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Computation of multiple functional integrals in quantum physics

Yu.Yu. Lobanov*, R.R. Shahbagian, E.P. Zhidkov

Laboratory of Computing Techniques and Automation, Joint Institute for Nuclear Research, 141980 Dubna, Russia

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Abstract

The new method of computation of multiple functional integrals of quantum physics is elaborated. The method is based on the numerical integration over complete separable metric spaces via approximations exact on a class of polynomial functionals of given degree. New approximation formulas for the functional integrals with respect to Gaussian measure are constructed. The convergence of approximations to an exact value of integral is proved, the estimate of the remainder is obtained. In the particular case of conditional Wiener measure the approximation formulas with the weight are derived. The method is applied to the study of the multidimensional Calogero model and to computation of the binding of nucleons in the nucleus of tritium.

Keywords: Functional integral; Gaussian measure; Quantum physics; Approximation formula; Numerical integration; Hamiltonian operator; Calogero model; Nucleus of tritium; Binding energy

1. Introduction

The functional integration method first applied in quantum mechanics by R. Feynman is now one of the most effective mathematical methods in contemporary quantum physics [3]. The wide scope of application of functional integrals [9] stimulated the development of their theory and methods for the numerical evaluation (see, e.g., [2]). In our previous works [4, 6] we derived for the functional integrals over complete separable metric spaces some new approximation formulas which have been proved to have important advantages versus the traditional lattice Monte Carlo method, including the higher efficiency with respect to computer resources [7]. In many physical problems when studying quantum systems with many degrees of freedom, one has to evaluate the multiple functional integral

$$\int_X F(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}), \quad \boldsymbol{x} = (x_1, x_2, \ldots, x_m), \tag{1}$$

* Corresponding author.

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over the Cartesian product of m copies of a complete separable metric space X. Here $\mu(\boldsymbol{x})$ is a Gaussian measure on X, uniquely determined by the correlation functional $K(\xi, \eta)$ and the mean value $M(\xi)$; $\xi, \eta \in X'$ [2].

One of the means of computation of integral (1) is the successive employment of some approximation formulas for the one-dimensional functional integrals [4] (e.g., formulas exact on a class of polynomial functionals of degree $\leqslant 2n_k + 1$ for the variable $x_k \in X$).

It turned out however [8] that the higher efficiency of computations can be provided by the approximation formulas with the given total degree of accuracy $2k + 1$, i.e., formulas which are exact for the constant functional and for the functionals

$$F(\boldsymbol{x}) = \prod_{i=1}^{m} F_{k_i}(x_i), \quad k_1 + k_2 + \cdots + k_m \leqslant 2k + 1,$$

where $F_{k_i}(x_i)$ is a homogeneous polynomial functional of degree k_i with respect to argument x_i.

In the present paper we derive and study the approximation formulas of this kind and demonstrate their efficiency by the numerical investigation of the multidimensional Calogero model and by the computation of the binding energy of nucleons in the nucleus of tritium.

2. Approximation formulas

The example of approximation formulas of the third total degree of accuracy is given by the following.

Theorem 1 (Egorov et al. [2]). *Let L be a linear homogeneous functional defined on a manifold of the functionals integrable with respect to the measure μ. Let, also, the following conditions be satisfied:*

(1) *$L\{F\} = 0$ for any odd functional $F(x)$.*

(2) *$L\{\langle\xi,\cdot\rangle\langle\eta,\cdot\rangle\} = K(\xi,\eta)$ for arbitrary $\xi,\eta \in X'$, $K(\xi,\eta)$ is a correlation functional of the measure μ.*

(3) *Either*

$$L\left\{\prod_{i=1}^{2l} \langle\xi_i,\cdot\rangle\right\} \neq 0 \quad \textit{and} \quad L\{1\} \neq 0, \tag{2}$$

or

$$L\left\{\prod_{i=1}^{2l} \langle\xi_i,\cdot\rangle\right\} \equiv 0 \quad \textit{for any } \xi_i \neq 0,\ \xi_i \in X',\ i = 2,3,\ldots,m.$$

Let b_i ($i = 2,3,\ldots,m$) be arbitrary positive numbers. Then the approximation formula

$$\int_X F(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) \approx \left(1 - \sum_{i=1}^{m} b_i L\{1\}\right) F(0,0,\ldots,0) + \sum_{i=1}^{m} b_i L_{x_i}\{F(0,0,\ldots,0,x_i/\sqrt{b_i},0,\ldots,0)\} \tag{3}$$

is exact for all polynomial functionals of third total degree on $\boldsymbol{X}$.

Remark. The designation $L_{x_i}(F)$ means that the functional L is applied to F as to the functional of argument $x_i \in X$ only.

