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ON THE DETERMINISTIC COMPUTATION OF FUNCTIONAL INTEGRALS IN APPLICATION TO QUANTUM MECHANICAL PROBLEMS

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1. INTRODUCTION

One of the most powerful mathematical techniques in the contemporary quantum field theory [1] is the method of functional integration (see, e.g., ref. [2]). One of the great successes of the method is the development of the lattice gauge theory [3]. The introduction of space-time lattice turns functional integrals into ordinary ones of high multiplicity ($\geq 10^5$) that are usually evaluated by the Monte Carlo method. In order to do it one needs to use fast computers with large memory. At present there are in some works [4] (see also [2]) being developed the ways of computation of functional integrals that do not need the lattice discretization methods. In the latter sense the approach, based on the mathematically rigorous study of functional integrals with Gaussian measure [5] appears to be promising. Within the framework of the mentioned approach in the present paper we derive for functional integrals several new approximate formulae exact on a class of polynomial functionals of a given degree. Using these formulae, we show, how to compute certain characteristics in Euclidean quantum mechanics and on the models of linear quantum oscillator and anharmonic oscillator we compare our results with the results of computations of the functional integrals that have been obtained in [4] via the approximation of paths in the functional and also in [6] and [7] by the Monte Carlo method on lattice. The employment of the derived approximate formulae replaces the evaluation of the considered functional integral by the evaluation of an ordinary integral of small multiplicity, allowing the use of the deterministic methods (Gaussian quadrature, Tchebyshev, etc.) and leading to a significant economy of computer time and memory. The comparison of the numerical results confirms the higher efficiency of the method employed.

2. APPROXIMATE FORMULAS FOR INTEGRALS WITH GAUSSIAN MEASURE

We will study a functional integral $\int_X F[x]d\mu(x)$, where $F[x]$ is a real functional defined on a separable Frechet space X. $\mu(x)$ is a Gaussian measure on X defined by a correlation functional $K(\xi,\eta)$ and by a mean value $m(\eta)$, $\xi, \eta \in X'$. In the sequel we will use the "formula of mixed integration" [8]

$$\int_X F[x]d\mu(x) = (2\pi)^{-\frac{n}{2}} \int_{R^n} \exp\{-\frac{1}{2}(u,u)\} \int_X F[x - S_n(x) + \Psi_n(u)]d\mu(x)du,$$

where

$$S_n(x) = \sum_{k=1}^{n} (e_k, x)_{\tilde H} e_k, \quad \Psi_n(u) = \sum_{k=1}^{n} u_k e_k \quad \text{and} \quad \{e_k\}_{k=1}^{\infty}$$

is an orthogonal basis in Hilbert space $\tilde H$ that is generated by the measure μ and also the approximate formula

$$\int_X F[x]d\mu(x) \approx \int_{R^m} F[\theta_m(v)]d\nu_m(v), \qquad (1)$$

exact for polynomial functionals of degree $\leq 2m+1$, where a measure ν_m in R^m is a cartesian product of symmetric probabilistic measures ν in R; $\theta_m(v) = \sum_{k=1}^{m} c_k^{(m)} \rho(v_k)$; $[c_k^{(m)}]^2$ are the roots of the polynomial $Q_m(t) = \sum_{k=0}^{m} (-1)^k t^{m-k}/k!$; $\rho(r): R \to X$ is an odd function that satisfies the conditions

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

$$\prod_{i=1}^{j} \langle \xi_i, \rho(r) \rangle \in L(R,\nu), \quad 1 \leq j \leq 2m+1$$

for any $\xi, \eta, \xi_i \in X'$.

Combining these formulas we get the following "composite approximate formula"

$$\int_X F[x]d\mu(x) = (2\pi)^{-\frac{n}{2}} \int_{R^n} \exp\{-\frac{1}{2}(u,u)\} \int_{R^m} F[\theta_m(v) - \theta_m^n(v) + \Psi_n(u)]d\nu_m(v)du + R_m^n(F) \quad (2)$$

exact for polynomial functionals of degree $\leq 2m+1$, where $\theta_m^n(v) = S_n(\theta_m(v))$. We will prove the convergence of the approximations, obtained according to (2), to the exact value for $n \to \infty$. We will assume, that for almost all $v \in R^m$ with respect to measure ν holds the convergence $\theta_m^n(v) \xrightarrow[n\to\infty]{} \theta_m(v)$. If $X = C[a,b]$ this assumption is fulfilled.

<u>Theorem 1.</u> Let $F[x]$ be a continuous functional on X, satisfying the condition $|F[x]| \leq h(A(x,x))$, where $A(x,x) = \sum_{k=1}^{\infty} \gamma_k (x, e_k)_{\tilde H}^2$ is a non-negative quadratic functional, $\sum_{k=1}^{\infty} \gamma_k < \infty$, $\gamma_k \geq 0$; $h(r)$ is a nondecreasing function, and $\int_{R^m}\int_X h[A(\theta_m(v), \theta_m(v)) + A(x,x)]d\mu(x)d\nu_m(v) < \infty$. Then $R_m^n \to 0$ for $n \to \infty$.

