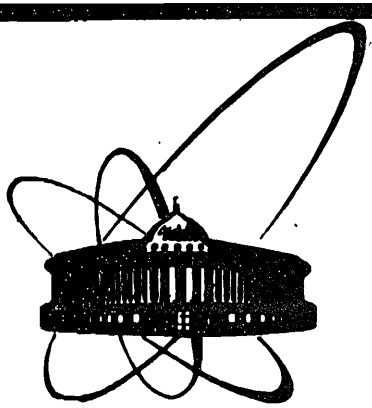

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EVALUATION OF QUANTUM MECHANICS PATH INTEGRALS BY THE APPROXIMATIONS EXACT ON A CLASS OF POLYNOMIAL FUNCTIONALS

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INTRODUCTION

Functional integration first applied in quantum mechanics by R.Feynman[1] is now one of the most powerful mathematical techniques in the contemporary quantum physics[2]. The method of functional integration lies at the foundation of quantum lattice gauge theory[3]. The introduction of space-time lattice turns functional integrals into ordinary ones of high multiplicity. This approach causes the serious problems: how do lattice calculations concern the continuum limit; how does the result depend on the lattice spacing, etc. Besides that, the basic method of lattice computations is Monte-Carlo one that guarantees the convergence of approximations only in probabilistic sence and needs too much computer time and memory. Thus the development of effective numerical methods different from lattice Monte-Carlo ones for the evaluation of functional integrals is of great importance. In the latter sence the approach based on the mathematically rigorous study of functional integrals with Gaussian measure[2] appears to be promising. The important results in this area have been obtained in works[4-7]. In the framework of the mentioned approach we derived[8,9] for the functional integrals with Gaussian measure in separable Fréchet spaces some new approximate formulae exact on a class of polynomial functionals of a given degree.

Feynman path integrals in Euclidean quantum mechanics can be represented in the form of functional integral with conditional Wiener measure[10] that is the special case of Gaussian ones. The search of continuum quantum mechanics models is of interest because it provides the better understanding of some problems in quantum field theory, e.g. ones concerned the topological structure of vacuum[11]. The values of topological susceptibility computed in various works by lattice Monte-Carlo simulations differ each from other and from the phenomenological estimate by 1-2 orders[12]. The reason of such a discrepancy can consist e.g. (see ref.[12]) in the difference of lattice topological charge definitions and also in the presence of specific finite-size effects. Some authors are engaged now in more consistent study of these problems on the models of quantum mechanics[13-16].

In the present paper we consider the computation of functional integrals using the derived approximate formulae in the case of condi-

tional Wiener measure in Euclidean quantum mechanics. The non-perturbative characteristics concerned the topological effects in double - well potential and in quantum pendulum model are investigated. The computations allowed us to search the validity bounds of the dilute instanton gas approximation in these models. The use of the derived formulae instead of Monte-Carlo method for the evaluation of path integrals yields the mathematically well-grounded results with greater accuracy and the significant economy of computer time and memory.

1. APPROXIMATE FORMULAE FOR FUNCTIONAL INTEGRALS

We consider the functional integral

$$\int_X F[x]\, d\mu(x)\,, \qquad (1)$$

where $F[x]$ is a real functional defined on a separable Fréchet space X /6/, $\mu(x)$ is a Gaussian measure on X. Some experience in the development of methods for numerical evaluation of integral (1) has already been accumulated/7/. One of the approaches that is being most intensively developed now is the creation of approximate formulae exact on a given class of functionals. The example of such a formula in a special case of normalized conditional Wiener measure $d_{w*}x$ $(X=C\equiv\{C[0,1], x(0)=x(1)=0\})$ can be presented by the following relation/6/

$$\int_C F[x]\, d_{w*}x \approx \frac{1}{2^m}\int_{-1}^{1}\dots\int_{-1}^{1} F[\theta_m(v,\cdot)]\, dv_1 \dots dv_m \qquad (2)$$

exact on a class of polynomial functionals of degree $\le 2m+1$. Here

$$\theta_m(v,\cdot)=\sum_{j=1}^{m} c_j^{(m)}\,\theta(v_j,\cdot)\,; \qquad \theta(w,t)=\begin{cases}-t\,\operatorname{sign} w, & t\le|w|\\ (1-t)\operatorname{sign} w, & t>|w|\end{cases};$$

$[c_j^{(m)}]^2$ are the roots of polynomial $Q_m(t)=\sum_{k=0}^{m}(-1)^k t^{m-k}/k!$. Formulas of the type (2) give the good approximation of the exact result when $F[x]$ is "closed" to the polynomial functional of degree $\le 2m+1$, i.e. to the functional

$$P_{2m+1}[x]=\sum_{k=0}^{2m+1} p_k[x]$$

where $p_k[x]$ is a continuous on X homogeneous form of order k.