Formulas like (3) give a good approximation to the integrals of functionals which are close to the polynomial functional of third total degree on X. More precise approximations can be achieved for the large class of functionals if one uses the method of construction of the so-called "composite approximation formulas" which we derive in [4] for the one-dimensional functional integrals. The advantages of the "composite approximation formulas" over the "elementary" ones have been determined in [4]. Analogously to the case of one-dimensional functional integrals, the construction of the composite approximation formulas for integral (1) is based on the use of the relation called "mixed integration formula" [2]. Applying this formula to integral (1) with respect to each component x_i, we obtain the mixed integration formula for the multiple functional integrals

$$\int_X F(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) = \int_{R^N} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m}(\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)})\right\}\int_X F(x_1 - S_{n_1}(x_1) + U_{n_1}(\boldsymbol{u}^{(1)}),\ldots$$
$$x_m - S_{n_m}(x_m) + U_{n_m}(\boldsymbol{u}^{(m)}))\,\mathrm{d}\mu(\boldsymbol{x})\,\mathrm{d}\boldsymbol{u}^{(1)}\ldots\boldsymbol{u}^{(m)}. \tag{4}$$

Here

$$S_{n_i}(x_i) = \sum_{j=1}^{n_i}(e_j, x_i)e_j, \quad U_{n_i}(\boldsymbol{u}^{(i)}) = \sum_{j=1}^{n_i} u_j^{(i)} e_j, \tag{5}$$
$$N = \sum_{i=1}^{m} n_i, \quad \boldsymbol{u}^{(i)} \in R^{n_i}, \quad (\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)}) = \sum_{j=1}^{n_i}(u_j^{(i)})^2,$$

n_i are arbitrary positive numbers, $\{e_k\}_{k=1}^{\infty}$ is an orthonormal basis formed by eigenfunctions of a correlation functional $K(\xi, \eta)$ in the Hilbert space H which is dense almost everywhere in X and generated by the measure μ, and $(\cdot,\cdot)$ is a scalar product in H.

Substituting the integral over X on the right-hand side of (4) by the approximation formula (3), we obtain the composite approximation formula of the third summary degree of accuracy for integral (1). Thus, the following theorem appears to be proved.

Theorem 2. *Under conditions* (2) *and* (5) *the approximation formula*

$$\int_X F(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) = (2\pi)^{(-N/2)}\int_{R^N}\exp\left\{-\frac{1}{2}\sum_{i=1}^{m}(\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)})\right\}$$
$$\times\Bigg[\left(1-\sum_{i=1}^{m} b_i L\{1\}\right)F(\Sigma_1(x_1\equiv 0,\boldsymbol{u}^{(1)}),\ldots,\Sigma_m(x_m\equiv 0,\boldsymbol{u}^{(m)}))$$
$$+\sum_{i=1}^{m} b_i L x_i\{F(\Sigma_1(x_1\equiv 0,\boldsymbol{u}^{(1)}),\ldots,\Sigma_i(x_i/\sqrt{b_i},\boldsymbol{u}^{(i)}),\ldots$$
$$\Sigma_m(x_m\equiv 0,\boldsymbol{u}^{(m)}))\}\Bigg]\,\mathrm{d}\boldsymbol{u} + R_N(F) \tag{6}$$

is exact for all polynomial functionals of third total degree on X.

Here

$$\Sigma_i(x_i, \boldsymbol{u}^{(i)}) = x_i - S_{n_i}(x_i) + U_{n_i}(\boldsymbol{u}^{(i)}),$$

$R_N(F)$ is a remainder of formula (6).

Consider the particular case

$$L\{F\} = \int_R F[\rho(v)]\, \mathrm{d}\nu(v), \tag{7}$$

where ν is the symmetric probabilistic measure on R. Let a function $\rho(r): R \mapsto X$ satisfy the conditions

$$\rho(r) = -\rho(r),$$

$$\int_R \langle \xi, \rho(r) \rangle \langle \eta, \rho(r) \rangle\, \mathrm{d}\nu(r) = K(\xi, \eta),$$

$$\prod_{i=1}^{j} \langle \xi_i, \rho(r) \rangle \in L(R, \nu), \quad 1 \leqslant j \leqslant 3, \;\; \eta, \xi, \xi_i \in X',$$

and let $b_i = 1/m$, $i = 1, 2, \ldots, m$. Then the following theorem is valid:

Theorem 3 (Zhidkov et al. [10]). *Let $F(\boldsymbol{x})$ be an arbitrary integrable real functional. Then the approximation formula*

$$\int_X F(\boldsymbol{x})\, \mathrm{d}\mu(\boldsymbol{x}) = (2\pi)^{(-N/2)} \int_{R^N} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m} (\boldsymbol{u}^{(i)}, \boldsymbol{u}^{(i)})\right\}$$
$$\times \frac{1}{m}\sum_{i=1}^{m} \int_R F(U_{n_1}(\boldsymbol{u}^{(1)}), \ldots, \Sigma_i(\sqrt{m}\, \rho(v, \cdot), \boldsymbol{u}^{(i)}), \ldots$$
$$U_{n_m}(\boldsymbol{u}^{(m)}))\, \mathrm{d}\boldsymbol{u}\, \mathrm{d}\nu(v) + R_N(F), \tag{8}$$

where

$$\Sigma_i = \rho(v, t) - S_{n_i}(\rho(v, t)) + U_{n_i}(\boldsymbol{u}^{(i)}),$$

is exact for functional polynomials of the third total degree on $\boldsymbol{X}$.

