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NUMERICAL EVALUATION OF WIENER INTEGRALS IN THE PROBLEMS OF QUANTUM PHYSICS [1]

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Abstract. In the framework of Feynman's formulation of quantum mechanics on a basis of path integration, the method of numerical study of quantum systems in Euclidean metric is elaborated. This method is based on representation of quantum characteristics in the form of functional integrals with respect to Wiener measure and on the use of our approximation formulas for computation of this kind of integrals. The approximation formulas satisfy the condition of being exact on a given class of functionals, particularly for polynomial functionals of a given degree. This approach enables one to reduce calculation of functional integrals to evaluation of Riemann integrals of low dimension that allows using more preferable deterministic numerical methods instead of traditional stochastic (Monte Carlo) ones for solution of these problems. Examples of application of the method to solution of some quantum-mechanical problems are presented.

Key words: functional integral, Wiener measure, density matrix, propagator, approximation formula, binding energy, computations

1. Introduction

Numerical functional integration is an effective method of solution of the wide scope of problems in various areas of physics and mathematics [2]. Used for the first time in quantum mechanics by Feynman, functional integration is now a basis of a modern constructive quantum field theory, the main method of numerical study of nonperturbative phenomena in the quantum gauge theory. Functional integrals are widely used in quantum mechanics, field theory, statistical physics, nuclear physics, solid state physics, quantum statistics, theory of a super-conductivity, quantum optics, statistical radio engineering, radiation physics of particles of high energies and in many other areas [6].

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The wide application of functional integrals stimulated the development of their theory and methods of approximate calculation. As the "Feynman measure" does not meet the condition of countable additivity, i.e. it is not a measure in a mathematically rigorous sense, many approaches to Feynman integrals appeared, justifying their constructions and offering appropriate ways of their approximate calculation. Study of the functional integrals with countable-additive measures was launched by Wiener. He introduced the measure of functional integration in the space of continuous functions, which is now carrying his name. For a long time the most investigated were Wiener integrals, connected with the Feynman ones by transition to imaginary time. However, recently major attention is given to their generalization and to study of the functional integrals with other measures in appropriate spaces.

For the functional integrals with respect to measures of the Gaussian type in complete separable metric spaces we developed a method of approximate calculation that does not require preliminary discretization of space and time [8]. Our method allows one to use the deterministic (as against probabilistic – Monte Carlo methods) algorithms of calculation in quantum physics.We proved the convergence of approximations to the exact value of functional integral and obtained estimate of the remainder [5].

2. Functional Integrals in Quantum Mechanics

In the Euclidean statement of quantum mechanics matrix element of the evolution operator $\exp\{-\beta H\}$

$$Z(\mathrm{x}_i, \mathrm{x}_f, \beta) = < \mathrm{x}_f \mid \mathrm{e}^{-\beta H} \mid \mathrm{x}_i >,$$

where H is a Hamiltonian of the system $H = \frac{1}{2}\hat{p}^2 + V$, according to the Feynman – Kac formula is written in the form of the Wiener integral

$$Z(\mathrm{x}_i, \mathrm{x}_f, \beta) = \int\limits_C \exp\Big\{-\int\limits_0^\beta V\big(x(t)\big)\,dt\Big\}\,d_W x, \tag{2.1}$$

where the integration is performed over all functions $x(t) \in C[0,\beta]$ satisfying the conditions $x(0) = \mathrm{x}_i$, $x(\beta) = \mathrm{x}_f$. The Green function Z with periodic boundary conditions $\mathrm{x}_i = \mathrm{x}_f = \mathrm{x}$ is a basis for finding various physical characteristics of the quantum system.

We have found in [8] that after appropriate change of variables the functional integral $Z(\mathrm{x},\mathrm{x},\beta)$ can be written in the form of integral with normalized conditional Wiener measure in the space $C_0 \equiv \big\{x(t):\ x(t) \in C[0,1],\ x(0) = x(1) = 0\big\}$:

$$Z(\mathrm{x},\mathrm{x},\beta) = \frac{1}{\sqrt{2\pi\beta}} \int\limits_{C_0} \exp\Big\{-\beta \int\limits_0^1 V\big(\sqrt{\beta}x(t) + \mathrm{x}\big)\,dt\Big\}\,dW(x). \tag{2.2}$$

Expressions for Helmholtz free energy $f(\beta)$, energy of a ground state E_0, propagator $G(\tau)$, wave function $\psi_0(x)$, the energy gap between the ground and first excited states $\triangle E$ can be found in the form of functional integrals with conditional Wiener measure [4]. This approach gives an opportunity of studying quantum mechanics by statistical methods and reveals the correlation between quantum and statistical physics, where the value

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

is treated as the statistical sum if one takes into account that $\beta = \dfrac{1}{kT}$, where k is the Boltzmann factor, T is a Kelvin temperature. We have shown in [4] that this approach provides an effective method of numerical study of multiparticle quantum systems.