We have obtained/8,9/ for integral (1) the "composite approximate formulae" of arbitrary degree of accuracy. These formulae can be used for the wide set of functionals. In the case of conditional Wiener measure the derived formula/9/ is written as follows:

$$\int_C F[x]\, d_{w*}x = (2\pi)^{-\frac{n}{2}}\int_{R^n}\exp\Big\{-\frac{1}{2}\sum_{k=1}^{n}u_k^2\Big\}\frac{1}{2^m}\int_{-1}^{1}\dots\int_{-1}^{1} F[\theta_m(v,\cdot)-\theta_m^n(v,\cdot)+\varphi_n(u,\cdot)]\,dv\,du+\mathcal{R}_m^n(F), \qquad (3)$$

where

$$\theta_m^n(v,t)=2\sum_{k=1}^{n}\sum_{i=1}^{m}\frac{1}{k\pi}\sin k\pi t\cdot c_i^{(m)}\operatorname{sign} v_i\cos k\pi v_i$$

$$\varphi_n(u,t)=\sqrt{2}\sum_{k=1}^{n}\frac{1}{k\pi}\sin k\pi t\cdot u_k\,.$$

Approximate formula (3) is exact for every polynomial functional of degree $\le 2m+1$. In the works/8,9/ we investigated the convergence to zero of the remainder $\mathcal{R}_m^n(F)$ and its estimate in dependence on m and n. Particularly we have found that under certain conditions on F the order of convergence $\mathcal{R}_m^n \xrightarrow[n\to\infty]{} 0$ is equal to $O(n^{-(m+1)})$. Note that the convergence of lattice approximations has the order $1/\sqrt{n}$ that indicates the advantage of the considered formulas over the lattice Monte-Carlo method.

In the work/17/ we derived and investigated some approximate formulas for conditional Wiener integrals with the weight. This result extends the class of functionals where the formulas are exact. In particular, we have proved the following

Theorem 1.

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

$$(1-s)K'(s)-(1-s)^2K^2(s)-3K(s)-2\lambda p(s)=0\,, \quad s\in[0,1]$$

$$K(1)=-\frac{2}{3}\lambda p(1)\,;$$

$\lambda\in R$; $p(t), g(t)\in C[0,1]$;

$$V(t)=\exp\Big\{\int_0^t(1-s)K(s)\,ds\Big\};$$

$$\alpha(t)=\int_0^t L(s)\,ds-\frac{1-t}{V(t)}\int_0^t K(s)V(s)\Big[\int_0^s L(u)\,du\Big]ds;$$

$$L(t)=\int_0^t[K(s)V(s)H(s)-g(s)]\,ds+C\,; \qquad H(t)=\int_t^1 g(s)\frac{1-s}{V(s)}\,ds$$

and the constant C is determined by the condition $\int_0^1 L(s)\,ds=0$.

Then the approximate formula

$$\int_C \exp\Big\{\int_0^1[\lambda p(t)x^2(t)+g(t)x(t)]\,dt\Big\}F[x]\,d_{w*}x =$$

$$=[V(1)]^{-\frac{1}{2}}\exp\Big\{\frac{1}{2}\int_0^1 L^2(t)\,dt\Big\}\frac{1}{2^m}\int_{-1}^{1}\dots\int_{-1}^{1}F[\tilde\theta_m(v,\cdot)+\alpha(\cdot)]\,dv_1\dots dv_m+\mathcal{R}_m(F), \qquad (4)$$

where

$$\tilde\theta_m(v,\cdot)=\sum_{k=1}^{m}c_k^{(m)}\,\tilde\theta(v_k,\cdot)\,;$$

$$\tilde{\theta}(w,\cdot) = f(w,\cdot) - \rho(w,\cdot); \qquad \rho(w,t) = \begin{cases} sign\, w, & t \le |w| \\ 0, & t > |w| \end{cases}$$

$$f(w,t) = sign\, w \cdot \frac{1-t}{V(t)} \cdot \left[1 + \int_0^{\min\{|w|,t\}} K(s)\, V(s)\, ds\right],$$

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

The proof of Theorem 1 is based on the employment of special linear transformation $x(t) \mapsto y(t)$ that we have found and investigated in /18/. This transformation maps the space $C = \{C[0,1], x(0) = x(1) = 0\}$ onto itself in one-to-one correspondence.