Proof. Using the mixed integration formula we transform the integral

$$\int_X \int_{R^m} F[\theta_m(v) - \theta_m^n(v) + S_n(x)]d\nu(v)d\mu(x) = \int_X T[x]d\mu(x) =$$

$$= (2\pi)^{-\frac{n}{2}} \int_{R^n} \exp\{-\frac{1}{2}(u,u)\} \int_X T[x - S_n(x) + \Psi_n(u)]d\mu(x)du.$$

However

$$T[x - S_n(x) + \Psi_n(u)] = \int_{R^m} F[\theta_m(v) - \theta_m^n(v) + S_n(x - S_n(x) + \Psi_n(u))]d\nu_m(v) =$$

$$= \int_{R^m} F[\theta_m(v) - \theta_m^n(v) + \Psi_n(u)]d\nu_m(v).$$

Hence

$$\int_X T[x]d\mu(x) = (2\pi)^{-\frac{n}{2}} \int_{R^n} \exp\{-\frac{1}{2}(u,u)\} \int_X \int_{R^m} F[\theta_m(v) - \theta_m^n(v) + \Psi_n(u)]d\nu_m(v)d\mu(x)du =$$

$$= (2\pi)^{-\frac{n}{2}} \int_{R^n} \exp\{-\frac{1}{2}(u,u)\} \int_{R^m} F[\theta_m(v) - \theta_m^n(v) + \Psi_n(u)]d\nu_m(v)du.$$

For almost all v and x with respect to measures ν and μ respectively the sequence $\theta_m(v) - \theta_m^n(v) + S_n(x)$ converges to x as $n \to \infty$. Consequently, at these points

$$\lim_{n\to\infty} F[\theta_m^{\cdot} - \theta_m^n + S_n(x)] = F[x].$$

On the other hand, for almost all v and x

$$|F[\theta_m(v) - \theta_m^n(v) + S_n(x)]| \leq h[A(\theta_m, \theta_m) + A(x,x)].$$

Indeed,

$$|F[\sum_{i=n+1}^{\infty} (\theta_m(v), e_i)_{\tilde{H}} e_i + \sum_{i=1}^{n} (x, e_i)_{\tilde{H}} e_i]| \leq$$

$$\leq h[\sum_{i=1}^{n} \gamma_i (x_i e_i)_{\tilde{H}}^2 + \sum_{i=n+1}^{\infty} \gamma_i (\theta_m(v), e_i)_{\tilde{H}}^2] \leq h[A(\theta_m(v), \theta_m(v)) + A(x,x)].$$

Now we can apply the Lebesgue theorem "on the passage to the limit under the integral sign" to the right side, and that proves the theorem.

The estimate of the remainder $R_m^n(F)$ in dependence on m and n establishes the following

Theorem 2[9] If the functional $F[x]$ integrable with respect to measure μ can be expressed in the form

$$F[x + x_0] = P_{2m+1}[x] + r_{2m+1}(x, x_0) \qquad \text{for all } x, x_0 \in X,$$

where P_{2m+1} is a polynomial functional of degree $\leq 2m+1$, and the remainder r_{2m+1} is estimated by the expression

$$|r_{2m+1}(x, x_0)| \leq [A(x,x)]^{m+1} \cdot \{k_1 \exp[k_2 A(x + x_0, x + x_0)] +$$

$$+ k_3 \exp[k_2 A(x_0, x_0)]\}, \quad k_i > 0, \quad i = 1, 2, 3;$$

$$1 - 2k_2\gamma_j > \alpha > 0, \quad j = 1, 2, \ldots; \quad \sum_{j=1}^{\infty} \gamma_j a_j < \infty, \quad (e_j, \theta_m(v))_{\tilde{H}}^2 \leq a_j,$$

then for the remainder of the approximate formula (2) there holds an estimate

$$|R_m^n(F)| \leq G_m(\sum_{j=n+1}^{\infty} \gamma_j)^{m+1} + H_m(\sum_{j=n+1}^{\infty} \gamma_j a_j)^{m+1},$$

where G_m and H_m are positive constants, dependent on m.

Remark. The proof of Theorem 1,2, for the special case m=1 is given in[8].

Practical example. Here we estimate the speed of convergence of Formula (2). We consider an integral with a conditional Wiener measure $d_{w*}x: X = C \equiv \{C[0,1], x(0) = x(1) = 0\}$, mean value $m(t) = 0$ and correlation function $B(t,s) = \min\{t,s\} - ts$. Then

$$\int_C F[x]d_{w*}x = (2\pi)^{-\frac{n}{2}} \int_{R^n} \exp\{-\frac{1}{2}(u,u)\} \frac{1}{2^m} \underbrace{\int_{-1}^{1} \ldots \int_{-1}^{1}}_{m} F[\theta_m(v,\cdot) - \theta_m^n(v,\cdot) + \Psi_n(u,\cdot)]dvdu + R_m^n(F), \tag{3}$$

$$\theta_m(v,t) = \sum_{i=1}^{m} c_i^{(m)} \theta(v_i, t); \qquad \theta(r,t) = \begin{cases} -t \cdot \operatorname{sign} r, & t \leq |r|; \\ (1-t)\operatorname{sign} r, & t > |r|; \end{cases}$$

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

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

And, if we choose $A(x,x) = \int_0^1 x^2(t)dt$ then we get the order of convergence equal to $O(n^{-(m+1)})$.