3. Approximate Calculation of Wiener Integrals

In many cases it appears to be convenient to select a part of an integrand as a weight functional and to use the approximation formulas with weight. We constructed such a formula for functional integrals with respect to conditional Wiener measure with the weight functional

$$P[x] = \exp\Big\{\int\limits_0^1 \big[p(t)\,x^2(t) + q(t)\,x(t)\big]\,dt\Big\}, \quad p(t), q(t) \in C[0,1] \tag{3.1}$$

Theorem 1. *Let $B(s)$ satisfy the initial differential problem*

$$\begin{cases} (1-s)\,B'(s) - (1-s)^2\,B^2(s) - 3\,B(s) - 2\,p(s) = 0, \quad s \in [0,1], \\ B(1) = -\dfrac{2}{3}\,p(1). \end{cases} \tag{3.2}$$

Let

$$Q(t) = \exp\Big\{\int\limits_0^1 (1-s)\,B(s)\,ds\Big\}, \tag{3.3}$$

$$a(t) = \int\limits_0^t L(s)\,ds - \frac{1-t}{Q(t)} \int\limits_0^t B(s)\,Q(s)\Big[\int\limits_0^s L(u)\ du\Big]\,ds,$$

$$L(t) = \int\limits_0^t \Big[B(s)\,Q(s)\,H(s) - q(s)\Big]\,ds + C, \quad H(t) = \int\limits_t^1 q(s)\,\frac{1-s}{Q(s)}\,ds,$$

where the constant C is determined from a condition $\int\limits_0^1 L(s)\,ds = 0$.

Then the approximation formula

$$\int\limits_{C_0} P[x]F[x]\,dW(x) = \big[Q(1)\big]^{-1/2} \exp\Big\{\frac{1}{2}\int\limits_0^1 L^2(t)\,dt\Big\}$$

$$\times\, 2^{-m} \underbrace{\int\limits_{-1}^{1} \dots \int\limits_{-1}^{1}}_{m} F\big[\Psi_m(v,\cdot) + a(\cdot)\big]\; dv_1 \cdots dv_m + \mathcal{R}_m(F), \qquad (3.4)$$

where

$$\Psi_m(v,\cdot) = \sum_{k=1}^{m} c_{m,k}\,\Psi(v_k,\cdot),$$

$$\Psi(r,\cdot) = f(r,\cdot) - \sigma(r,\cdot), \quad \sigma(r,t) = \begin{cases} \operatorname{sign}(r), & t \le |r| \\ 0, & t > |r| \end{cases}$$

$$f(r,t) = \operatorname{sign}(r)\,\frac{1-t}{Q(t)}\Big[1 + \int\limits_0^{\min\{|r|,t\}} B(s)\,Q(s)\;ds\Big],$$

is exact for any polynomial functional of degree $\le 2m+1$.

The proof of the theorem is based on properties of the linear transformation $x(t) \mapsto y(t)$, which we have found and studied just for this purpose. This transformation is given by a relation $y = x + A\,x$, where

$$A\,x(t) = (1-t)\int\limits_0^t B(s)\,x(s)\;ds, \qquad B(s) \in C[0,1].$$

It maps the space C_0 onto itself in one-to-one correspondence. The inverse transformation is the following:

$$x(t) = \hat{A}\,y(t) = y(t) - \frac{1-t}{Q(t)}\int\limits_0^1 B(s)\,Q(s)\,x(s)\;ds,$$

where $Q(t)$ satisfies (3.3).

The approximation (3.4) assumes computation of the low-dimensional Riemann integrals ($\le$ 10-fold ones for accuracy 0.1%). This is especially important in the case of systems with many degrees of freedom [5].

