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COMPUTATION OF GREEN FUNCTION OF THE SCHRÖDINGER-LIKE PARTIAL DIFFERENTIAL EQUATIONS BY THE NUMERICAL FUNCTIONAL INTEGRATION

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1. INTRODUCTION

Numerical functional integration is one of the perspective means of computation in many branches of contemporary science, especially in quantum and statistical physics [1]. One of the important areas of application of functional integrals [2] is the computation of various characteristics of physical systems which consist of many particles interacting with each other. The basis for the computations is the Green function $Z(x,x_0,t)$ which in Euclidean metrics ($t=i\tau$) is the solution of the following problem

$$\frac{\partial Z}{\partial t} = \frac{1}{2}\sum_{i=1}^{n} \frac{\partial^2 Z}{\partial x_i^2} - V(x)\, Z \equiv H\, Z$$

$$Z(x,x_0,0) = \delta\,(x-x_0) \qquad (1)$$

$$Z(x,x_0,t) \to 0 \quad \text{when } |x_k| \to \pm\infty\ ,\ k=1,2,\dots,n$$

where $V(x)$ is a given function. The Green function method is an effective means of solution of multidimensional problems in statistical mechanics, nuclear physics, quantum optics etc. The solution of (1) without any simplifying assumptions (mean field approximation, collective excitations) is a rather complicated computational problem. In the case of high dimensions ($n>3$) the traditional methods (finite element, finite difference) lose their efficiency because of the presence of singularities and of the necessity of solving the algebraic systems of extreme high orders. The approach based on the computation of matrix elements of the time evolution operator $\exp\left\{-TH\right\}$

$$Z(x_i,x_f,t) = \langle x_f|e^{-TH}|x_i\rangle \qquad (2)$$

appears to be perspective [3]. This approach enables one to replace the differential formulation of the problem (1) by the evaluation of the functional integrals. The stochastic methods (Monte Carlo algorithms) are often used in this case. It provides the way of solution of the variety of multidimensional problems, e.g. problems of nuclear physics [4]. This approach is of particular importance when the other methods (perturbative, variational, stationary-phase approximation etc.) cannot be applied [5]. In connection with the recent development of the methods of approximate evaluation of functional integrals with respect to Gaussian measures (see [6]), the approach based on the use of the expression of matrix element (2) in the form of the integral with conditional Wiener measure $d_W x$

$$\langle x_f|e^{-TH}|x_i\rangle = \int \exp\left\{ -\int_0^T V\big(x(t)\big)dt \right\} d_W x \qquad (3)$$

appears to be of particular interest. The integration in (3) is performed over all functions $x(t) \in C\,[0,T]$, satisfying $x(0)=x_i$, $x(T)=x_f$. One of the advantages of this approach is the possibility of solution of the problem (1) in unbounded region, without replacement of the boundary conditions at the infinity by the conditions at some large x_k^{max}.

In the framework of the deterministic approach which we are successively developing [7] we derived for the functional integrals with Gaussian measures μ

$$\int_X F[x]\ d\mu(x) \qquad (4)$$

some new approximation formulas exact on a class of polynomial functionals [8]. Here X is a full separable metric space, F is a real functional. In particular case of conditional Wiener measure the family of approximation formulas with the weight is derived [9]. The use of the formulas in the problems of quantum mechanics show [10] that these formulas provide the higher efficiency of computations versus other methods of evaluation of functional integrals.

The employment of our formulas gives the significant (by an order) economy of computer time and memory compared to the lattice Monte Carlo method in the problems wich we have considered (with the equal accuracy of results). Moreover, while solving the problem (1) by finite difference methods one needs to discretise both space and time variables, the integral formulation via lattice Monte Carlo method assumes the discretization of time only and the continuum approach based on the use of our formulas does not need any discretization at all. The discretization is performed here only at the final step of computation of the ordinary (Rimanian) integrals which arise in the formulas.

In order to solve the problem (1) by the functional integration method in the case n>1 one has to evaluate the multiple functional integrals [11]. In the present paper we derive and study the approximation formulas for such integrals. We prove the theorem on convergence of approximations to the exact value of integral and estimate the speed of this convergence for some class of functionals. We illustrate the employment of our formulas by examples of computation in statistical mechanics.

2. CONSTRUCTION OF APPROXIMATION FORMULAS.

Let $X^m = X\cdot\ldots\cdot X$ be a Cartesian product of the full separable metric spaces X. The m-dimensional integral with Gaussian measure is defined as an integral built on X^m with respect to Cartesian product of the Gaussian measures μ on X.

$$\int_X \overset{(m)}{\cdots} \int_X F(x_1,\ldots,x_m)\,d\mu(x_1)\ldots d\mu(x_m) \equiv \int_{X^m} F(x)\,d\mu^{(m)}(x) \qquad (5)$$

One of the means of computation of integral (5) is the successive employment of some approximation formulas for the "one-dimensional" functional integrals (e.g. formulas exact on a class of polynomial functionals of degree $\le 2n_k+1$ for the variable $x_k \in X, k=1,2,\ldots,m$, which we constructed in paper