In the special case

$$X = \{C[0, 1],\, x(0) = x(1) = 0\} \equiv C$$

when X is a functional space with conditional Wiener measure, determined by the correlation functional

$$K(t, s) = \min(t, s) - ts,$$

we obtain [10] the following approximation formula for an m-dimensional conditional Wiener integral:

$$\int_C F(\boldsymbol{x})\,\mathrm{d_W}\boldsymbol{x} = (2\pi)^{-N/2}\int_{R^N}\exp\left\{-\frac{1}{2}\sum_{i=1}^{m}(\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)})\right\}$$
$$\times\frac{1}{m}\sum_{i=1}^{m}\int_R F(\tilde{U}_{n_1}(\boldsymbol{u}^{(1)}),\ldots,\tilde{\Sigma}_i(\sqrt{m}\,\rho(v,\cdot),\boldsymbol{u}^{(i)}),\ldots$$
$$\tilde{U}_{n_m}(\boldsymbol{u}^{(m)}))\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}v + R_N(F), \tag{9}$$

where

$$\mathrm{d}\nu = \tfrac{1}{2}\mathrm{d}v,\quad \rho(v,t) = \begin{cases} -\,t\,\mathrm{sign}(v), & t \leqslant |v|,\\ (1-t)\,\mathrm{sign}(v), & t > |v|,\end{cases}$$

$$\tilde{\Sigma}_i(\rho(v,t),\boldsymbol{u}^{(i)}) = \rho(v,t) - S_{n_i}(\rho(v,t)) + \tilde{U}_{n_i}(\boldsymbol{u}^{(i)}),$$

$$S_{n_i}(\rho(v,t)) = 2\sum_{j=1}^{n_i}\frac{1}{j\pi}\sin(j\pi t)\,\mathrm{sign}(v)\cos(j\pi v),$$

$$\tilde{U}_{n_i}(\boldsymbol{u}^{(i)}) = \sqrt{2}\sum_{j=1}^{n_i}u_j^{(i)}\frac{1}{j\pi}\sin(j\pi t)\quad\text{for all } i=1,2,\ldots,m.$$

Let us now study the convergence of the approximations (8) (and (9) respectively) to the exact value of the integral.

Theorem 4. *Assume that for almost all $v \in R$ we have*

$$S_{n_i}(\rho(v)) \to \rho(v),\quad n_i\to\infty,\ i=1,2,\ldots,m, \tag{10}$$

with respect to the measure $\nu(v)$. Let $F(\boldsymbol{x})$ be a continuous on $\boldsymbol{X}$ functional satisfying the conditions

$$|F(\boldsymbol{x})| \leqslant g(A^1(x_1,x_1),\ldots,A^m(x_m,x_m)), \tag{11}$$

where $A^k(x_k,x_k)$ is a nonnegative quadratic functional

$$A^k(x_k,x_k) = \sum_{i=1}^{\infty}\gamma_i^k(x_k,e_i)^2,\quad k=1,2,\ldots,m, \tag{12}$$

$$\sum_{i=1}^{\infty}\gamma_i^k < \infty,\quad \gamma_i \geqslant 0,\ i=1,2,\ldots, \tag{13}$$

$g(x)$ is a nondecreasing positive function and

$$\int_X\int_R g\Big(A^1(x_1,x_1),\ldots,\underbrace{A^k(\sqrt{m}\rho(v),\sqrt{m}\rho(v)) + A^k(x_k,x_k)}_{k},\ldots A^m(x_m,x_m)\Big)\,\mathrm{d}\nu(v)\,\mathrm{d}\mu^{(m)}(x) < \infty. \tag{14}$$

Then the remainder of the approximation formula (8)

$$R_N(F) \to 0 \quad \text{as } n_i \to \infty,\ i = 1,2,\ldots,m.$$

Proof. Without any restrictions of generality we suppose that

$$\gamma_i^k \equiv \gamma_i \quad \text{for all } k = 1,2,\ldots,m$$

and

$$A^k(x_k, x_k) \equiv A(x_k, x_k).$$

Using (11)–(13), we obtain

$$\begin{aligned}
&|F(S_{n_1}(x_1),\ldots,\sqrt{m}(\rho(v) - S_{n_k}(\rho(v))) + S_{n_k}(x_k),\ldots,S_{n_m}(x_m))| \\
&= \left| F\left(\sum_{i=1}^{n_1} (x_1, e_i)e_i, \ldots, \sum_{i=1}^{n_k} (x_k, e_i)e_i + \sqrt{m} \sum_{i=n_k+1}^{\infty} (\rho(v), e_i)e_i, \ldots, \sum_{i=1}^{n_m} (x_m, e_i)e_i \right) \right| \\
&\leqslant g\left(\sum_{i=1}^{n_1} \gamma_i (x_1, e_i)^2, \ldots, \sum_{i=1}^{n_k} \gamma_i (x_k, e_i)^2 + m \sum_{i=n_k+1}^{\infty} \gamma_i (\rho(v), e_i)^2, \ldots, \sum_{i=1}^{n_m} \gamma_i (x_m, e_i)^2 \right) \\
&\leqslant g(A(x_1, x_1), \ldots, A(\sqrt{m}\rho(v), \sqrt{m}\rho(v)) + A(x_k, x_k), \ldots, A(x_m, x_m))
\end{aligned} \tag{15}$$

for all $k = 1,2,\ldots,m$.