4. Numerical Calculations in Nuclear Physics

Functional integrals provide a convenient way of studying the wide scope of nuclear systems, which are making difficulty for numerical investigation by other methods (perturbation theory, variational method, method of stationary phase etc.). However, the most popular Monte Carlo method for calculation of functional integrals requires excessively large computer memory and high calculation time. In this sense the deterministic method of calculation of functional integrals, which we are developing, seems to be perspective, since it does not require lattice discretization [3]. We studied the nuclear model offered in [7], in which the interaction potential between particles in a nucleus is the following:

$$V(\mathrm{x}) = \sum_{k=1}^{2} \frac{V_k}{\sigma_k \sqrt{\pi}} \exp\Big\{-\frac{\mathrm{x}^2}{\sigma_k^2}\Big\}, \tag{4.1}$$

$$V_1 = 12, \quad V_2 = -12, \quad \sigma_1 = 0.2, \quad \sigma_2 = 0.8, \quad \hbar = m = 1,$$

in terms of lengths $l_0 = 1.89$ Fm and energy $E_0 = \hbar^2/(m\, l_o^2) = 11.6$ MeV.

For the system consisting of two nucleones (nucleus of deuterium, or deuteron) the outcome of our calculation of a binding energy is $E_d = 2.4$ MeV, which it is possible to compare with experimental data $E_{ex} = 2.2$ MeV and with predictions of the semi-empirical mass formula $E_{se} = 3.5$ MeV. Our results obtained in the framework of such a simple model can be considered as satisfactory.

For the system consisting of four nucleons (α - particle) the outcome of our calculation of a binding energy is $E_F = 27.6$ MeV, that corresponds to experimental value $E_{ex} = 28.3$ MeV . The prediction of semi-empirical formula constitutes $E_{se} = 18.8$ MeV. We can compare our result to the value obtained in [7] within the framework of the same model by the Monte Carlo method on a lattice. As the values in [7] are represented in a graphics form, we reproduce them on Fig. 1. Binding energy of nucleons in dimensionless form E/E_0, obtained in [7] by simulation of 10^4 events, is shown as the function of a lattice spacing ε. E_T and E_N designate trial and normalized energy accordingly, and E_M are values obtained with the help of Metropolis algorithm [7]. The problem of extrapolation of outcomes on a continuum limit ($\varepsilon \to 0$) was discussed in [7] and was considered as rather complicated. At the same time in our approach these problems do not arise, since we do not use lattice discretization. Our outcome E_F/E_0 is exhibited in Fig. 1 at a point $\varepsilon = 0$.

One of the perspective directions of application of functional integrals is investigation of open quantum systems (OQS), i.e. systems interacting with their environment. It allows one to study nonequilibrium irreversible processes with dissipation of energy. For the description of OQS the density operator $\hat{\rho}(t)$ is used. In case of Markov systems this operator satisfies the known Lindblad master equation. Within the formulation of quantum mechanics on a basis of functional integrals Feynman and Vernon have offered the model, in which the propagator is expressed through a double Feynman integral. By transition to the Euclidean metrics with the help of Wick's rotation on a complex plane we

obtained expression of a propagator in the form of double functional integral with conditional Wiener measure. We considered application of our method for calculation of the physical characteristics in the framework of the dinuclear system model (DNS) [1] that has been recently elaborated in JINR, Dubna. This model allows one to correctly evaluate the probability of creation of a compound nucleus at the deeply inelastic collisions of heavy ions, which is important for preparation of experiments on synthesis of superheavy elements. The evolution of the DNS can be considered as a process of tunneling with dissipation in the open quantum system. In Fig. 2 the outcomes of our calculations of a density matrix $\rho(\mathrm{x}, t)$ for various moments of time are exhibited.

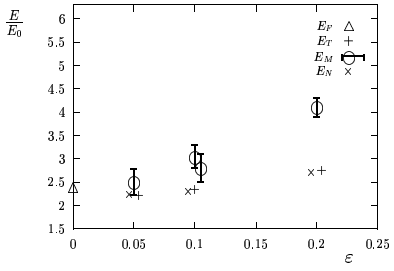

Figure 1. Binding energy of 4 nucleons.

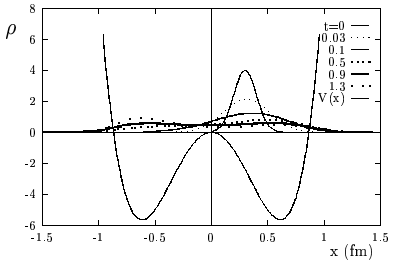

Figure 2. Density matrix of the DNS.

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