3. APPROXIMATE FORMULAS WITH WEIGHT FOR CONDITIONAL WIENER INTEGRALS

Here we will study in more detail a significant to quantum mechanics case of Gaussian measure, namely the conditional Wiener measure. An important role in constructing the approximate formulae for

$$I(P\cdot F)=\int_C P[x]\cdot F[x]\,d_{w^*}x \tag{4}$$

with weight

$$P[x]=\exp\{\int_0^1 [\lambda p(t)x^2(t)+g(t)x(t)]dt\}, \tag{5}$$

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

Theorem 3. An integral (4) with weight (5) can be written in the form

$$I(P\cdot F)=\exp\{-\frac{1}{2}\int_0^1 (1-s)K(s)ds\}\exp\{\frac{1}{2}\int_0^1 L^2(t)dt\}\cdot\int_C F[\phi(x)+a]\,d_{w^*}x, \tag{6}$$

where

$$\phi(x(t))=x(t)-\frac{1-t}{V(t)}\int_0^t K(s)V(s)x(s)ds;\quad V(t)=\exp\{\int_0^t (1-s)K(s)ds\};$$

$K(s)$ is the solution of the differential equation

$$(1-s)K'(s)-(1-s)^2K^2(s)-3K(s)-2\lambda p(s)=0,\quad s\in[0,1], \tag{7}$$

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

$$a(t)=\int_0^t L(s)ds-\frac{1-t}{V(t)}\int_0^t K(s)V(s)[\int_0^s L(u)du]ds; \tag{8a}$$

$$L(t)=\int_0^t [K(s)V(s)H(s)-g(s)]ds+c;\quad H(t)=\int_t^1 g(s)\frac{1-s}{V(s)}ds, \tag{8b}$$

and the constant c in (8b) is determined by the condition

$$\int_0^1 L(s)ds=0. \tag{9}$$

Proof. We will consider a transformation $x(t)\to y(t)$ /10/ defined by the relation

$$y(t)=x(t)+(1-t)\int_0^t K(s)x(s)ds,\quad K(s)\in C[0,1]. \tag{10}$$

Transformation (10) maps the space C onto itself in one-to-one correspondence. The inverse transformation $x(t)=\phi(y(t))$ is given by the relation

$$\phi(y(t))=y(t)-(1-t)\exp\{-\int_0^t (1-s)K(s)ds\}\times\int_0^t \exp\{\int_0^s (1-u)K(u)du\}K(s)y(s)\,ds. \tag{11}$$

For a general case of linear transformation

$$y=x+Ax=(E+A)x, \tag{12}$$

where $Ax(t)=\int_0^1 Q(t,s)x(s)ds$, analogously with the formulae for the Wiener measure /11/, we obtain a formula for the change of variables in conditional Wiener integral

$$\int_C F[y]\,d_{w^*}y=|D|\int_C F[x+Ax]\exp\{-\frac{1}{2}\int_0^1 [\frac{d}{dt}(Ax)]^2dt-\int_0^1 \dot{x}\frac{d}{dt}(Ax)dt\}\,d_{w^*}x, \tag{13}$$

where D is the Fredholm determinant of the kernel $Q(t,s)$. For the special case of transformation (10)

$$Q(t,s)=\begin{cases}(1-t)K(s), & s\le t;\\ 0, & s>t;\end{cases}$$

and $D=\exp\{\frac{1}{2}\int_0^1 Q(s,s)ds\}=\exp\{\frac{1}{2}\int_0^1 (1-s)K(s)ds\}$.

After some transformations of the expression in the exponent of the right side of (13), we get

$$\int_C F[y]\,d_{w^*}y=|D|\int_C F[x+Ax]\times$$

$$\times\exp\{\frac{1}{2}\int_0^1 [(1-t)^2K^2(t)+3K(t)-(1-t)K'(t)]x^2(t)dt\}\,d_{w^*}x.$$

Hence, if $K(t)$ is the solution of (7), then

$$\int_C F[x]\exp\{\lambda\int_0^1 p(t)x^2(t)dt\}\,d_{w^*}x=|D|^{-1}\int_C F[\phi(y)]\,d_{w^*}y. \tag{14}$$

Substituting $F[x]=\exp\{\int_0^1 g(t)x(t)dt\}\cdot\Phi[x]=G[x]\,\Phi[x]$ into (14) and performing still one more change of variables

$$y(t)=z(t)+\int_0^t L(s)ds\equiv z(t)+w(t),$$

where L(s) satisfies (9), after some transformations we obtain

$$\int_C P[x]\Phi[x]d_{w*}x = |D|^{-1}\exp\{-\frac{1}{2}\int_0^1 \dot{w}^2(t)dt\}\times$$

$$\times\int_C G[\phi(z+w)]\cdot\Phi[\phi(z+w)]\cdot\exp\{-\int_0^1 \dot{w}(t)\dot{z}(t)dt\}d_{w*}z =$$

$$= |D|^{-1}\exp\{\frac{1}{2}\int_0^1 L^2(s)ds\}\int_C \exp\{\int_0^1 z(t)[g(t)-K(t)V(t)\times$$

$$\times[\int_t^1 g(s)\frac{1-s}{V(s)}ds]+L'(t)]dt\}\cdot\Phi[\phi(z(t)+\int_0^t L(s)ds)]d_{w*}z.$$

Assuming the conditions (8) hold the assertion of the theorem follows directly from the last equality.