Consider the functional

$$T_N(x_1, x_2, \ldots, x_m) = \sum_{k=1}^{m} \int_R F(S_{n_1}(x_1), \ldots, \sqrt{m}(\rho(v) - S_{n_k}(\rho(v))) + S_{n_k}(x_k), \ldots, S_{n_m}(x_m))\, \mathrm{d}\nu(v).$$

It follows from (14) and (15) that $T_N(\boldsymbol{x})$ is integrable on $\boldsymbol{X}$ with respect to measure μ. Using the mixed integration formula (4) we get

$$\begin{aligned}
\int_X T_N(\boldsymbol{x})\, \mathrm{d}\mu(\boldsymbol{x}) &= (2\pi)^{-N/2} \int_R \exp\left\{ \frac{1}{2} \sum_{i=1}^{m} (\boldsymbol{u}^{(i)}, \boldsymbol{u}^{(i)}) \right\} \\
&\quad \times \int_X T_N(x_1 - S_{n_1}(x_1) + U_{n_1}(\boldsymbol{u}^{(1)}, \ldots, x_m - S_{n_m}(x_m) + U_{n_m}(\boldsymbol{u}^{(m)}))\, \mathrm{d}\mu\, \mathrm{d}\boldsymbol{u}.
\end{aligned} \tag{16}$$

One can transform the functional

$$T_N(x_1 - S_{n_1}(x_1) + U_{n_1}(\boldsymbol{u}^{(1)}), \ldots, x_m - S_{n_m}(x_m) + U_{n_m}(\boldsymbol{u}^{(m)}))$$

as follows:

$$\begin{aligned}
&T_N(x_1 - S_{n_1}(x_1) + U_{n_1}(\boldsymbol{u}^{(1)}), \ldots, x_m - S_{n_m}(x_m) + U_{n_m}(\boldsymbol{u}^{(m)})) \\
&= \sum_{k=1}^{m} \int_R F(U_{n_1}(\boldsymbol{u}^{(1)}), \ldots, \sqrt{m}(\rho(v) - S_{n_k}(\rho(v))) + U_{n_k}(\boldsymbol{u}^{(k)}), \ldots, U_{n_m}(\boldsymbol{u}^{(m)}))\, \mathrm{d}\nu(v).
\end{aligned} \tag{17}$$

Substituting (17) into (16) and taking into account

$$\int_X \mathrm{d}\mu = 1,$$

we obtain

$$\int_X T_N(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) = (2\pi)^{-N/2}\int_R \exp\left\{\frac{1}{2}\sum_{i=1}^{m}(\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)})\right\}$$

$$\times \int_X \left\{\sum_{k=1}^{m}\int_R F(U_{n_1}(\boldsymbol{u}^{(1)}),\ldots,\sqrt{m}(\rho(v)-S_{n_k}(\rho(v)))+U_{n_k}(\boldsymbol{u}^{(k)}),\ldots\right.$$

$$\left. U_{n_m}(\boldsymbol{u}^{(m)}))\,\mathrm{d}v(v)\right\}\mathrm{d}\mu\,\mathrm{d}\boldsymbol{u} = (2\pi)^{-N/2}\int_R \exp\left\{\frac{1}{2}\sum_{i=1}^{m}(\boldsymbol{u}^{(i)},\boldsymbol{u}^{(i)})\right\}$$

$$\times \sum_{k=1}^{m}\int_R F(U_{n_1}(\boldsymbol{u}^{(1)}),\ldots,\sqrt{m}(\rho(v)-S_{n_k}(\rho(v)))+U_{n_k}(\boldsymbol{u}^{(k)}),\ldots$$

$$U_{n_m}(\boldsymbol{u}^{(m)}))\,\mathrm{d}v(v)\,\mathrm{d}\boldsymbol{u}.$$

Hence, the integral (1) can be presented in the form

$$\int_X F(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) = \frac{1}{m}\int_X T_N(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) + R_N(F).$$

For almost all $\boldsymbol{x}\in \boldsymbol{X}$ with respect to the measure μ there holds the convergence

$$S_{n_i}(x_i)\to x_i \quad \text{when } n_i\to\infty, \quad i=1,2,\ldots,m,$$

therefore

$$\sqrt{m}(\rho(v)-S_{n_k}(\rho(v)))+S_{n_k}(x_k)\to x_k \quad \text{when } n_k\to\infty, \quad k=1,2,\ldots,m.$$

Consequently, at these points

$$F\left(S_{n_1}(x_1),\ldots,\underbrace{\sqrt{m}(\rho(v)-S_{n_k}(\rho(v)))+S_{n_k}(x_k)}_{k},\ldots,S_{n_m}(x_m)\right)\to F(\boldsymbol{x})$$

by the simultaneous approach of all n_k to infinity.

