ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ
СО АН СССР

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FEYNMAN FORMULATION OF QUANTUM MECHANICS AND COMPUTER EVALUATION OF PATH INTEGRALS

PREPRINT 83-47

НОВОСИБИРСК

FEYNMAN FORMULATION OF QUANTUM MECHANICS AND COMPUTER EVALUATION OF PATH INTEGRALS

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A b s t r a c t

The Metropolis method of Monte-Carlo computer simulation of paths in imaginary time is applied to several quantum-mechanical problems such as nonlinear double-well oscillator, atoms with one or two electrons and light nuclei up to He^4. A method of calculation of path integrals with the absolute normalization is proposed and used for the calculation of the Green functions.

We have really found this method capable to evaluate integrals with about $10^{3\div4}$ variables. So, the properties of quantum systems with a number of degrees of freedom up to 10-15 can be calculated starting from the first principles.

1. Introduction

Feynman formulation of quantum mechanics [1] differs crucially from more traditional Schrödinger and Heizenberg ones. As in classical mechanics, the main object is the particle trajectory $x(t)$. The statistical nature of quantum mechanics becomes in this language very transparent: the trajectory $x(t)$ is not governed by any equations of motion and can be arbitrary, but with some probability. The corresponding weight is $exp(iS[x(t)])$ (where S is the action). Such approach naturally explains the physical meaning of Minimal Action Principle of classical mechanics.

From computational point of view, the striking feature of this approach is the absence of any differential equations. In some sence, the answer is written in quadratures, but as a path integrals. So, the problem is to develop effective methods of their evaluation.

The important case in which it can be done analytically is the Gaussian one, when action depends quadratically on its variables. We remind that a number of famous results were obtained by such a method, in particular the Feynman rules for perturbation series in quantum electrodynamics and, more recently, for nonabelian gauge theories. One should also mention here semiclassical methods, e.g. related with the famous "instanton" solution [2] in QCD.

However, it is desirable to evaluate the path integrals of arbitrary type, at least numerically. The most urgent is the situation in quantum chromodynamics, where no evident small parameter is present and neither perturbation theory nor semiclassical methods can describe the bulk properties of the ground state. So, it is not surprizing that the possibility of numerical evaluation of functional integrals was first studied in this context.

Historically, the work by K.Wilson [3] was very important because it has stressed the analogy between the gauge field on the lattice and spin systems, discussed for long time in statistical mechanics by various numerical methods. The crucial step was made by M.Creutz [4], who has shown correct beha-

viour of the Wilson loop in the continuum limit. During last few years many calculations were done by this method, see e.g. reviews [5].

However, as it often happens at the discovery of a new approach, the desire to obtain results as soon as possible goes ahead of real understanding of the accuracy obtained. It should be stressed, that in QCD there exist no competing theoretical method to compare with. Experimental data are not directly relevant because of several reasons, in particular, due to the (completely uncontrolled!) neglect of virtual quark fields.

We think that it is reasonable to start with the most difficult problem of physics, and it is much more reasonable to consider first several examples of increasing complexity in which the results are known. This is the main aim of the present paper.

The first step in this direction was made by Creutz and Freedman [6], who has considered linear and nonlinear oscillators. However, they do not consider methodical questions in details, using these problems just for illustration of the essence of the method to wide audience*.

In the present paper we discuss the following questions. After the introduction and discussion of the method used (§ 2) we consider nonlinear two-well oscillator in § 3. We discuss methodical questions concerning the accuracy of the results obtained. We have found, in particular, rather nontrivial dependence on the discrete time step a in the case when the barrier penetration probability is low. We also present the comparison of our results with semiclassical formulae for level splitting and discuss their validity region and the mechanism of their breakdown.

However, the main interest of the method considered is related with its potential applications to systems with lar-

* By the way, it is written in short and clear manner, so it can really be recommended as an introduction to the subject.

ge number D of degrees of freedom, for which the straighforward methods based on Schrödinger equation evidently fail. It is easy to understand that using standard finite difference methods with about K steps over each variable, one has to consider K^D points, which is not practical at $D \gg 1$. Usually, people apply some simplifying assumptions like perturbation expansion, starting from some soluable system; variational methods; K-harmonic expansion etc. We think that if the method considered can be used, it provides the result in much simpler and direct manner starting from first principles.

In section 4 we discuss atomic systems. Starting from hydrogen atom we proceed to helium one and other ions with two electrons. The important methodical question discussed in this section is the behaviour of the trajectory, simulated by the computer algorithm, near the singular attractive center.