Now, if we apply the approximate formula (1) in the case of $d\mu(x) = d_{w*}x$ (this case has been studied in [12]) to the functional integral in the right side of (6), then for an integral (4) with weight (5) we obtain a family of approximate formulas, dependent on a natural parameter m.

Theorem 4 [13] Under the conditions of the above theorem the approximate formula

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

$$\approx \exp\{-\frac{1}{2}\int_0^1(1-s)K(s)ds\}\exp\{\frac{1}{2}\int_0^1 L^2(t)dt\}\times \tag{15}$$

$$\times\frac{1}{2^m}\int_{-1}^{1}\dots\int_{-1}^{1}F[\tilde{\theta}_m(v,\cdot)+a(\cdot)]dv_1\dots dv_m,$$

where

$$\tilde{\theta}_m(v,\cdot) = \sum_{k=1}^{m} c_k^{(m)}\tilde{\theta}(v_k,\cdot), \qquad \tilde{\rho}(r,t) = \begin{cases} \operatorname{sign} r, & t \le |r|; \\ 0, & t > |r|; \end{cases}$$

$$\tilde{\theta}(r,\cdot) = \phi(\theta(r,\cdot)) = f(r,\cdot) - \tilde{\rho}(r,\cdot),$$

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

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

Particularly, if $p(t)\equiv 1$; $g(t)\equiv g = \mathrm{const}$; $\lambda < \pi^2/2$ the formula (15) acquires the form

$$I(P\cdot F) = \int_C \exp\{\int_0^1[\lambda x^2(t)+gx(t)]dt\}F[x]d_{w*}x \approx I_m(P\cdot F) =$$

$$= \sqrt{\frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}}\exp\{\frac{g^2}{2\lambda\sqrt{2\lambda}}[\operatorname{tg}\sqrt{\frac{\lambda}{2}}-\sqrt{\frac{\lambda}{2}}]\}\frac{1}{2}\underbrace{\int_{-1}^{1}\dots\int_{-1}^{1}}_{m}F[\tilde{\theta}_m(v,\cdot)+a(\cdot)]dv_1\dots dv_m. \tag{16}$$

It ought to be noted, that in this case the function a(t) can be represented in explicit form:

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

the fact that must not be generally disregarded in actual application of formulas. The transformation $\phi(x)$ acquires a simple form, too:

$$\phi(x) = x - \hat{A}x \tag{17}$$

where $\hat{A}x(t) = \sin\sqrt{2\lambda}(1-t)\cdot\int_0^t \hat{f}(s)x(s)ds$,

$$\hat{f}(s) = \frac{\sqrt{2\lambda}(1-s)\cdot\cos\sqrt{2\lambda}(1-s)-\sin\sqrt{2\lambda}(1-s)}{(1-s)\cdot\sin^2\sqrt{2\lambda}(1-s)}.$$

To estimate the remainder of Formula (16) we need some preliminary results.

Lemma. Linear operator ϕ, defined on $C = \{C[0,1],\ x(0)=x(1)=0\}$ according to (17), is bounded on C in L_2-norm.

Proof. The parallelogram law in L_2 yields

$$||\phi(x)||_{L_2}^2 \le 2||x||_{L_2}^2 + 2||\hat{A}x||_{L_2}^2.$$

From the inequality

$$[\int_0^t \hat{f}(s)x(s)ds]^2 \le t\int_0^t \hat{f}^2(s)x^2(s) \le \int_0^t \hat{f}^2(s)x^2(s)ds, \quad 0\le t\le 1,$$

after the change of order of integration with respect to t and s we get

$$||\hat{A}x||_{L_2}^2 \le \int_0^1 \hat{f}^2(s)x^2(s)\int_s^1 \sin^2\sqrt{2\lambda}(1-t)dt\,ds = \int_0^1 x^2(s)\omega(s)ds,$$

where

$$\omega(s)=\hat{f}^2(s)\cdot\frac{1}{2}\left(1-s-\frac{\sin 2\sqrt{2\lambda}(1-s)}{2\sqrt{2\lambda}}\right).$$

If $\tau\equiv\tau(s)=\sqrt{2\lambda}(1-s)$ we have

$$\omega(s)=\left(\frac{\tau\cos\tau-\sin\tau}{\tau\sin^2\tau}\right)^2\cdot\frac{\sqrt{2\lambda}}{2}\left(\tau-\frac{\sin 2\tau}{2}\right)\le\left(\frac{1}{6}\cdot\frac{\tau^2}{\sin^2\tau}+\frac{\tau}{2\sin\tau}\right)^2\frac{\sqrt{2\lambda}}{2}\cdot\frac{2\tau^3}{3}.$$