It follows from (14) and (15) that the sequence

$$\{T_N(\boldsymbol{x})\}_{n_i=1}^{\infty}, \quad i=1,2,\ldots,m,$$

is bounded by the integrable function. Now we can apply the Lebesque theorem "on the passage to the limit under the integral sign"

$$\int_X T_N(x)\,\mathrm{d}\mu(x) \to m \int_X F(x)\,\mathrm{d}\mu(x),$$

which completes the proof of the theorem. □

The estimate of the remainder $R_N(F)$ in dependence on N is given by the following.

Theorem 5. *If the integrable with respect to measure $\mu(x)$ functional $F(x)$ can be expressed in the form*

$$F(x + x_0) = P_3(x) + r(x, x_0), \tag{18}$$

where $P_3(x)$ is a polynomial functional of the third total degree on X and the remainder $r(x, x_0)$ is estimated by the expression

$$|r(x, x_0)| \leqslant \prod_{i=1}^{m} (A^i(x_i, x_i))^2 (c_1 \exp\{c_2 A^i(x_i + x_i^0, x_i + x_i^0)\} + c_3 \exp\{c_2 A^i(x_i^0, x_i^0)\}), \tag{19}$$

where c_i are positive constant such that

$$\tfrac{1}{2} - c_2 \gamma_k^{(i)} \geqslant 0, \quad k = 1, 2, \ldots, \; i = 1, \ldots, m, \tag{20}$$

$$\sum_{k=1}^{\infty} \gamma_k^{(i)} a_k < \infty; \quad (e_k, \sqrt{m}\,\rho(v))^2 \leqslant a_k; \; a_k, v \in R,$$

then for the remainder of approximation formula (8) *there holds the estimate*

$$R_N(F) = \mathrm{O}\left(\prod_{i=1}^{m} \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} \right)^2 \right) + \sum_{i=1}^{m} \mathrm{O}\left(\left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} a_k \right)^2 \right). \tag{21}$$

Proof. Since the formula (8) is exact for all polynomial functionals of the third summary degree, it follows that its remainder $R_N(F)$ can be expressed as follows:

$$R_N(F) = (2\pi)^{-N/2} \int_R \exp\left\{ \frac{1}{2} \sum_{i=1}^{m} (u^{(i)}, u^{(i)}) \right\} \left\{ \int_X r(x - S_n(x);\, U_n(u))\,\mathrm{d}\mu(x) \right.$$
$$\left. - \frac{1}{m} \sum_{i=1}^{m} \int_R r\Big(0, \ldots, \underbrace{\sqrt{m}(\rho(v) - S_{n_i}(\rho(v)))}_{i}, \ldots, 0;\, U_n(u)\Big)\,\mathrm{d}\nu(v) \right\} \mathrm{d}u \equiv K_1 - K_2. \tag{22}$$

According to (19), we get

$$|K_1| \leqslant (2\pi)^{-N/2} \int_R \exp\left\{\frac{1}{2}\sum_{i=1}^{m} (\boldsymbol{u}^{(i)}, \boldsymbol{u}^{(i)})\right\} \int_X \prod_{i=1}^{m} \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(x_i, e_k)^2\right)^2$$
$$\times\left(c_1 \exp\left\{c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(x_i, e_k)^2 + c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)}(u_k^{(i)})^2\right\}\right.$$
$$\left. + c_3 \exp\left\{c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)}(u_k^{(i)})^2\right\}\right) \mathrm{d}\mu(\boldsymbol{x})\, \mathrm{d}\boldsymbol{u},$$

and after some transformations

$$|K_1| \leqslant \prod_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2\gamma_k^{(i)})^{-1/2} \int_X \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(x_i, e_k)^2\right)^2$$
$$\times\left(c_1 \exp\left\{c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(x_i, e_k)^2\right\} + c_3\right)\mathrm{d}\mu(x_i)$$
$$\equiv \prod_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2\gamma_k^{(i)})^{-1/2} I_1^{(i)}.$$

Analogously for K_2 we have

$$|K_2| \leqslant \sum_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2\gamma_k^{(i)})^{-1/2} \int_R \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(\sqrt{m}\rho(v), e_k)^2\right)^2$$
$$\times\left(c_1 \exp\left\{c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(\sqrt{m}\rho(v), e_k)^2\right\} + c_3\right)\mathrm{d}\nu(v)$$
$$\equiv \sum_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2\gamma_k^{(i)})^{-1/2} I_2^{(i)}.$$

In order to evaluate $I_1^{(i)}$ let us consider the integral

$$I_i(\lambda) = \int_X \exp\left(\lambda c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)}(x_i, e_k)^2\right) \mathrm{d}\mu(x_i), \quad i = 1, 2, \ldots, m.$$

It is well known [2] that its analytic value

$$I_i(\lambda) = \prod_{k=n_i+1}^{\infty} (1 - 2\lambda c_2\gamma_k^{(i)})^{-1/2}. \tag{23}$$