Particularly, if $\rho(t) \equiv 1$; $g(t) \equiv g = const$; $\lambda < \pi^2/2$ the formula (4) acquires the form

$$\int_C \exp\left\{\int_0^1 [\lambda x^2(t) + g x(t)]\, dt\right\} F[x]\, d_{W^*}x =$$

$$= \sqrt{\frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}} \cdot \exp\left\{\frac{g^2}{(2\lambda)^{3/2}}\left[tg\sqrt{\frac{\lambda}{2}} - \sqrt{\frac{\lambda}{2}}\right]\right\} \frac{1}{2^m} \int_{-1}^{1}\cdots\int_{-1}^{1} F[\tilde{\theta}_m(v,\cdot) + a(\cdot)]\, dv_1 \cdots dv_m + \mathcal{R}_m^{(F)}. \quad (5)$$

In this case

$$a(t) = \frac{g}{\lambda \cos\sqrt{\frac{\lambda}{2}}} \cdot \sin\sqrt{\frac{\lambda}{2}}t \cdot \sin\sqrt{\frac{\lambda}{2}}(1-t);$$

$$K(t) = \frac{1}{1-t}\left[\sqrt{2\lambda}\, ctg\sqrt{2\lambda}(1-t) - \frac{1}{1-t}\right].$$

The estimate of the remainder $\mathcal{R}_m(F)$ in (5) is given by the following

Theorem 2 /9/.

Suppose the functional $F[x]$ can be expressed in the form

$$F[x] = P_{2m+1}[x] + r_{2m+1}[x],$$

where $P_{2m+1}[x]$ is a polynomial functional of degree $\le 2m+1$;

$$|r_{2m+1}[x]| \le c_1(m) \cdot \exp\left\{c_2(m) \int_0^1 x^2(t)\, dt\right\};$$

$$c_1(m),\ c_2(m) \ge 0; \qquad 0 \le \lambda + c_2(m) < \frac{\pi^2}{2}.$$

Then

$$|\mathcal{R}_m(F)| \le c_1(m) \cdot \left\{\tilde{c}_2(m) \cdot M(g,\lambda) \cdot \left[\frac{8}{3}\exp\left(\frac{2}{3}\alpha \cdot c_2(m)\right)\right]^m + M(g, \lambda + c_2(m))\right\},$$

where

$$\tilde{c}_2(m) = \exp\left\{2c_2(m)\int_0^1 a^2(t)\, dt\right\} = \exp\left\{\frac{c_2(m) g^2}{\lambda^2 \cos^2\frac{\sqrt{\lambda}}{2}}\left(2 + \cos\sqrt{2\lambda} - 5\,\frac{\sin\sqrt{2\lambda}}{\sqrt{2\lambda}}\right)\right\},$$

$$M(g,\lambda) = \int_C \exp\left\{\int_0^1 [\lambda x^2(t) + g x(t)]\, dt\right\} d_{W^*}x = \sqrt{\frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}} \cdot \exp\left\{\frac{g^2}{(2\lambda)^{3/2}}\left[tg\sqrt{\frac{\lambda}{2}} - \sqrt{\frac{\lambda}{2}}\right]\right\},$$

$$\alpha = 2\left[1 + \frac{1}{3}\beta^2\lambda^2\left(\frac{\beta}{3} + 1\right)^2\right]; \qquad \beta = \frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}.$$

Practical computations based on the use of the approximate formulae (2) - (5) have been performed in /19/. The comparison of numerical results confirms the higher efficiency of these formulae versus lattice Monte-Carlo computation.