Considering, that for $0\le s\le 1$ we have $\tau\le\sqrt{2\lambda}$; $\tau/\sin\tau\le\sqrt{2\lambda}/\sin\sqrt{2\lambda}\equiv r_0$ we obtain the following estimate

$$\omega(s)\le\frac{r_0^2\lambda^2}{3}\left(\frac{r_0}{3}+1\right)^2.$$

Therefore, the inequality $\|\phi(x)\|^2_{L_2}\le\alpha\|x\|^2_{L_2}$ where $\alpha=2[1+\frac{1}{3}r_0^2\lambda^2(\frac{r_0}{3}+1)^2]$ holds for all $x(t)\in C$. Thus the proof of the lemma is complete.

Theorem 5. 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 $\le 2m+1$;

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

$$c_1(m),\ c_2(m)\ge 0;\quad 0\le\lambda+c_2(m)<\frac{\pi^2}{2}. \tag{18}$$

Then for the remainder $R_m(P\cdot F)=I(P\cdot F)-I_m(P\cdot F)$ of Formula (16) we have the estimate

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

where

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

$$M(g,\lambda)=\int_C P[x]\,d_{w*}x=\sqrt{\frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}}\exp\{\frac{g^2}{2\lambda\sqrt{2\lambda}}[\mathrm{tg}\sqrt{\frac{\lambda}{2}}-\sqrt{\frac{\lambda}{2}}]\}. \tag{19}$$

Proof. Since Formula (16) is exact for $P_{2m+1}[x]$, it follows that

$$|R_m(P\cdot F)|=|R_m(P\cdot r_{2m+1})|\le|I(P\cdot r_{2m+1})|+|I_m(P\cdot r_{2m+1})|,$$

where, according to (18) and (19),

$$|I(P\cdot r_{2m+1})|\le c_1(m)\cdot M(g,\lambda+c_2(m))$$

$$|I_m(P\cdot r_{2m+1})|\le c_1(m)\cdot M(g,\lambda)\cdot\frac{1}{2^m}\underbrace{\int_{-1}^{1}\cdots\int_{-1}^{1}}_{m}\exp\{c_2(m)\times\int_0^1[\phi(\theta_m(v,t))+a(t)]^2dt\}\,dv.$$

Using the result formulated in the preceeding lemma we have

$$\exp\{c_2(m)\int_0^1[\phi(\theta_m(v,t))+a(t)]^2dt\}\le\tilde{c}_2(m)\cdot\exp\{2c_2(m)\cdot\alpha\cdot\int_0^1[\theta_m(v,t)]^2dt\}.$$

Applying the Cauchy - Bunyakovskii inequality and the property $\sum_{j=1}^m[c_j^{(m)}]^2=1$ we obtain

$$[\theta_m(v,t)]^2=[\sum_{j=1}^m c_j^{(m)}\theta(v_j,t)]^2\le\sum_{j=1}^m[\theta(v_j,t)]^2.$$

Since $\int_0^1[\theta(v_j,t)]^2dt=v_j^2-|v_j|+\frac{1}{3}$, there follows for $w\in R$

$$|I_m(P\cdot r_{2m+1})|\le c_1(m)M(g,\lambda)\tilde{c}_2(m)[2\int_0^{1/2}\exp\{2c_2(m)\alpha(w^2-w+\frac{1}{3})\}dw]^m.$$

If we take into account that for $a\le x\le b$

$$\exp x\le(b-a)^{-1}[\exp b-\exp a](x-a)+\exp a,$$

we get

$$\int_0^{1/2}\exp\{2c_2(m)\alpha(w^2-w+\frac{1}{3})\}dw\le 2\left(\frac{4}{3}\exp\frac{2}{3}\alpha c_2(m)-\exp\frac{1}{6}\alpha c_2(m)\right)\le$$

$$\le\frac{8}{3}\exp\{\frac{2}{3}\alpha c_2(m)\}.$$

Therefore

$$|I_m(P\cdot r_{2m+1})|\le c_1(m)M(g,\lambda)\tilde{c}_2(m)[\frac{8}{3}\exp(\frac{2}{3}\alpha c_2(m))]^m.$$

Q.E.D.

