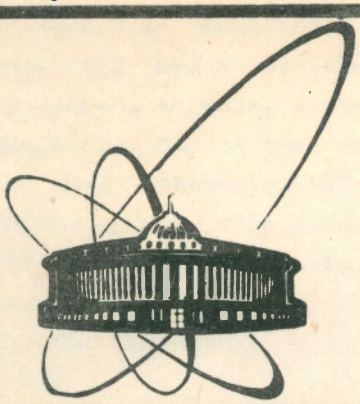

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MODELLING OF MULTIDIMENSIONAL QUANTUM SYSTEMS BY THE NUMERICAL FUNCTIONAL INTEGRATION

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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 $G(x,x_0,t)$ which in Euclidean metrics ($t=i\tau$) is the solution of the following problem

$$\frac{\partial G}{\partial t} = \frac{1}{2}\sum_{k=1}^{n}\frac{\partial^2 G}{\partial x_k^2} - V(x)\,G = -H\,G; \qquad x \in \mathbb{R}^n, \quad t>0;$$

$$G(x,x_0,0) = \delta(x-x_0); \qquad x=(x_1,\ldots,x_k,\ldots,x_n), \qquad (1)$$

$$G(x,x_0,t)\Big|_{|x_k|\to\infty} = 0, \qquad k=1,2,\ldots,n,$$

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 elements, 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 comoutation of matrix elements of the time evolution operator e^{-TH}

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

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 the matrix element (2) in the form of the integral with conditional Wiener measure $d_w x$

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

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}, $k=1,2,\ldots,n$.

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

$$\int_{\mathfrak{X}} F[x]\, d\mu(x) \qquad (4)$$

some new approximation formulas exact on a class of polynomial functionals [8]. Here $\mathfrak{X}$ is a full separable metric space, F is a real functional. The theorems on the convergence of approximations to the exact value of integral are proved, the estimate of the remainder is obtained. 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 with the equal accuracy of results compared to the lattice Monte Carlo method in the problems which we have considered. Moreover, while solving the problem (1) by finite difference methods one has 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 space-time 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.

For the multiple functional integrals with respect to the Gaussian measures

$$\int_{\mathfrak{X}}\cdots\int_{\mathfrak{X}} F[x_1,\ldots,x_n]d\mu(x_1)\ldots d\mu(x_n) \equiv \int_{\mathfrak{X}^n} F[x]d\mu^{(n)}(x) \qquad (5)$$

we derived [11] the new approximation formulas of the given summary degree of accuracy. In particular case of normalized conditional Wiener measure $d_w x$, $\mathfrak{X}=\{C[0,1], x(0)=x(1)=0\}\equiv C$ we obtained the family of approximation formulas with the weight.

Theorem.

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

$$(1-s)B_i'(s)-(1-s)^2 B_i^2(s)-3B_i(s)-2p_i(s)=0, \quad i=1,\ldots,n$$
$$B_i(1)=-\frac{2}{3}p_i(1) \qquad s \in [0,1], \quad p_i \in C[0,1], \qquad (6)$$

and let the following definitions hold

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

$$K_i(s)=\int_s^1 q_i(u)\frac{1-u}{W_i(u)}du, \qquad q_i \in C[0,1],$$

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

$$a_i(t)=\int_0^t L_i(s)ds- \frac{1-t}{W_i(t)}\int_0^t B_i(s)W_i(s)\int_0^s L_i(u)du\,ds,$$

where the constants c_i are determined by the condition

$$\int_0^1 L_i(s)ds = 0.$$

Then the approximation formula

$$\int_{C^n} P[x_1,\dots,x_n]\,F[x_1,\dots,x_n]\,d_w x_1\dots d_w x_n \simeq$$

$$\simeq \exp\left\{-\frac{1}{2}\sum_{i=1}^n\int_0^1 (1-s)B_i(s)ds\right\}\exp\left\{\frac{1}{2}\sum_{i=1}^n\int_0^1 L_i^2(t)dt\right\}\cdot \tag{7}$$

$$\cdot\,(2n)^{-1}\sum_{i=1}^n\int_{-1}^1 F[a_1(\cdot),\dots,a_{i-1}(\cdot),\sqrt{n}\Psi_i(v,\cdot)+a_i(\cdot),$$

$$a_{i+1}(\cdot),\dots,a_n(\cdot)]\,dv,$$

where $$P[x_1,\dots,x_n]=\exp\left\{\sum_{i=1}^n\int_0^1 [p_i(t)x_i^2(t)+q_i(t)x_i(t)]dt\right\}$$

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

Here $\Psi_i(v,\cdot) = f_i(v,\cdot) - \omega(v,\cdot)$,

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

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

The proof of the theorem is based on the employment of the special linear transformation which maps the space C onto itself in one-to-one correspondence. We have found and studied this transformation in [12].