[8]). The more interesting is to construct the approximation formulas with the given summary degree of accuracy 2k+1, i.e. formulas which are exact for the constant functional and for the functionals

$$F(x_1,\ldots,x_m) = \prod_{i=1}^{m} F_{k_i}(x_i)$$

where $k_1+k_2+\ldots+k_m \le 2k+1$, $F_{k_i}(x_i)$ is a homogeneous polynomial of degree k_i with respect to argument x_i. The example of such a formula is given by the following

Theorem 1.[6] let L be a linear homogeneous functional defined on a manifold of the functionals integrable with respect to the measure μ. Let L satisfy the following conditions

1. $L(F) = 0$ for any odd functional $F(x)$.
2. $L\left\{\langle\xi,\cdot\rangle\langle\eta,\cdot\rangle\right\} = K(\xi,\eta)$ for arbitrary $\xi,\eta\in X'$

$K(\xi,\eta)$ is a correlation functional of the measure μ.

3. Either $L\left\{\prod_{i=1}^{2}\langle\xi_i,\cdot\rangle\right\} \not\equiv 0$ and $L(1)\neq 0$, (6)

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

Let b_i $(i=1,2,\ldots,m)$ be arbitrary positive numbers.

Then the approximation formula

$$\int_{X^m} F(x)\,d\mu^{(m)}(x) \approx \left(1-\sum_{i=1}^{m} b_i L(1)\right) F(0,0,\ldots,0) + \sum_{i=1}^{m} b_i L_{x_i}\left\{ F(0,0,\ldots,x_i/\sqrt{b_i},0,\ldots,0) \right\} \qquad (7)$$

is exact for all polynomial functionals of the third summary degree on X^m.

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 (7) give a good approximation to the exact value of integral when F[x] is close to the polynomial functional of the third summary degree on X^m. 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 derived in [8,9] for the 1-dimensional functional integrals. The advantages of the composite approximation formulas over the "elementary" ones have been determined in [9]. Analogously to the case of 1-dimensional functional integrals the construction of the composite approximation formulas for integral (5) is based on the use of the relation called "mixed integration formula" [6]. Applying this formula to integral (5) with respect to each component x_i we obtain the mixed integration formula for the multiple functional integrals

$$\int_{X^m} F(\mathbf{x})\,d\mu^{(m)}(\mathbf{x}) = \int_{R^N} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\right\}\times$$

$$\times\int_{X^m} F(x_1-S_{n_1}(x_1)+U_{n_1}(u^{(1)}),\dots,x_m-S_{n_m}(x_m)+U_{n_m}(u^{(m)}))\times \qquad (8)$$

$$\times\, d\mu(x_1)\cdots d\mu(x_m)\,du^{(1)}\cdots du^{(m)}.$$

Here

$$S_{n_i}(x_i) = \sum_{j=1}^{n_i}(e_j,x_i)_{\tilde H}e_j \qquad U_{n_i}(u^{(i)}) = \sum_{j=1}^{n_i}u_j^{(i)}e_j \qquad (9)$$

$$N = \sum_{i=1}^{m} n_i\ ,\quad u^{(i)}\in R^{n_i}\ ,\quad (u^{(i)},u^{(i)}) = \sum_{j=1}^{n_i}\left(u_j^{(i)}\right)^2$$

n_i are arbitrary positive numbers.

$\left\{e_k\right\}_{k=1}^{\infty}$ is an orthonormal basis in the Hilbert space $\tilde H$ which is generated by the measure μ and is dense almost everywhere in X [6]. This basis is formed by eigenfunctions of correlation functional $K(\xi,\eta)$.

Substituting the integral over X^m in the right-hand side of (8) by the approximation formula (7), we obtain the

composite approximation formula of the third summary degree of accuracy for integral (5). Thus, the following theorem appears to be proved

Theorem 2. Under conditions (6) and (9) the approximation formula

$$\int_{X^m} F(\mathbf{x})\,d\mu^{(m)}(\mathbf{x}) = (2\pi)^{-N/2}\int_{R^N} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\right\}\times$$

$$\times\left[\left(1-\sum_{i=1}^{m} b_i L(1)\right) F(\Sigma_1(x_1\equiv 0,u^{(1)}),\dots,\Sigma_m(x_m\equiv 0,u^{(m)})) + \right.$$

$$+\sum_{i=1}^{m} b_i L_{x_i}\Big\{F(\Sigma_1(x_1\equiv 0,u^{(1)}),\dots, \qquad (10)$$

$$\left.\Sigma_i(x_i/\sqrt{b_i},u^{(i)}),\dots,\Sigma_m(x_m\equiv 0,u^{(m)}))\Big\}\right]\,du + R_N(F)$$

is exact for all polynomial functionals of the third summary degree on X^m.

Here

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

$$du = du^{(1)}\cdots du^{(m)}$$

$R_N(F)$ is a remainder of the formula (10).