2. FUNCTIONAL INTEGRALS IN EUCLIDEAN QUANTUM MECHANICS

Let us consider the quantum-mechanical system characterized by the Hamiltonian

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x), \qquad x \in (-\infty, \infty), \quad \hbar = c = 1. \quad (6)$$

The investigation of some important phenomena such as the instanton effects, concerned the topological structure of the ground state, is to be performed in Euclidean metrics (i.e. in imaginary time). In this case the Schrödinger equation is written in the form

$$\frac{\partial \Psi^E(x,t)}{\partial t} = -H\,\Psi^E(x,t), \quad t \ge 0. \quad (7)$$

The general solution of (7) with arbitrary initial conditions $\Psi^E(x,0) = \Psi_0^E(x)$ is

$$\Psi^E(x,t) = \int_{-\infty}^{\infty} \Psi_0^E(x_0)\, Z(x_0, x, t)\, dx_0,$$

where $Z(x_0, x, t)$ is a fundamental solution of equation (7). The main problem is to find the evolution matrix elements $Z(x_0,x,t) = \langle x | e^{-Ht} | x_0 \rangle$ that satisfy the equation

$$\frac{\partial Z}{\partial t} = \frac{1}{2}\frac{\partial^2 Z}{\partial x^2} - V(x)\, Z$$
$$Z(x_0, x, 0) = \delta(x - x_0). \quad (8)$$

Analogously with the well-known result of R. Feynman the solution of (8) is represented in the form of the conditional Wiener integral /4,2/:

$$Z(x_i, x_f, T) = \int_{C_{0,x_i,T,x_f}} \exp\left\{-\int_0^T V[x(t)]\, dt\right\} d_W x. \quad (9)$$

Integration in (9) is performed over the space of continuous on $[0,T]$ functions $x(t)$ with boundary conditions

$$x(0) = x_i,$$
$$x(T) = x_f.$$

Note that in distinction from the conventional Feynman path integral the exponent argument in (9) contains not the action functional but the integral of the potential energy. The kinetic term is included into $d_W x$. The extension of (6)-(9) to the systems with many degrees of freedom is obvious (see ref. /4/).

Suppose the Hamiltonian H has the discrete spectrum

$$H\psi_n(x) = E_n \psi_n(x).$$

Then there holds the following expansion[4]:

$$Z(x_i, x_f, T) = \sum_n e^{-E_n T} \psi_n(x_i) \psi_n(x_f). \qquad (10)$$

Hence the ground state energy E_0 can be calculated as follows:

$$E_0 = \lim_{T\to\infty} \left[-\frac{1}{T} \ln Z(T)\right], \qquad (11)$$

where

$$Z(T) = \sum_n e^{-E_n T} = \int_{-\infty}^{\infty} Z(X, X, T)\, dX.$$

After the appropriate change of variables in functional integral[19] the expression for $Z(X, X, T)$ is written in the form of the following integral

$$Z(X, X, T) = \frac{1}{\sqrt{2\pi T}} \int_C \exp\left\{-T \int_0^1 V[\sqrt{T}x(t) + X]\, dt\right\} d_{w^*}x \qquad (12)$$

with respect to normalized conditional Wiener measure in the space $C = \{C[0,1],\ x(0) = x(1) = 0\}$. The energy gap between the ground and the first excited states is defined[19] as

$$\Delta E = E_1 - E_0 = -\lim_{\tau\to\infty} \frac{d}{d\tau} \ln G(\tau), \qquad (13)$$

where the propagator

$$G(\tau) = \langle 0 | x(0)\, x(\tau) | 0 \rangle = \qquad (14)$$

$$= \lim_{T\to\infty} \frac{1}{Z(T)} \frac{1}{\sqrt{2\pi T}} \int_{-\infty}^{\infty} dx \cdot x \int_C \exp\left\{-T \int_0^1 V[\sqrt{T}x(t) + X]\, dt\right\} \cdot [\sqrt{T} \cdot x(\tau/T) + X]\, d_{w^*}x.$$

Using the values of (9) one can calculate also the ground state wave function squared:

$$|\psi_0(x)|^2 = \lim_{T\to\infty} \left[e^{E_0 T} \cdot Z(x, x, T)\right]. \qquad (15)$$

In the next sections we will consider the computation of functional integrals using the derived approximate formulae. We investigate the topological structure of the ground state in some quantum-mechanical models.