4. LINEAR QUANTUM OSCILLATOR

We will illustrate the use of the formulae with examples of simple quantum-mechanical models characterized by the Hamiltonian

$$H = \frac{1}{2} p^2 + V(X), \qquad X \in (-\infty, \infty).$$

The ground state energy E_0 of the system is defined [14] as

$$E_0 = \langle 0|H|0\rangle = \lim_{T\to\infty} \frac{1}{Z(T)} \frac{1}{\sqrt{2\pi T}} \int_{-\infty}^{\infty} dX \int_C \exp\{-T\int_0^1 V[\sqrt{T}\,x(t) + X]dt\}[\frac{1}{2} X V'(X) + V(X)]d_{w^*}x \tag{20}$$

where $Z(T) = \int_{-\infty}^{\infty} \tilde{Z}(X,T)dX$;

$$\tag{21}$$

$$\tilde{Z}(X,T) = \frac{1}{\sqrt{2\pi T}} \int_C \exp\{-T\int_0^1 V[\sqrt{T}\,x(t) + X]dt\}d_{w^*}x. \tag{22}$$

The energy gap between the ground and the first excited states is

$$\Delta E = E_1 - E_0 = -\lim_{\tau\to\infty} \frac{d}{d\tau} \ln G(\tau), \tag{23}$$

where the propagator

$$G(\tau) = \langle 0|x(0)x(\tau)|0\rangle = \lim_{T\to\infty} \frac{1}{Z(T)} \frac{1}{\sqrt{2\pi T}} \int_{-\infty}^{\infty} dX\cdot X \int_C \exp\{-T\times \int_0^1 V[\sqrt{T}\,x(t)+X]dt\}[\sqrt{T}\,x(\frac{\tau}{T}) + X]d_{w^*}x. \tag{24}$$

For a wave function of the ground state we have

$$|\Psi_0(X)|^2 = \lim_{T\to\infty} [e^{E_0 T} \tilde{Z}(X,T)]. \tag{25}$$

The functional integral (22) for a harmonic oscillator with $V(X) = \frac{1}{2} X^2$ may be evaluated explicitly using the formula with weight (16):

$$\tilde{Z}(X,T) = \frac{1}{\sqrt{2\pi\,\mathrm{sh}\,T}} \exp\{-\mathrm{th}\frac{T}{2} X^2\}.$$

Consequently, for finite T,

$$E_0^{(T)} = \frac{\int_{-\infty}^{\infty} X^2 \tilde{Z}(X,T)dX}{\int_{-\infty}^{\infty} \tilde{Z}(X,T)dX} = \frac{1}{2}\mathrm{cth}\frac{T}{2};$$

$$|\Psi_0^{(T)}(X)|^2 = e^{E_0^{(T)}T}\tilde{Z}(X,T) = \frac{e^{\frac{T}{2}\mathrm{cth}\frac{T}{2}}}{\sqrt{2\,\mathrm{sh}\,T}} \cdot \frac{1}{\sqrt{\pi}} e^{-\mathrm{th}\frac{T}{2}X^2}; \tag{26}$$

$$G^{(T)}(\tau) = \frac{1}{2}\mathrm{cth}\frac{T}{2}\cdot(\mathrm{ch}\,\tau - \mathrm{th}\frac{T}{2}\mathrm{sh}\,\tau), \quad \Delta E^{(T)} = \mathrm{th}\frac{T}{2}.$$

The values of $E_0^{(T)}$, $|\Psi_0^{(T)}(X)|^2$ for various T, and also of $E_0^{(T,n)}$, obtained on the CDC-6500 computer using the composite formula (3) with m = 1, are given in Table 1. We remined that the theoretical values are: $E_0 = 1/2$; $\Delta E = 1$; $|\Psi_0(X)|^2 = \frac{1}{\sqrt{\pi}} e^{-X^2}$. It follows from Table 1 that good approximations $E_0^{(T,n)}$ of the theoretical value are achieved at relatively small values of T and n. We cite, for comparison, the results [6], obtained on a lattice of N = 51 points and the step a = 0.5. The result of an exact evaluation of the Gaussian N -dimensional integral has been $E_0^{(N)} = 0.447$; the computation of the integral via the simulations of $N_E = 100$ lattice configurations has given the result $E_0^{(N,N_E)} = 0.45$. In paper [4] the result of computations of N = 4-dimensional integral obtained in $N_R = 100$ runs each consisting of 10000 path simulations is $E_0^{(N,N_R)} = 0.4932 \pm 0.145$, which took 19×100 s of CPU time on the Vax 780. For N = 10, $N_R = 100$ the result is $E_0^{(N,N_R)} = 0.4979 \pm 0.051$ in 67×100 s.

Table 1

T	$E_0^{(T)}$ Formula (16)	$\lvert\Psi_0^{(T)}(X)\rvert^2$ Formula (16)	n	$E_0^{(T,n)}$ Formula (3)	CPU time, s
5	0.50678	$1.0345\,(1/\sqrt{\pi})\ \exp\{-0.9866X^2\}$	1	0.5077	1.8
6	0.50248	$1.0150\,(1/\sqrt{\pi})\ \exp\{-0.9951X^2\}$	2	0.5073	3.1
7	0.50091	$1.0064\,(1/\sqrt{\pi})\ \exp\{-0.9982X^2\}$	3	0.5010	5.5
8	0.50034	$1.0027\,(1/\sqrt{\pi})\ \exp\{-0.9993X^2\}$	5	0.5002	9.7

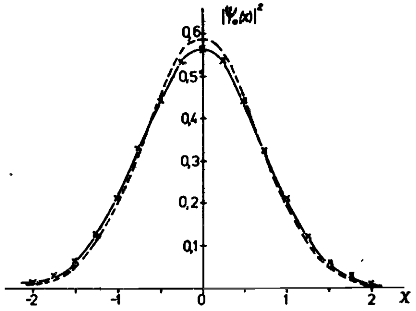

Fig.1. Wave function of the ground state of harmonic oscillator.