Corollary. In particular case of conditional Wiener measure $d_W x$ in the space $X = \left\{ C\ [0,1];\ x(0)=x(1)=0 \right\} \equiv C$ the composite approximation formula of the third summary degree of accuracy for the multiple conditional Wiener integrals is written as follows

$$\int_{C^m} F(\mathbf{x})\, d_W\mathbf{x} = (2\pi)^{-N/2}\int_{R^N} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\right\}\times$$

$$\times\frac{1}{2m}\sum_{i=1}^{m}\int_{-1}^{1} F(\tilde U_{n_1}(u^{(1)}),\dots,\tilde\Sigma_i(\sqrt{m}\ \rho(v,\cdot),u^{(i)}),\dots, \quad (11)$$

$$\tilde{U}_{n_m}(u^{(m)})\ )\ du\, dv + R_N^{(m)}(F)$$

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

$$\tilde{\Sigma}_1(\rho(v,t),u^{(1)}) = \rho(v,t) - S_{n_1}(\rho(v,t)) + \tilde{U}_{n_1}(u^{(1)})$$

$$S_{n_1}(\rho(v,t),u^{(1)}) = 2\sum_{j=1}^{n_1}\frac{1}{j\pi}\sin(j\pi t)\operatorname{sign}(v)\cos(j\pi v)$$

$$\tilde{U}_{n_1}(u^{(1)}) = \sqrt{2}\sum_{j=1}^{n_1}u_j^{(1)}\frac{1}{j\pi}\sin(j\pi t).$$

Proof. Since in the space C [0,1] the following relation holds

$$<\xi,x> = \int_0^1 x(t)\, d\xi(t)$$

we can write

$$K(\xi,\eta) = \int_0^1\int_0^1 \mathfrak{K}(t,s)\, d\xi(t)\, d\eta(s)$$

where

$$\mathfrak{K}(t,s) = \int_C x(t)\, x(s)\, d_W x.$$

In the case of conditional Wiener measure we have [6]

$$\mathfrak{K}(t,s) = \min(t,s) - ts\ ;\ e_k = \sqrt{\lambda_k}\ \Phi_k(t)$$

where λ_k and $\Phi_k(t)$ are the eigenvalues and the eigenfunctions of the kernel $\mathfrak{K}(t,s)$

$$\lambda_k = 1/k^2\pi^2\ ;\ \Phi_k(t) = \sqrt{2}\sin(k\pi t).$$

Taking the functional L(F) in the form

$$L(F) = \int_R F[\ \rho(v)\ ]d\nu(v),$$

ν is the symmetric probabilistic measure on R, satisfying

$$d\nu(v) = \tfrac{1}{2}\, dv,\ v \in [-1,1]$$

and substituting the last relations into (10) with

$$b_k = 1/m\ ,\ k=1,2,\dots,m,$$

we obtain formula (11).

In many cases the use of approximation formulas with weight is preferable. For the multiple conditional Wiener integrals

$$I = \int_{C^m} P(\mathbf{x})\ F(\mathbf{x})\ d_W\mathbf{x} \tag{12}$$

$$\mathbf{x} = (x_1,\dots,x_m)\ ,\ d_W\mathbf{x} = d_W x_1\, d_W x_2 \cdots d_W x_m$$

with the weight

$$P(\mathbf{x}) = \exp\left\{\sum_{i=1}^m\int_0^1\Big(\ p_i(t)x_i^2(t) + q_i(t)x_i(t)\ \Big)\, dt\right\} \tag{13}$$

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

we obtained the following approximation formula

Theorem 3. Let $B_i(s)$ be the solution of differential equation

$$(1-s)\ B_i'(s) - (1-s)^2\ B_i^2(s) - 3\ B_i(s) = 2\ p_i(s),\ s \in [0,1]$$

$$B_i(1) = -2/3\ p_i(1) \tag{14}$$

and let the following definitions hold

$$W_i(t) = \exp\left\{\int_0^t (1-s)\ B_i(s)\, ds\right\}$$

$$\alpha_i(t) = \int_0^t L_i(s)\, ds - \frac{1-t}{W_i(t)}\int_0^t B_i(s)\ W_i(s)\ \times$$

$$\times\left[\int_0^s L_i(u)\, du\right] ds \tag{15}$$

$$L_i(t) = \int_0^t\Big[\ B_i(s)\ W_i(s)\ H_i(s) - q_i(s)\ \Big]\, ds + c_i$$

$$H_i(s) = \int_s^1 q_i(u) \frac{1-u}{W_i(u)} du \quad , \quad \int_0^1 L_i(u)\, du = 0 .$$

Then the approximation formula

$$I \approx \exp\left\{ -\frac{1}{2} \sum_{i=1}^{m} \int_0^1 (1-s)\ B_i(s)\ ds \right\} \exp\left\{ \frac{1}{2} \sum_{i=1}^{m} \int_0^1 L_i^2(t) dt \right\} \times \tag{16}$$

$$\times \frac{1}{2m} \sum_{i=1}^{m} \int_{-1}^{1} F(\alpha_1, \dots, \sqrt{m}\ \Psi_i(v,\cdot) + \alpha_i(\cdot), \dots, \alpha_m)\ dv$$

is exact for any polynomial functional of the third summary degree on C^m.