After some more transformations we obtain

$$I_1^{(i)} = c_1 \prod_{k=n_i+1}^{\infty} (1 - 2c_2\gamma_k^{(i)})^{-1/2} \left\{ \left(\sum_{j=n_i+1}^{\infty} \gamma_j^{(i)} (1 - 2c_2\gamma_j^{(i)})^{-1} \right)^2 \right.$$
$$\left. + 2 \sum_{j=n_i+1}^{\infty} (\gamma_j^{(i)})^2 (1 - 2c_2\gamma_j^{(i)})^{-2} \right\} + c_3 \left(\sum_{j=n_i+1}^{\infty} \gamma_j^{(i)} \right)^2 + 2c_3 \sum_{j=n_i+1}^{\infty} (\gamma_j^{(i)})^2,$$

and it follows from the last expression that

$$I_1^{(i)} = \mathrm{O}\left\{ \left(\sum_{j=n_i+1}^{\infty} \gamma_j^{(i)} \right)^2 \right\}, \quad K_1 = \mathrm{O}\left\{ \prod_{i=1}^{m} \left(\sum_{j=n_i+1}^{\infty} \gamma_j^{(i)} \right)^2 \right\}.$$

Using condition (20) we get

$$I_2^{(i)} \leqslant \left(c_1 \exp\left\{ c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} a_k \right\} + c_3 \right) \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} a_k \right)^2,$$

$$I_2^{(i)} = \mathrm{O}\left\{ \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} a_k \right)^2 \right\}, \quad K_2 = \sum_{i=1}^{m} \mathrm{O}\left\{ \left(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} a_k \right)^2 \right\}.$$

Thus the proof of the theorem is complete. □

3. Approximation formulas with weight

In the real physical problems it is often convenient to use the approximation formulas for multiple conditional Wiener integrals

$$I = \int_C P(\boldsymbol{x}) F(\boldsymbol{x}) \, \mathrm{d_W}\boldsymbol{x}, \quad \boldsymbol{x} = (x_1, \ldots, x_m), \ \mathrm{d_W}\boldsymbol{x} = \mathrm{d_W}x_1 \ldots \mathrm{d_W}x_m \tag{24}$$

with the weight

$$P(\boldsymbol{x}) = \exp\left\{ \sum_{i=1}^{m} \int_0^1 (p_i(t) x_i^2(t) + q_i(t) x_i(t)) \, \mathrm{d}t \right\}, \tag{25}$$

$$p_i(t), q_i(t) \in C[0, 1] \quad \text{for all } i = 1, 2, \ldots, m.$$

For such integrals we obtained the following approximation formula:

Theorem 6. *Let $B_i(s)$ be a solution of the differential equation*

$$\begin{gathered} (1 - s) B_i'(s) - (1 - s)^2 B_i^2(s) - 3B_i(s) = 2p_i(s), \quad s \in [0, 1], \\ B_i(1) = -2/3 p_i(1) \end{gathered} \tag{26}$$

and let the following definitions hold:

$$
\begin{aligned}
W_i(t) &= \exp\left\{\int_0^t (1-s)B_i(s)\,\mathrm{d}s\right\},\\
\alpha_i(t) &= \int_0^t L_i(s)\,\mathrm{d}s - \frac{1-t}{W_i(t)}\int_0^t B_i(s)W_i(s)\left[\int_0^s L_i(u)\,\mathrm{d}u\right]\mathrm{d}s,\\
L_i(t) &= \int_0^t (B_i(s)W_i(s)H_i(s) - q_i(s))\,\mathrm{d}s + c_1,\\
H_i(s) &= \int_0^1 q_i(u)\frac{1-u}{W_i(u)}\,\mathrm{d}u, \quad \int_0^1 L_i(u)\,\mathrm{d}u = 0.
\end{aligned}
\tag{27}
$$

Then the approximation formula

$$
\begin{aligned}
I \approx{}& \exp\left\{\frac{1}{2}\sum_{i=1}^m \int_0^1 (1-s)B_i(s)\,\mathrm{d}s\right\}\exp\left\{\frac{1}{2}\sum_{i=1}^m\int_0^1 L_i^2(t)\,\mathrm{d}t\right\}\\
&\times\frac{1}{2m}\sum_{i=1}^m\int_{-1}^1 F(\alpha_1,\ldots,\sqrt{m}\Psi_i(v,\cdot)+\alpha_i(\cdot),\ldots,\alpha_m)\,\mathrm{d}v
\end{aligned}
\tag{28}
$$

is exact for any polynomial functional of the third total degree on $\mathbf{C}$.