3. DOUBLE-WELL POTENTIAL

Due to existence of tunneling the wave function of the ground state of the system characterized by the Hamiltonian (6) with the potential

$$V(x) = \frac{1}{2}(x^2 - f^2) \qquad (16)$$

is an even superposition of wave functions at each of the wells. The basic effect caused by instantons is the splitting of the energy levels. (Assuming absence of instantons the levels are doubly degenerated). In the approximation of dilute instanton gas[20]:

$$E_0 = f - d; \quad \Delta E = 2d \qquad (17)$$

$$d = 4f \sqrt{\frac{2f^3}{\pi}}\, e^{-\frac{4}{3}f^3}$$

$$|\psi_0(\pm f)|^2 = \frac{1}{2}\sqrt{\frac{2f}{\pi}}. \qquad (18)$$

Our results for E_0 and ΔE computed using approximate formula (3) with $n = m = 1$ are given in Figures 1 and 2 by the dots. CPU time of the CDC-6500 computer was about 10 s per point f^2.

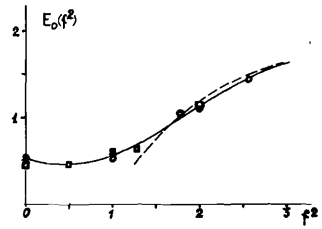


Fig.1

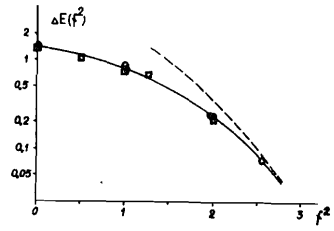
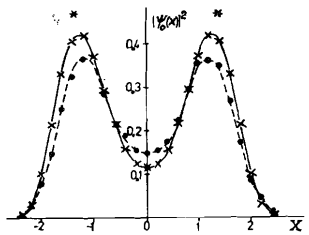


Fig.2

The solid lines represent "exact" results[21], the dashed lines correspond to (17). For comparison, the circles show the results[13] of lattice Monte-Carlo computations. The squares represent the results of [14], obtained evaluating N-fold integral via averaging over 10 Monte-Carlo iterations on lattice with N=303 points and spacing $a=0.25$. The information on CPU time and a type of computer in [13,14] is missing, the results are given in diagram form. Figures 1 and 2 show that the values of considered quantities can be obtained using (3) with accuracy equal to, and in some cases with even a greater accuracy, than in Monte-Carlo method on lattice, but with the multiplicity of the evaluated integrals smaller by two orders.

The ground state wave function squared, computed according to (15) using (3) with $n = m = 1;\ T = 4.5;\ f^2 = 2$ is shown in Fig.3 by crosses. The dots represent the results of the paper [14] that have been obtained via averaging over 100 Monte-Carlo iterations



on lattice with $N=200$, $a=0.25$; the stars correspond to (18). The solid and the dashed lines unite the points for easier comprehension.

Fig.3

4. QUANTUM PENDULUM

Let us consider now the quantum system with the Hamiltonian

$$H = \frac{1}{2}\lambda p^2 + V, \qquad (19)$$

where

$$V(x) = \frac{\omega^2}{\lambda}(1-\cos x), \qquad (20)$$

ω is a frequency of small oscillations, λ is a coupling constant. In the case of bounded periodic $V(x)$, $x\in(-\infty,\infty)$ the analysis of Hamiltonian (19) is reduced[22] to the study of

$$H(\theta) = -\frac{1}{2}\left(\frac{d^2}{dx^2}\right)_\theta + V(x). \qquad (21)$$

Here $\left(\frac{d^2}{dx^2}\right)_\theta$ is the operator $\frac{d^2}{dx^2}$ on $L^2[0,2\pi]$ with boundary conditions

$$\psi(2\pi) = e^{i\theta}\psi(0); \qquad \psi'(2\pi) = e^{i\theta}\psi'(0).$$

Therefore in this case we have

$$Z(x, x+2\pi N, T) = e^{i\theta N} Z(x,x,T). \qquad (22)$$

Performing the transformation (see ref. [15])

$$\psi(x) \to e^{-i\frac{x}{2\pi}\theta}\psi(x)$$

that removes the phase factor, we find that the expression (9) is valid for the new action functional ("θ-action"):

$$S_\theta = S - i\theta Q,$$

where Q is a topological charge, $|\theta| \le \pi$. The definition of the topological charge follows from (22):

$$Q(x) = -\frac{1}{2\pi}\int_0^T \dot{x}\,dt = \left[\frac{x}{2\pi}\right] \qquad (x(0)=x;\ x(T)=x_{mod\,2\pi}),$$

where $[\ ]$ denotes the integer part of the value.