Here

$$\Psi_i(v,\cdot) = f_i(v,\cdot) - \sigma_i(v,\cdot),$$

$$f_i(v,t) = \text{sign } v \frac{1-t}{W_i(t)} \left(1 + \int_0^{\min(v,t)} B_i(s)\ W_i(s)\ ds \right)$$

$$\sigma_i(v,t) = \begin{cases} \text{sign } v, & t \le |v| \\ 0 \quad , & t > |v| . \end{cases}$$

Proof. We employ the linear transformation $x(t) \longrightarrow y(t)$, given by the relation $y_i = x_i + A_i x_i$, $x_i \in C$, $i=1,2,\dots,m$ where

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

The transformation

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

maps the space C onto itself in one-to-one correspondence [12]. Using this transformation analogous to the result which we derived in [13] for the case of integration in one dimension, we obtain now

$$\int_{C^m} F(\mathbf{x}) d_W \mathbf{x} = \prod_{i=1}^{m} D_i \int_{C^m} F\left[\hat{A}_1 x_1, \dots, \hat{A}_m x_m \right] \times$$

$$\exp\left\{ -\sum_{i=1}^{m} \int_0^1 \left(\frac{1}{2} \left[\frac{d}{dt} (A_i x_i) \right]^2 + \dot{x}_i \frac{d}{dt} (A_i x_i) \right) dt \right\} d_W \mathbf{x} =$$

$$= \prod_{i=1}^{m} D_i \int_{C^m} \Phi\ [x_1, \dots, x_m]$$

$$\exp\left\{ \frac{1}{2} \sum_{i=1}^{m} \int_0^1 \left[(1-s) B_i'(s) - (1-s)^2 B_i^2(s) - 3B_i(s) \right] x_i^2(s) ds \right\} d_W \mathbf{x},$$

where

$$\Phi\ [x_1, \dots, x_m] = F\left[\hat{A}_1 x_1, \dots, \hat{A}_m x_m \right],$$

D_i is the Fredholm determinant

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

Therefore, if $B_i(t)$ is the solution of the problem (14), we have

$$\int_{C^m} \Phi\ [x_1, \dots, x_m] \exp\left\{ \sum_{i=1}^{m} \int_0^1 p_i(t)\ x_i^2(t)\ dt \right\} d_W \mathbf{x} =$$

$$= \prod_{i=1}^{m} D_i^{-1} \int_{C^m} \Phi \left[\hat{A}_1^{-1} x_1, \dots, \hat{A}_m^{-1} x_m \right] d_W \mathbf{x}$$

where

$$\hat{A}_i^{-1} x_i(t) = x_i(t) - \frac{1-t}{W_i(t)} \int_0^t B_i(s)\ W_i(s)\ x_i(s)\ ds,$$

$W_i(s)$ corresponds to (15).

Performing one more change of variables

$$y_i(t) = z_i(t) + \int_0^t L_i(s)\ ds,$$

where $L_i(s)$ satisfy (15) after some transformations we obtain for integral (12) with the weight (13)

$$\int_{C^m} P(x)\ F(x)\ d_W x =$$

$$= \exp\left\{-\frac{1}{2}\sum_{i=1}^{m}\int_0^1 (1-s)\ B_i(s)\ ds\right\}\exp\left\{\frac{1}{2}\sum_{i=1}^{m}\int_0^1 L_i^2(t)dt\right\}\times \tag{17}$$

$$\int_{C^m} F\left[\hat{A}_1^{-1}x_1+\alpha_1,\dots,\hat{A}_m^{-1}x_m+\alpha_m\right] d_W x$$

where α_i correspond to (15).

For the integral over C^m in the right-hand side of (17) we apply the approximation formula (7). The assertion of Theorem 3 follows now from Theorem 1 due to continuity of $\hat{A}_i^{-1}$ and α_i and to the linearity of $\hat{A}_i^{-1}$.

Remark. Equation (14) is in fact a Riccati equation. Its solution for

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

is

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

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

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

$$i=1,2,\dots,m$$

and the approximation formula (16) acquires the form

$$I \approx \prod_{i=1}^{m}\left[\left(\frac{\sqrt{2p_i}}{\sin\sqrt{2p_i}}\right)^{1/2}\exp\left\{\frac{q_i^2}{(2p_i)^{3/2}}\left[\text{tg}\sqrt{p_i/2} - \sqrt{p_i/2}\right]\right\}\right]\times \tag{18}$$

$$\times\frac{1}{2m}\sum_{i=1}^{m}\int_{-1}^{1}F(\alpha_1(\cdot),\dots,\sqrt{m}\ \Psi_i(v,\cdot)+\alpha_i(\cdot),\dots,\alpha_m(\cdot))dv.$$

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

3. CONVERGENCE OF THE APPROXIMATIONS

Theorem 4. Let for almost all $v\in R$, with respect to measure $\nu(v)$ the following convergence hold

$$S_{n_i}(\rho(v)) \longrightarrow \rho(v)\ \text{when}\ n_i\longrightarrow\infty,\quad i=1,2,\dots,m. \tag{19}$$

Let $F(x)$ be a continuous on X^m functional, satisfying the condition

$$|F(x)| \le g(A^1(x_1,x_1),\dots,A^m(x_m,x_m)) \tag{20}$$

where $A^k(x_k,x_k)$ - is a non-negative quadratic functional

$$A^k(x_k,x_k) = \sum_{i=1}^{\infty}\gamma_i^k\ (x_k,e_i)_{\tilde{H}}^2 \tag{21}$$

$$\sum_{i=1}^{\infty}\gamma_i^k < \infty,\quad \gamma_i \ge 0,\quad i=1,2,\dots \tag{22}$$