Here

$$
\begin{aligned}
\Psi_i(v,\cdot) &= f_i(v,\cdot) - \sigma(v,\cdot),\\
f_i(v,t) &= \operatorname{sign}(v)\frac{1-t}{W_i(t)}\left(1+\int_0^{\min\{|v|,t\}} B_i(s)W_i(s)\,\mathrm{d}s\right),\\
\sigma(v,t) &= \begin{cases}\operatorname{sign}(v), & t \leqslant |v|\\ 0, & t > |v|\end{cases} \quad \textit{for all } i = 1,2,\ldots,m.
\end{aligned}
$$

Proof. Analogously to the one-dimensional case (see [6]) we employ the linear transformation $\boldsymbol{x}(t) \mapsto \boldsymbol{y}(t)$, given by the relation

$$y_i = x_i + A_i x_i, \quad x_i \in C, \ i = 1,2,\ldots,m,$$

where

$$A_i x_i(t) = (1-t)\int_0^t B_i(s)x_i(s)\,\mathrm{d}s, \quad B_i(s) \in C[0,1].$$

The transformation

$$\boldsymbol{A}_i = 1 + A_i$$

maps the space C onto itself in one-to-one correspondence. Using this transformation we obtain

$$\int_C F(\boldsymbol{x})\,\mathrm{d_W}\boldsymbol{x} = \prod_{i=1}^m D_i \int_C F(A_1x_1,\ldots,A_mx_m)\exp\left\{-\sum_{i=1}^m \int_0^1 \left(\frac{1}{2}\left[\frac{\mathrm{d}}{\mathrm{d}t}(A_ix_i)\right]^2 + x_i\frac{\mathrm{d}}{\mathrm{d}t}(A_ix_i)\right)\mathrm{d}t\right\}\mathrm{d_W}\boldsymbol{x} = \prod_{i=1}^m D_i \int_C \Phi(x_1,\ldots,x_m)$$
$$\times\exp\left\{\frac{1}{2}\sum_{i=1}^m \int_0^1 ((1-s)B_i'(s) - (1-s)^2B_i^2(s) - 3B_i(s))x_i^2(s)\,\mathrm{d}s\right\}\mathrm{d_W}\boldsymbol{x},$$

where

$$\Phi(x_1,\ldots,x_m) = F(A_1x_1,\ldots,A_mx_m),$$

D_i is the Fredholm determinant

$$D_i = \exp\left\{\frac{1}{2}\int_0^1 (1-s)B_i(s)\,\mathrm{d}s\right\}.$$

Therefore, if $B_i(t)$ is the solution of the problem (26), we have

$$\int_C \Phi(x_1,\ldots,x_m)\exp\left\{\sum_{i=1}^m \int_0^1 p_i(t)x_i^2(t)\,\mathrm{d}t\right\}\mathrm{d_W}\boldsymbol{x}$$
$$= \prod_{i=1}^m D_i^{-1}\int_C \Phi(A_1^{-1}x_1,\ldots,A_m^{-1}x_m)\,\mathrm{d_W}\boldsymbol{x},$$

where

$$A_i^{-1}x_i(t) = x_i(t) - \frac{1-t}{W_i(t)}\int_0^t B_i(s)W_i(s)x_i(s)\,\mathrm{d}s,$$

$W_i(s)$ corresponds to (27).

Performing one more change of variables

$$y_i(t) = z_i(t) + \int_0^t L_i(s)\,\mathrm{d}s,$$

where the $L_i(s)$ satisfy (27), after some transformation we obtain for integral (24) with weight (25)

$$\int_C P(\boldsymbol{x})F(\boldsymbol{x})\,\mathrm{d_W}\boldsymbol{x} = \exp\left\{-\frac{1}{2}\sum_{i=1}^m \int_0^1 (1-s)B_i(s)\,\mathrm{d}s\right\}$$
$$\times\exp\left\{\frac{1}{2}\sum_{i=1}^m \int_0^1 L_i^2(t)\,\mathrm{d}t\right\}\int_C F(A_1^{-1}x_1+\alpha_1,\ldots,A_m^{-1}x_m+\alpha_m)\,\mathrm{d_W}\boldsymbol{x}, \quad (29)$$

where the α_i correspond to (27).

For the integral over C on the right-hand side of (29) we apply the approximation formula (3) with $L\{F\}$ satisfying (7). The assertion of Theorem 6 follows now from Theorem 1 due to the continuity of A_i^{-1} and α_i and due to the linearity of A_i^{-1}. □

Remark. Eq. (26) is in fact a Riccati equation. Its solution for

$$p_i(t) \equiv p_i = \text{const.} < \pi^2/2$$

is

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

If we set also $q_i(t) \equiv q_i = \text{const.}$, then $\alpha_i(t)$ can be expressed explicitly as

$$\alpha_i(t) = \frac{q_i}{p_i \cos\sqrt{p_i/2}} \sin(\sqrt{p_i/2}t) \sin(\sqrt{p_i/2}(1-t)),$$

and the approximation formula (28) acquires the form

$$I \approx \prod_{i=1}^{m} \left(\frac{\sqrt{2p_i}}{\sin\sqrt{2p_i}}\right)^{1/2} \exp\left\{\frac{q_i^2}{(2p_i)^{3/2}}\left(\mathrm{tg}\sqrt{\frac{p_i}{2}} - \sqrt{\frac{p_i}{2}}\right)\right\}$$
$$\times \frac{1}{2m}\sum_{i=1}^{m}\int_{-1}^{1} F\Bigl(\alpha_1(\cdot), \ldots, \underbrace{\sqrt{m}\Psi_i(v,\cdot) + \alpha_i(\cdot)}_{i}, \ldots, \alpha_m(\cdot)\Bigr)\,dv \tag{30}$$

(for $p < 0$ the trigonometric functions are converted into hyperbolic ones).