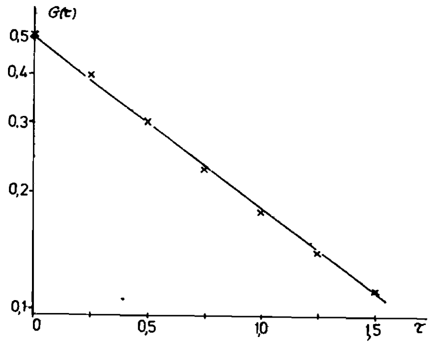

Fig.2. Dependence of the propagator $G(\tau) = \langle 0|x(0)x(\tau)|0\rangle$ *on* τ *for harmonic oscillator. Its theoretical value is illustrated with the straight line.*

On a lattice with N = 1000, a = 1 in paper /6/ they have given, using the exact evaluation of the integral, the value

$$|\Psi_0^{(N)}(X)|^2 = 0{,}59\, e^{-1.1 X^2} = 1.05 \frac{1}{\sqrt{\pi}} e^{-1.1 X^2} . \qquad (27)$$

In Fig.1 the solid curve gives the theoretical value, the dashed curve gives the best result (27) on lattice /6/ and the crosses are our results obtained via the composite formula (3) with m = 1, T = 6, n = 2. CPU time of the CDC-6500 computer at each point X was less than 0.1 s. The information on CPU time and a type of computer in /6/ is missing.

In Fig.2 with logarithmic scale, the crosses represent our values of $G(\tau)$. These results were computed using the formula (3) with m = 1, n = 2, T = 6. CPU time on the CDC-6500 has been within the range of 10 s per point τ. Fitting a straight line by the method of least squares, we have got $G^{(T,n)}(0) = E^{(T,n)} = 0.5053$; $\Delta E^{(T,n)} = 1.0198$. In /6/, on a lattice with N = 51, a = 0.5, the authors have obtained, using the exact value of the integral, $\Delta E^{(N)} = 0.9875$; while in modelling $N_E = 100$ lattice configurations they obtained $\Delta E^{(N,N_E)} = 0.99$. In /4/, through $N_R = 100$ runs with 10000 paths each, the authors have found

for N = 4 $\quad \Delta E^{(N,N_R)} = 0.8801 \pm 0.202$, time = 100×19 s;
for N = 10 $\quad \Delta E^{(N,N_R)} = 0.9331 \pm 0.129$, time = 100×67 s.

Table 2

g	E_0^* /15/	G^* /4/ (0)	$G^{(N)}(0)$ N=4 /4/	$G^{(N)}(0)$ N=20 /4/	T	$E_0^{(T,1)}$ Formula (16)	$G^{(T,1)}(0)$ Formula (16)
0.1	0.559146	0.4125	0.433±0.16	0.409±0.06	3	0.552	0.406
0.2	0.602405	-	-	-	2.5	0.592	0.364
0.5	0.696176	0.3058	0.296±0.07	0.293±0.04	2	0.685	0.293
1.0	0.803771	0.2571	0.269±0.08	0.267±0.08	1.5	0.774	0.257

Table 3

g	ΔE^* /15/	$\Delta E^{(N)}$ N=20 /4/	T	$\Delta E^{(T,1)}$ Formula (3)	$E_0^{(T,1)}$ Formula (3)	$G^{(T,1)}(0)$ Formula (3)
0.1	1.2104	1.03±0.29	4.5	1.14	0.570	0.419
0.2	1.3481	-	4	1.32	0.616	0.377
0.5	1.6282	1.50±0.67	3	1.55	0.707	0.313
1.0	1.9341	1.56±0.81	2.5	1.88	0.832	0.263

5. ANHARMONIC OSCILLATOR

Our results for an anharmonic oscillator with $V(X)=1/2X^2+gX^4$, obtained using Formulae (16) and (3) with $n=m=1$ are illustrated in Tables 2 and 3, respectively. The overall time of computation for $E_0^{(T,1)}$ and $G^{(T,1)}(0)$ at each point g has been ≈ 10 min for (16) and ≈ 0.5 min for (3) on the CDC-6500. Exact values are denoted through E_0^*, $G^*(0)$ and ΔE^*. The results, obtained in [4] via 10 simulations of 3000 paths each, are denoted $G^{(N)}(0)$ and $\Delta E^{(N)}$. The time of computation for each point g was 10×25 s for N = 4 and 10×17 min for N = 20 on the Vax 780. $\Delta E^{(T,1)}$ denotes the logarithmic derivative of $G^{(T,1)}(\tau)$ [16] that we find, analogously with the case of harmonic oscillator, graphically from the points obtained using (3) with $n=m=1$.