$g(x)$ is a non-decreasing function, and

$$\int\int_{X^m R} g\ (A^1(x_1,x_1),\dots,A^k(\rho(v),\rho(v))+A^k(x_k,x_k),\dots, \tag{23}$$

$$A^m(x_m,x_m))\ d\nu(v)\ d\mu^{(m)}(x) < \infty.$$

Then the remainder of the approximate formula (10)

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

Proof. Without any restrictions of generality we suppose that

$$\gamma_i^k \equiv \gamma_i$$

and

$$A^k(x_k,x_k) \equiv A(x_k,x_k),\quad k=1,2,\dots,m.$$

Using (20)-(22) we obtain

$$|F(S_{n_1}(x_1),\dots,\sqrt{m}\,(\rho(v)-S_{n_k}(\rho(v)))+S_{n_k}(x_k),\dots,S_{n_m}(x_m))| =$$

$$|\ F\Big(\sum_{i=1}^{n_1}(x_1,e_i)_{\tilde{H}}\ e_i,\dots,\sqrt{m}\,\Big(\sum_{i=1}^{n_k}(x_k,e_i)_{\tilde{H}}\ e_i+\sum_{i=n_k+1}^{\infty}(\rho(v),e_i)_{\tilde{H}}e_i\Big),$$

$$\ldots, \sum_{i=1}^{n_m}(x_m,e_i)_{\tilde H}\, e_i) \mid \le \tag{24}$$

$$g\Big(\sum_{i=1}^{n_1}\gamma_i(x_1,e_i)_{\tilde H}^2,\ldots, \sum_{i=1}^{n_k}\gamma_i(x_k,e_i)_{\tilde H}^2+\sum_{i=n_k+1}^{\infty}\gamma_i(\rho(v),e_i)_{\tilde H}^2,\ldots,$$

$$\sum_{i=1}^{n_m}\gamma_i(x_m,e_i)_{\tilde H}^2 \Big) \le$$

$$g(\, A(x_1,x_1),\ldots,A(\rho(v),\rho(v))+A(x_k,x_k),\ldots,A(x_m,x_m)\,),$$

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

Consider the functional

$$T_N(x_1,\ldots,x_m) =$$

$$\sum_{k=1}^{m}\int_R F(S_{n_1}(x_1),\ldots,\sqrt{m}(\rho(v)-S_{n_k}(\rho(v)))+S_{n_k}(x_k),\ldots,$$

$$S_{n_m}(x_m))\, d\nu(v).$$

$T_N(\mathbf{x})$ is integrable on X^m with respect to measure μ. Using the mixed integration formula (8) we get

$$\int_{X^m} T_N(\mathbf{x})\, d\mu^{(m)}(x) = (2\pi)^{-N/2}\int_{R^N}\exp\Big\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\Big\}\times \tag{25}$$

$$\times\int_{X^m} T_N(x_1-s_{n_1}(x_1)+U_{n_1}(u^{(1)}),\ldots,x_m-S_{n_m}(x_m)+U_{n_m}(u^{(m)}))\,d\mu^{(m)}x\,du.$$

One can transform the functional

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

as follows

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

$$= \sum_{k=1}^{m}\int_R F(\, S_{n_1}(x_1+S_{n_1}(x_1)+U_{n_1}(u^{(1)})),\ldots,$$

$$\sqrt{m}(\rho(v)-S_{n_k}(\rho(v)))+S_{n_k}(x_k+S_{n_k}(x_k)+U_{n_k}(u^{(k)})),\ldots,$$

$$S_{n_m}(x_m+S_{n_m}(x_m)+U_{n_m}(u^{(m)}))\,)\, d\nu(v) = \tag{26}$$

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

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

Substituting (26) into (25) and taking into account

$$\int_{X^m} d\mu^{(m)}(x) = 1$$

we obtain

$$\int_{X^m} T_N(\mathbf{x})\, d\mu^{(m)}(\mathbf{x}) = (2\pi)^{-N/2}\int_{R^N}\exp\Big\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\Big\}\times$$

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

$$\ldots, U_{n_m}(u^{(m)})\,)\, d\nu(v)\Big\}\, d\mu^{(m)}x\, du =$$

$$= (2\pi)^{-N/2}\int_{R^N}\exp\Big\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\Big\}\times$$

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

$$U_{n_m}(u^{(m)})\,)\, d\nu(v)\, du.$$

Hence, the integral

$$\int_{X^m} F(x)\,d\mu^{(m)}(x)$$

can be represented in the form

$$\int_{X^m} F(x)\,d\mu^{(m)}(x) = \frac{1}{m}\int_{X^m} T_N(x)\ d\mu^{(m)}(x) + R_N(F).$$

For almost all $x\in X^m$ with respect to the measure μ there holds the convergence