4. Numerical calculations

The basis of our computations in Euclidean quantum mechanics is the matrix element

$$Z_{if}(\beta) = \langle x_f | \mathrm{e}^{-\beta H} | x_i \rangle \tag{31}$$

for the Hamiltonian $H = -\frac{1}{2}\Delta + V$. The partition function $Z_{if}(\beta) = Z(x_i, x_f, \beta)$ can be expressed in the form of an integral with respect to conditional Wiener measure $\mathrm{d_W}x$ [3]:

$$Z(x_i, x_f, \beta) = \int \exp\left\{-\int_0^{\beta} V(x(t))\,dt\right\} \mathrm{d_W}x. \tag{32}$$

The integration in (32) is performed over the manifold of continuous functions $x(t) \in C[0, \beta]$ with $x(0) = x_i$, $x(\beta) = x_f$.

Table 1

ω	E_0	E_{mc}	E_{ex}
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

Various characteristics of a quantum system, such as the free energy $f(\beta)$, the ground-state energy E, the wave function $\Psi_0(x)$, are expressed as follows:

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

$$Z(\beta) = \operatorname{Tr}\exp(-H\beta) = \int_{-\infty}^{\infty} Z(x, x, \beta)\,dx,$$

$$Z(x, x, \beta) = (2\pi\beta)^{-1/2}\int_C \exp\left\{-\beta\int_0^1 V(\sqrt{\beta}x(t) + x)\,dt\right\} d_W x,$$

$$E = \lim_{\beta\to\infty} f(\beta),$$

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

Using our approximation formulas we computed [7] the various physical quantities in some quantum models, such as the system with the double-well potential and the quantum pendulum model. In that case we studied the problems of tunnelling. Our numerical results appeared to be in good agreement with the theoretical prediction of dilute instanton gas approximation.

We have also investigated the Calogero model which corresponds to the system of n particles ($n = 3, 5, \ldots, 11$) in one-dimensional space with pairwise interaction via centrifugal potential repulsion forces and linear attraction forces. This model is characterized by the Hamiltonian

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

where ω and g are known coupling constants.

The values of the energy E_0 computed for $g = 1.5$ using formula (30) for various ω at $n = 3$ and various n at $\omega = 0.25$ are given in Tables 1 and 2, respectively. Here E_{mc} are the solutions obtained by the Monte Carlo method and E_{ex} are the exact (theoretical) values [5].

For $n = 11$, the computation of E_0 required 3 min on CDC 6500, whereas the computation of E_{mc} took as long as 15 min on a similar computer. Comparison with the data of other authors shows that the use of our deterministic method gives significant economy of computer time and memory versus other methods while obtaining the results with the same accuracy.

Table 2

ω	E_0	E_{mc}	E_{ex}
5	13.447	13.37 ± 0.04	13.4397
7	32.249	32.34 ± 0.09	32.2718
9	61.473	61.31 ± 0.01	61.5183
11	102.865	102.31 ± 0.14	102.6028

Now let us consider the numerical investigation of the interaction of particles (nucleons) in the nucleus of tritium. This three-body problem is of fundamental interest in physics (see [1]). The Hamiltonian describing the system of three particles interacting pairwise in three-dimensional space is the following:

$$H = \sum_{i=1}^{3} \frac{\hbar^2}{2m_i} \frac{\partial}{\partial \boldsymbol{x}_i^2} + \sum_{i<j} V(|\boldsymbol{r}_{ij}|). \tag{33}$$

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

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

We have studied the following model of triton:

$$V(\boldsymbol{r}) = -51.5 \exp\left\{-\frac{r^2}{b^2}\right\} \text{MeV}, \quad b = 1.6F, \tag{34}$$

$m_1 = m_2 = m_3 = m_p$, where $m_p = 938.279$ MeV is a proton mass. This model is an object of investigation of many authors (see, e.g., [5] and the references therein). The main attention in these works has been paid to the calculation of the binding energy of the nucleons. The following values of the ground-state energy have been obtained there by means of variational E_v and Monte Carlo E_{mc} methods:

$$E_{mc} = -9.77 \pm 0.06 \text{ MeV},$$

$$E_v = -9.42 \text{ MeV},$$

$$E_v = -9.47 \pm 0.4 \text{ MeV},$$

$$-9.99 \pm 0.05 \text{ MeV} < E_v < -97.5 \pm 0.04 \text{ MeV},$$

$$E_v = -9.78 \text{ MeV}.$$

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 methods is of interest for obtaining the more precise result.

We consider the problem (33)–(34) in the framework of the functional integral approach (31)–(32). In order to compute the nine-dimensional functional integral Z we use our numerical techniques mentioned above. The computations have been performed on the CDC 6500 computer with the relative accuracy $\varepsilon = 0.01$. Our result $E = -9.7$ MeV agrees well with the data of other authors. The CPU time per point β was about 15 min, which is less than the times required in the other known works.

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