6. DOUBLE-WELL POTENTIAL

Here we will examine the example of tunneling in double-well potential $V(X)=1/2(X^2-f^2)^2$ on the existence of topological effects. The basic effect caused by instantons [17] is the splitting of the energy levels. (Assuming absence of instantons the levels are doubly degenerated). In this case, the wave function of the ground state is an even superposition of wave functions at each of the wells. In the approximation of dilute instanton gas

$$E_0 = f - d; \quad \Delta E = 2d; \quad \left(f \geq 0, \; d = 4\sqrt{\frac{2f^3}{\pi}}\, e^{-\frac{4}{3}f^3}\right); \tag{28}$$

$$|\Psi_0(\pm f)|^2 = \frac{1}{2}\sqrt{\frac{2f}{\pi}}. \tag{29}$$

Numerical results for E_0 and $E_1 = E_0 + \Delta E$, computed using Formula (3) with $n=m=1$ are given in Fig.3 by circles and squares, respectively. Our results, corresponding to the values of E_0 and denoted by crosses, were obtained from $E_0 = -(1/T)\ln Z(T)$. The solid lines represent exact results [18], the dashed line corresponds to (28). For comparison, the dots show the results [6], obtained evaluating N-fold integral via the averaging over 10 Monte Carlo iterations on lattice with N = 303 points and step a = 0.25; the triangles represent the result of [7]. In Fig.4 the crosses give the results of computations of $|\Psi_0(X)|^2$ performed using Formulas (25) and (3) with $n=m=1$, $T = 4.5$ for the case $f^2 = 2$. The dots represent the results of paper [6], that have been obtained via the averaging over 100 Monte Carlo iterations on lattice with N = 200, a = 0.25; the stars depict (29). The solid and the dashed lines unite the points for easier comprehension.

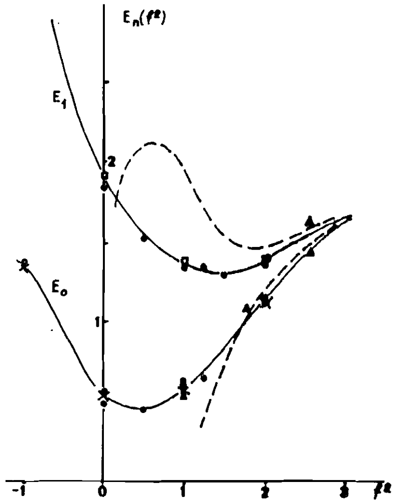

Fig.3. The ground state and the first excited state energy of a system with the potential $V(X)=\frac{1}{2}(X^2-f^2)^2$.

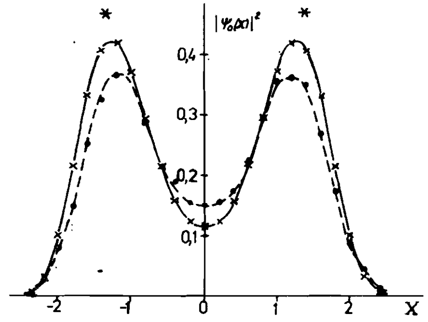

Fig.4. Wave function of the ground state of a system with the potential $V(X)=\frac{1}{2}(X^2-2)^2$.

7. CONCLUSIONS

Due to limitation of space we were not able to discuss the results and the wide spectrum of application in detail. The method of evaluation of functional integrals based on the use of conditional Wiener measure and the derived approximate formulae yields the values of the considered quantities with accuracy equal to, and in many cases with even a greater accuracy, than in the Monte Carlo method on lattice, while requiring essentially lesser-dimensional integrals. As we have already mentioned at the introduction, we evaluate these integrals using the quadrature formulae. Within the bounds of the method we use, there do not appear undesirable effects such as "jumping" of a particle over a potential barrier instead of tunneling through it, which were discovered in [7] and connected with the finiteness of the lattice step. Our work in the approximation theory of integration with respect to Gaussian measure is stimulated by recent advances of measure theory in quantum field theory.

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Грегуш М. и др. Е11-86-266
О детерминированном вычислении континуальных интегралов в применении к задачам квантовой механики

Получены новые приближенные формулы для континуальных интегралов по гауссовой мере в сепарабельном пространстве Фреше. Как частный случай рассмотрено интегрирование по мере Винера и по условной мере Винера. Для интегралов по условной мере Винера получено семейство приближенных формул с весом. Рассмотрены квантовомеханические модели, а именно линейный и ангармонический осцилляторы. Эффективность формул продемонстрирована на этих примерах путем численного сравнения с методом Монте - Карло на решетке.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1986

Greguš M. et al. E11-86-266
On the Deterministic Computation of Functional Integrals in Application to Quantum Mechanical Problems

New approximate formulae for functional integrals with the Gaussian measure in separable Frechet spaces are derived. As a special case, the integration with respect to the conditional Wiener measure is investigated. For conditional Wiener integrals a family of approximate formulae with weight is constructed. The quantum mechanical models, namely the linear and the anharmonic oscillators, are described. The efficiency of the formulas is demonstrated in the numerical comparison with the Monte Carlo method on lattice.

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

Preprint of the Joint Institute for Nuclear Research. Dubna 1986