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

Therefore

$$\sqrt{m}\,(\rho(v)-S_{n_k}(\rho(v))) + S_{n_k}(x_k) \longrightarrow x_k$$

$$\text{when } n_k \longrightarrow \infty, \quad k=1,2,\ldots,m.$$

Consequently, at these points

$$F\big(S_{n_1}(x_1),\ldots,\sqrt{m}\,(\rho(v)-S_{n_k}(\rho(v))) + S_{n_k}(x_k),\ldots,$$

$$S_{n_m}(x_m)\big) \longrightarrow F(x)$$

by the simultaneous approach of all n_k to the infinity.
It follows from (23) and (24) that the sequence

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

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

$$\int_{X^m} T_N(x)\ d\mu^{(m)}(x) \longrightarrow m\int_{X^m} F(x)\,d\mu^{(m)}(x) \text{ as } n_i\to\infty,\ i=1,2,\ldots,m$$

which completes the proof of the theorem.
The estimate of the remainder $R_N(F)$ in dependence on N is established by the following
Theorem 5. If the integrable with respect to measure $\mu^{(m)}(x)$ functional $F(x)$ can be expressed in the form

$$F(x+x_0) = P_3(x) + r(x;x_0) \tag{27}$$

where $P_3(x)$ is a polynomial functional of the third summary degree on X^m and the remainder $r(x;x_0)$ is estimated by the expression

$$|r(x;x_0)| \le \prod_{i=1}^{m}(A^i(x_i,x_i))^2\left[c_1\exp\left\{ c_2A^i(x_i+x_i^0,x_i+x_i^0)\right\} + \right.$$

$$\left. + c_3\exp\left\{ c_2A^i(x_i^0,x_i^0)\right\}\right], \tag{28}$$

$$c_i > 0,\quad (i=1,2,3)$$

$$\frac{1}{2} - c_2\gamma_k^{(i)} \ge 0,\quad k=1,2,\ldots,\quad i=1,2,\ldots,m$$

$$\sum_{k=1}^{\infty}\gamma_k^{(i)}a_k < \infty;\quad (e_k,\ \sqrt{m}\,\rho(v))^2 \le a_k;\ a_k,v\in R \tag{29}$$

then for the remainder of approximation formula (10) there holds the estimate

$$R_N(F) = O\Big(\prod_{i=1}^{m}\big(\sum_{k=1}^{\infty}\gamma_k^{(i)}\big)^2\Big) + \sum_{i=1}^{m}O\Big(\big(\sum_{k=n_i+1}^{\infty}\gamma_k^{(i)}a_k\big)^2\Big). \tag{30}$$

Proof. Since the formula (10) is exact for all polynomial functionals of the third summary degree, it follows that it's remainder can be expressed as follows

$$R_N(F) = (2\pi)^{-N/2}\int_{R^N}\exp\Big\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\Big\}\times$$

$$\times\Bigg[\int_{X^m} r(x-S_n(x);U_n(u))\,d\mu^{(m)}(x) -$$

$$\frac{1}{m}\sum_{i=1}^{m}\int_R r(0,\ldots 0,\sqrt{m}\,\rho(v)-S_{n_i}(\rho(v)),0,\ldots,0;U_n(u))\,d\nu(v)\Bigg]\,du=$$

$$= K_1 - K_2.$$

According to (28), we get

$$|K_1| \le (2\pi)^{-N/2}\int_{R^N}\exp\Big\{-\frac{1}{2}\sum_{i=1}^{m}(u^{(i)},u^{(i)})\Big\}\times$$

$$\times \int_{X^m} \prod_{i=1}^{m} \Big(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2\Big)^2 \times$$

$$\times \Bigg[c_1 \exp\Big\{ c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2 + c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)} (u_k^{(i)})^2 \Big\} +$$

$$+ c_3 \exp\Big\{ c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)} (u_k^{(i)})^2 \Big\} \Bigg] d\mu^{(m)}(\mathbf{x})\ du =$$

$$= \prod_{i=1}^{m} (2\pi)^{-n_i/2} \int_{R^{n_i}} \exp\Big\{ -\frac{1}{2} (u^{(i)}, u^{(i)}) \Big\} \times$$

$$\int_X \Big(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2\Big)^2 \times$$

$$\times \Bigg[c_1 \exp\Big\{ c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2 + c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)} (u_k^{(i)})^2 \Big\} +$$

$$+ c_3 \exp\Big\{ c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)} (u_k^{(i)})^2 \Big\} \Bigg] d\mu(x_i)\ du^{(i)} =$$

$$\prod_{i=1}^{m} (2\pi)^{-n_i/2} \int_X d\mu(x_i) \int_{R^{n_i}} \exp\Big\{ -\frac{1}{2} (u^{(i)}, u^{(i)}) \Big\} \times$$

$$\exp\Big\{ c_2 \sum_{k=1}^{n_i} \gamma_k^{(i)} (u_k^{(i)})^2 \Big\} \Big(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2\Big)^2 \times$$

$$\times \Bigg[c_1 \exp\Big\{ c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2 \Big\} + c_3 \Bigg] du^{(i)} =$$

$$= \prod_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2 \gamma_k^{(i)})^{-1/2} \int_X \Big(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2\Big)^2 \times$$

$$\times \Bigg[c_1 \exp\Big\{ c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2 \Big\} + c_3 \Bigg] d\mu(x_i) \equiv$$

$$\equiv \prod_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2 \gamma_k^{(i)})^{-1/2}\ I_i^{(1)}.$$

