as well as finite-difference methods usually fail. Moreover, it is of no importance for implementation of this method whether the interaction is pairwise or multiparticle, the function $V(x)$ can depend on its components $x_1, \ldots, x_m$ arbitrarily, because there is no need to reverse densely filled high-order matrices. The advantages mentioned above prove this method to be a promising tool for solving the many-body problems. We have found this approach to be convenient for study of the complicated quantum systems [29]. Further work in this area is in progress.

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