We obtain for $Z(T)$ the following expression:

$$Z(T) = \int_{-\infty}^{\infty} Z(x,x,T)\,dx = \frac{2e^{-\frac{T}{\lambda}\omega^2}}{\sqrt{2\pi}}\cdot\sqrt{\frac{\lambda}{T}}\cdot\sum_{n=0}^{\infty}\cos\theta n\cdot e^{-2\pi^2\frac{\lambda}{T}n^2}\cdot Z_n(T), \qquad (23)$$

where

$$Z_n(T) = \int_0^{\pi}\left[I_n(x,T) + I_n(-x,T)\right]dx \xrightarrow[n\to\infty]{} 2\pi,$$

$$I_n(x,T) = \int_C \exp\left\{-\frac{\omega^2 T}{\lambda}\int_0^1 \cos\left[\sqrt{\frac{T}{\lambda}}x(t) + 2\pi nt + x\right]dt\right\}d_{w*}x.$$

The dependence on $\beta = \frac{\omega}{\lambda}$ of the topological susceptibility

$$\frac{1}{T_0}\langle Q^2\rangle,$$

$$\langle Q^2\rangle = \frac{1}{Z(T)}\cdot\frac{2e^{-\frac{T}{\lambda}\omega^2}}{\sqrt{2\pi}}\sqrt{\frac{\lambda}{T}}\cdot\sum_{n=0}^{\infty}\cos\theta n\cdot n^2\cdot e^{-2\pi^2\frac{\lambda}{T}n^2}\cdot Z_n(T); \quad T_0=\omega T, \qquad (24)$$

computed using approximate formula (2) with $m=1$, $T_0=7$, $\theta=0$, $\lambda=1$ is given in Fig.4 by the dots. The calculations have shown that the accuracy in the form of 3 correct signs can be reached taking into account only two or three terms in the series (24), i.e. the main contribution give the configurations with $n<5$. The CPU time on CDC-6500 has been within the range of 10 s per point β.

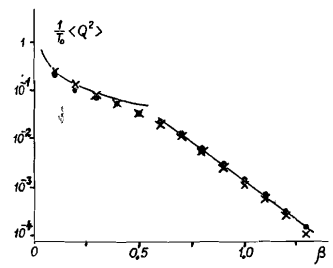


Fig.4

The crosses represent the β - dependence of the value

$$\frac{1}{\varepsilon N}\langle Q^2\rangle$$

that has been obtained in [15] by the Monte-Carlo method on lattice with $N=100$, $\varepsilon=\omega a=1$ (N is the number of points, i.e. the multiplicity of integrals, a is the lattice spacing). The solid line at $\beta>0.5$ denotes the dilute instanton gas approximation[15]:

$$\frac{1}{T_0}\langle Q^2\rangle = \frac{8}{\sqrt{\pi}}\sqrt{\beta}\,e^{-8\beta}\left[1-\frac{7}{64}\beta^{-1}-\dots\right]. \qquad (25)$$

The curve at $\beta<0.5$ represents the high-temperature expansion[15] in the continuum limit ($\varepsilon\to 0$, $N\to\infty$, εN fixed):

$$\frac{1}{T_0}\langle Q^2\rangle = \frac{1}{4\pi^2\beta}.$$

In order to compare $\langle Q^2\rangle$ more precisely to the theoretical expectations we consider the quantity

$$D = \frac{1}{T_0}\langle Q^2\rangle \cdot \beta^{-\frac{1}{2}} e^{S\beta}.$$

In the continuum limit (in this case $S = 8$) and for sufficiently large β (semiclassical region) there holds

$$D = \frac{8}{\sqrt{\pi}} \approx 4.51 . \qquad (26)$$

Our results are shown in Fig.5 by the dots. The values agree well with (26). The results[15] obtained with $\varepsilon = 1$, $N = 100$, $S = S_0 = 7.87$ (S_0 is an instanton action for this lattice) are denoted by the crosses. The deviation of these results from the theoretical predictions (26) cannot be explained by the presence of the two-loop correction factor in (25). To make the situation clear the computations in [15] were performed also with $\varepsilon = 0.6$ (at $\beta = 0.7$). In this case they have obtained the value $D = 3.3$, i.e. greater than the results with $\varepsilon = 1$ but still too smaller than theoretical estimate. The further decrease of ε in [15] has not been performed because of the arising difficulties connected with the growth of instanton size on the lattice and therefore with the serious metastabilities. It is clear that we have no these problems: the calculations are performed in the continuum, $\varepsilon = 0$.