Analogously for K_2 we have

$$|K_2| \le \sum_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2 \gamma_k^{(i)})^{-1/2} \int_R \Big(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (\sqrt{m}\ \rho(v), e_k)^2\Big)^2$$

$$\times \Bigg[c_1 \exp\Big\{ c_2 \sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (\sqrt{m}\ \rho(v), e_k)^2 \Big\} + c_3 \Bigg] d\nu(v) \equiv$$

$$\equiv \sum_{i=1}^{m} \prod_{k=1}^{n_i} (1 - 2c_2 \gamma_k^{(i)})^{-1/2}\ I_2^{(i)}.$$

Consider the integral

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

It is well known [6], that it's analytic value

$$I_i(\lambda) = \prod_{k=n_{i+1}}^{\infty} (1 - 2\lambda c_2 \gamma_k^{(i)})^{-1/2}. \tag{31}$$

After some more transformations we obtain

$$I_i''(\lambda) = \int_X \Big(\sum_{k=n_i+1}^{\infty} \gamma_k^{(i)} (x_i, e_k)^2\Big)^2 \times$$

$$\times \exp\left\{\lambda c_2 \sum_{k=n_1+1}^{\infty} \gamma_k^{(1)} (x_1, e_k)^2\right\} d\mu(x_1) =$$

$$= \prod_{k=n_{1+1}}^{\infty} (1-2\lambda c_2 \gamma_k^{(1)})^{-1/2} \left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)} (1-2\lambda c_2 \gamma_j^{(1)})^{-1}\right]^2 +$$

$$+ 2 \prod_{k=n_{1+1}}^{\infty} (1-2\lambda c_2 \gamma_k^{(1)})^{-1/2} \sum_{j=n_1+1}^{\infty} (\gamma_j^{(1)})^2 (1-2\lambda c_2 \gamma_j^{(1)})^{-2}.$$

Since

$$I_1''(1) = \prod_{k=n_{1+1}}^{\infty} (1-2c_2 \gamma_k^{(1)})^{-1/2} \left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)} (1-2c_2 \gamma_j^{(1)})^{-1}\right]^2 +$$

$$+ 2 \prod_{k=n_{1+1}}^{\infty} (1-2c_2 \gamma_k^{(1)})^{-1/2} \sum_{j=n_1+1}^{\infty} (\gamma_j^{(1)})^2 (1-2c_2 \gamma_j^{(1)})^{-2}$$

and

$$I_1''(0) = \left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)}\right]^2 + 2 \sum_{j=n_1+1}^{\infty} (\gamma_j^{(1)})^2$$

then

$$I_1^{(1)} = c_1 \prod_{k=n_{1+1}}^{\infty} (1-2c_2 \gamma_k^{(1)})^{-1/2} \left\{\left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)} (1-2c_2 \gamma_j^{(1)})^{-1}\right]^2 +\right.$$

$$\left. 2 \sum_{j=n_1+1}^{\infty} (\gamma_j^{(1)})^2 (1-2c_2 \gamma_j^{(1)})^{-2}\right\} +$$

$$+ c_3 \left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)}\right]^2 + 2c_3 \sum_{j=n_1+1}^{\infty} (\gamma_j^{(1)})^2$$

and there follows

$$I_1^{(1)} = O\left\{\left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)}\right]^2\right\}, \quad K_1 = O\left\{\prod_{l=1}^{m} \left[\sum_{j=n_1+1}^{\infty} \gamma_j^{(1)}\right]^2\right\}.$$

Using the condition (29) we get

$$I_2^{(1)} \le \left[c_1 \exp\left\{c_2 \sum_{k=n_1+1}^{\infty} \gamma_k^{(1)} a_k\right\} + c_3\right] \left[\sum_{k=n_1+1}^{\infty} \gamma_k^{(1)} a_k\right]^2$$

$$I_2^{(1)} = O\left\{\left[\sum_{k=n_1+1}^{\infty} \gamma_k^{(1)} a_k\right]^2\right\}, \quad K_2 = \sum_{l=1}^{m} O\left\{\left[\sum_{k=n_1+1}^{\infty} \gamma_k^{(1)} a_k\right]^2\right\}.$$

Thus the proof of the theorem is complete.

4. NUMERICAL CALCULATIONS.

We will illustrate the use of the formulas with examples of m-dimensional quantum models, characterized by the Hamiltonian

$$H = \frac{1}{2} \sum_{l=1}^{m} \frac{\partial^2}{\partial x_l^2} + V(x). \tag{32}$$

We shall study the energy E_0 of the ground state and wave function $\Psi_0(x)$. The basis for the computation is the Green function (2). The expressions for the principal quantities of Euclidean quantum mechanics in the form of functional integrals with conditional Wiener measure are [10]