Equation (6) is in fact a Riccati equation. Its solution for $p_i(t)\equiv p_i=\text{const.}$ is

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

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

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

and the approximation formula (7) for $p_i < \frac{1}{2}\pi^2$ acquires the form

$$\int_{C^n} P[x_1,\dots,x_n]\,F[x_1,\dots,x_n]\,d_w x_1\dots d_w x_n \simeq$$

$$\simeq \prod_{i=1}^n\left(\frac{\sqrt{2p_i}}{\sin\sqrt{2p_i}}\right)^{1/2}\exp\left\{\frac{q_i^2}{2p_i\sqrt{2p_i}}\left[\tan\sqrt{\tfrac{1}{2}p_i}-\sqrt{\tfrac{1}{2}p_i}\,\right]\right\}\cdot \tag{8}$$

$$\cdot\,(2n)^{-1}\sum_{i=1}^n\int_{-1}^1 F[a_1(\cdot),\dots,a_{i-1}(\cdot),\sqrt{n}\Psi(v,\cdot)+a_i(\cdot),$$

$$a_{i+1}(\cdot),\dots,a_n(\cdot)]\,dv$$

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

Consider the Calogero model which is characterised by the Hamiltonian

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

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 model serves as an object of investigations for many authors (see [13]-[15]). The convenience of the model is determined by the fact that the explicit analytic solution for it has been found (see [15]). We computed the Green function $G(x_i, x_f, T)$ for the various numbers of particles n. The Green function is the basis for computation of the physical characteristics, such as the bound states energies, the propagator, the wave function, etc. [10]. Particularly, the ground state energy E_o is defined as follows

$$E_o = \lim_{T\to\infty} \left[-\frac{1}{T} \ln \int_{-\infty}^{\infty} G(x,x,T)\, dx \right].$$

The values of E_o which we computed using our approximation formula with weight (8) for g=1.5 in the case n=3 with different values of ω, are listed in Table 1.

Table 1.

ω	E_o	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

The CPU time of computation of E_o is 11 sec per point ω on

the CDC-6500 comouter. The values obtained for ω=0.25 and different n are presented in Table 2.

Table 2.

n	E_o	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±0.10	61.5183
11	102.865	102.31±0.14	102.6028

For comparison, we cite the results obtained in [15] using Monte Carlo method (1000 points of discretisation, 100 iterations). These results are denoted by E_{mc}. The exact results are denoted by E_{ex}. The CPU time of computation of E_o for n=11 is 3 min on the CDC-6500 computer, whereas the computation of E_{mc} takes 15 min on the analogous comouter [15]. The presented results show that our formulas provide the higher efficiency of computations.

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Лобанов Ю.Ю., Шахбагян Р.Р., Жидков Е.П. E11-90-393

Моделирование многомерных квантовых систем методом приближенного континуального интегрирования

Рассматривается применение метода приближенного континуального интегрирования для описания многомерных систем в квантовой и статистической физике. Для кратных континуальных интегралов по гауссовым мерам в полных сепарабельных метрических пространствах получены новые приближенные формулы, точные на классе функциональных многочленов заданной суммарной степени. Использование формул демонстрируется на примере расчета функции Грина и энергии основного состояния в многомерной модели Калоджеро. Сравнение численных результатов с данными, полученными другими авторами методом Монте-Карло с применением итерационных алгоритмов свидетельствует о том, что построенные нами формулы обеспечивают высокую эффективность вычислений.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Modelling of Multidimensional Quantum Systems by the Numerical Functional Integration

The employment of the numerical functional integration for the description of multidimensional systems in quantum and statistical physics is considered. For the multiple functional integrals with respect to Gaussian measures in the full separable metric spaces the new approximation formulas exact on a class of polynomial functionals of a given summary degree are constructed. The use of the formulas is demonstrated on example of computation of the Green function and the ground state energy in multidimensional Calogero model. The comparison of numerical results with the data obtained by the other authors which used the Monte Carlo method combined with iterative algorithms indicates that our formulas provide the higher efficiency of computations.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

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