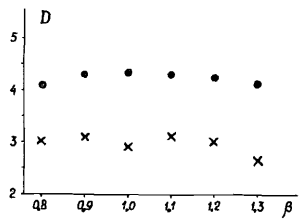


Fig.5

By the minimizing of χ^2 according to the relation

$$\ln\left[\frac{1}{T_0}\langle Q^2\rangle\right] = \ln D - S\beta + p\ln\beta$$

in ref.[15] they have obtained with $S = 7.87$ the values of parameters

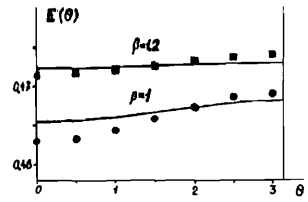
$$D = 2.98 ; \quad p = 0.46 .$$

Taking into account that in continuum limit $S = 8$ we have got from our data represented in Fig.5:

$$D = 4.25 ; \quad p = 0.493 .$$

that is in a good agreement with theoretical continuum predictions $D = 4.51$; $p = 0.5$.

Let us find now the value of the vacuum energy. Due to instanton effects the ground state energy E is washed away into a zone and is characterized by the CP-violating angle θ. The values of $E(\theta)$ obtained



using the approximate formula (2) with $m = 1$ according to (11), $\omega = 1$, $\beta = 1/\lambda$ are shown in Fig.6 for $\beta = 1$ and $\beta = 1.2$.

Fig.6

The solid lines represent the theoretical estimate obtained within the dilute instanton gas approximation[15]:

$$E(\theta) = \left(\frac{1}{2} - \frac{1}{8\cdot 4}\beta^{-1} - \frac{1}{32\cdot 16}\beta^{-2} - \ldots\right) - \cos\theta \cdot \frac{8}{\sqrt{\pi}}\beta^{-\frac{1}{2}} e^{-8\beta}\left[1 - \frac{7}{64}\beta^{-1} - \ldots\right] .$$

The characteristic COS-behaviour of our results is well seen in Fig.6.

5. CONCLUSIONS

The results of the above computations demonstrate the advantages of the considered method of evaluation of path integrals versus lattice Monte-Carlo method. The use of the conditional Wiener measure and the derived approximate formulae yields the more precise results while requiring essentially lesser-dimensional ordinary integrals to evaluate. The small multiplicity of integrals allowed us to use the deterministic methods (Gaussian quadrature, Tchebyshev, etc.) providing the results with guaranteed (not probabilistic) error estimate and the significant economy of computer time and memory. Due to the absence of lattice discretization in this method the problems concerned the finiteness of lattice spacing do not appear. All these considerations make the "deterministic approach" an attractive method for the computation of path integrals.

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Вычисление континуальных интегралов квантовой механики с помощью приближенных формул, точных на классе функциональных многочленов

Разработан метод приближенного вычисления интегралов по траекториям в евклидовой квантовой механике без решеточной дискретизации. Метод основан на представлении этих интегралов в виде континуальных интегралов по условной мере Винера и использовании построенных приближенных формул, точных на классе функциональных многочленов заданной степени. На примере расчета непертурбативных характеристик, связанных с топологической структурой вакуума, демонстрируются преимущества метода по сравнению с методом Монте-Карло расчетов на решетке.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Evaluation of Quantum Mechanics Path Integrals by the Approximations Exact on a Class of Polynomial Functionals

The method for numerical evaluation of path integrals in Euclidean quantum mechanics without lattice discretization is elaborated. The method is based on the representation of these integrals in the form of functional integrals with respect to the conditional Wiener measure and on the use of the derived approximate formulae exact on a class of polynomial functionals of a given degree. By the computations of non-perturbative characteristics, concerned the topological structure of vacuum, the advantages of this method versus lattice Monte-Carlo calculations are demonstrated.

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

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