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

$$Z(T) = \mathrm{Tr}\exp\left\{-TH\right\} = \int_{-\infty}^{\infty} Z(X,X,T)\, dX$$

$$Z(X,X,T) = (2\pi)^{-1/2} \int_C \exp\left\{-T \int_0^1 V(\sqrt{T}\, x(t) + X)\, dt\right\} d_W x \tag{33}$$

$$E_0 = \lim_{T\to\infty} f(T) \quad (34)$$

$$G(\tau) = \langle x(0)x(\tau)\rangle =$$

$$= \frac{1}{Z(T)} (2\pi T)^{-1/2} \int_{-\infty}^{\infty}\int_C \exp\left\{-T\int_0^1 V(\sqrt{T}\, x(t) + X)dt\right\} \times$$

$$\times [\sqrt{T}\, x(\tau/t) + X]\, d_W x\; X\; dx$$

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

$$|\Psi_0(x)|^2 = \lim_{T\to\infty} \left[\exp\left\{ E_0 T \right\} Z(X,X,T) \right]. \quad (35)$$

Consider the harmonic oscillator with

$$V(x) = \frac{1}{2}\sum_{i=1}^{n} x_i^2 . \quad (36)$$

The theoretical values are

$$E_m^* = (m+1/2)n \quad (37)$$

$$|\Psi_0^*(x)|^2 = (1/\pi)^{n/2} \exp\left\{ -\sum_{i=1}^{n} x_i^2 \right\}. \quad (38)$$

Using the formula with weight, one can evaluate the integral Z as follows

$$Z(y_1,\dots,y_n,T) = \prod_{i=1}^{n} 1/(2\pi\, \mathrm{sh}T)^{1/2} \exp\left\{-\mathrm{th}(T/2)y_i^2\right\}. \quad (39)$$

Consequently, the analytic values for finite T are

$$E_0^{(T)} = \frac{n}{2}\,\mathrm{cth}(T/2) \xrightarrow[T\to\infty]{} E_0^*$$

$$|\Psi_0^{(T)}(y)|^2 = \exp\left\{ E_0^{(T)} T\right\} Z(y,T) \xrightarrow[T\to\infty]{} |\Psi_0^*(y)|^2 .$$

The values of $E_0^{(T)}$ and E_0 for various T and N obtained on the CDC·6500 computer, using the composite formula (10) whith various n_1 and n_2 are given in Tables 1 and 3 for n = 2 and 3. The convergence of the numerical results of energy E_0 to $E_0^{(T)}$ (T=3) is represented in Tables 2 and 4.

Table 1

T	E_0	$E_0^{(T)}$	n_1/n_2
4	1.007	1.037	1
5	1.004	1.013	2
6	1.002	1.004	3

$$E_0^* = 1$$

Table 2

n_1/n_2	1	2	3	4
E_0	1.024	1.009	1.005	1.004

Table 3

T	E_0	$E_0^{(T)}$	n_1/n_2
4	1.507	1.555	1
5	1.503	1.520	2
6	1.500	1.500	3

$$E_0^* = 1.5$$

Table 4

n_1/n_2	1	2	3	4
E_0	1.515	1.511	1.509	1.507

The CPU time of computation of E_0 has been ca 20 sec. It follows from Tables 1 and 3 that the good approximations E_0 of the theoretical value are achieved at relatively small values of T and N.

Table 5

x_2	$\|\Psi_0(x)\|^2$	$\|\Psi_0^{(T)}(x)\|^2$
-2.8	.618E-04	.584E-04
-2.4	.805E-03	.777E-03
-1.6	.198E-01	.195E-01
-0.5	.173E+00	.173E+00
0.5	.173E+00	.173E+00
1.6	.198E-01	.195E-01
2.4	.805E-03	.777E-03
2.8	.618E-04	.584E-04

The numerical results of calculation $|\Psi_0(\mathbf{x})|^2$ and $|\Psi_0^{(T)}(\mathbf{x})|^2$ obtained using the composite formula (10) with T=6, $n_1=n_2=1$, n=2, are given in Table 5 in the form of dependence on the parameter x_2 with $x_1=0.5$.

We compute all integrals using the Gaussian quadrature with the relative accuracy 0.1 % . The CPU time of computation of $|\Psi_0(\mathbf{x})|^2$ has been ca 2 sec on the CDC·6500 computer.

Consider the Calogero model which is characterized by the Hamiltonian

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

This model corresponds to the system of n particles in one dimension, which interact pairwise via inverse cube repulsion ("centrifugal potential") and linear attraction ("harmonic oscillator potential"). This problem serves as an object of investigations for many authors (see [14]-[16]). The analytic solution for it has been found in [16]. We computed the energy E_0 of ground state, using our approximation formula with weight. The results of computation for g=1.5 in the case n=3 are listed in Table 6.

Table 6

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±.004	3.3680
0.50	6.738	——	6.7361

The values of E_0, obtained for ω = 0.25 and different n are presented in Table 7.

Table 7

n	E_0	E_{mc}	E_{ex}
5	13.447	13.37±.04	13.4397
7	32.249	32.34±.09	32.2718
9	61.473	61.31±.10	61.5183
11	102.865	102.31±.14	102.6028

For comparison, we cite the results obtained in [16] using Monte Carlo method (1000 points of discretization, 100 iterations). These results are denoted by E_{mc}. The exact values are denoted by E_{ex}. The CPU time of computation of E_0 for n = 11 is 3 min on the CDC·6500 computer, whereas the computation of E_{mc} takes 15 min on the analogous computer.

The presented results show that our formulas provide the higher efficiency of computations.

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