The atomic systems are very useful because their action is simple and well known, and the experimental values of the ground state energy are known with high accuracy. However, with more than 2 electrons we come across some difficulties connected with Pauli principle, or antisymmetrization of paths for identical fermions.

Therefore, we take as more complicated systems the light nuclei up to He^4, in which nucleons can be to some approximation considered as distinguishable. Unfortunately, the so called nuclear potentials are poorly defined, they are rather complicated (depend on spin and isospin; there are tensor and spin-orbital interactions etc.). In principle, all this can be included, but in the present paper we consider just some simple central potential, which is similar to Reid soft core one. After all, we are not so much interested in nuclei, but in the method ability to treat problems of such complexity.

In section 6 we consider the question of the calculation of the functional integrals in absolute normalization. We remind the reader, that the algorithms used generate only ensemble of paths suitable for calculation of average values, but not the partition functions themselves. However, average values are, generally speaking, derivatives of the statisti-

cal sum, so the integration over the suitable parameter solves the problem. The "integration constant" should, however, be known, which is the absolute value of path integral in some case. For example, considering Green functions, we know them in some cases, e.g. for free propagation. We demonstrate that such an approach really works, so that Green functions with various potentials can indeed be calculated by MC simulations.

Our conclusions and final comments are included in section 7.

2. The method

Our starting point is the famous Feynman formula, expressing the probability amplitude for some particle to come from point x_i to point x_f by the time t (the so called Green function) as the path integral:

$$G(x_i, x_f, t) = \langle x_f | \exp(-\tfrac{i}{\hbar} H t) | x_i \rangle = \qquad (1)$$
$$= \int \mathcal{D}x(t) \exp\{\tfrac{i}{\hbar} S[x(t)]\}$$

The first expression given in traditional terminology, using states vectors $|x\rangle$ and Hamiltonian operator H. The second one contains the action $S[x(t)]$ and the path integral $\int \mathcal{D}x(t)$ defined as follows. Let us split the time interval into N pieces with length $a = t/N$. The d-dimensional path can be approximately represented by $N \cdot d$ numbers, $x_\alpha(ka)$ $(k = 1, N;\ \alpha = 1, \mathcal{D})$. The limit of the integral over all of them at $N \to \infty$ is the path integral. Evidently, it should be defined with some N-dependent weight in order to be finite. These questions, as well as the derivation of formula (1), can be found in widely known text book by Feynman and Hibbs [1].

The first nontrivial step one makes is the transfer to imaginary time $\tau = it$, so that the oscillating weight $\exp\{\frac{i}{\hbar} S\}$ is changed to exponentially falling one, $\exp\{-S/\hbar\}$. Evidently, the latter is much easier to handle with. Moreover, such transformation reviels analogy between quantum and statistical mechanics, for in the latter one also

should calculate sums over all states of the system with the weight $\exp(-E/T)$, E being the energy and T the temperature. Note, that in imaginary time the sign of kynetic energy is reversed and the action now is as follows

$$S = \int d\tau \left[\sum_{\alpha=1}^{d} \frac{m_\alpha}{2} \left(\frac{dx_\alpha}{d\tau}\right)^2 + V(x) \right] \qquad (2)$$

After splitting of time into finite portions a, one can imagine some one-dimensional "cristal" with "spins", having their values in d-dimensional space. Using $\frac{dx_\alpha}{d\tau} = (x_\alpha[(k+1)a] - x_\alpha[ka])/a$ one observes that such spins are coupled to each other.

Now, as it will become obvious below, in order to make any useful calculation along such line one should consider $N \sim 10^2$, and simetimes much more. All traditional methods fail for evaluation of integrals with so many variables.

Explaining the methods actually used we first comment, that we do not directly calculate the integral, but generate an ensemble of paths $\{x(t)\}$ such that each one enters with the probability $\exp(-\frac{S}{\hbar})$.

The main idea of its generation is very simple and can be demonstrated with an example of only one variable $r \in [a,b]$, distributed with weight $W(r) \in [c,d]$. Let us choose randomly some r on $[a,b]$ and calculate $W(r)$. Then, we choose random ξ on $[c,d]$ and compare it with $W(r)$. If $W(r) > \xi$ the value of r is taken into ensemble, otherwise it is rejected. Repeating this many times we obtain the ensemble $\{r\}$ we need.

What this ensemble can be used for? Note, that if the rejected values of r are not recorded at all (as is really the case in real calculations), we are not even able to say what is $\int dr\, W(r)$.

The answer is that we can calculate average values of some functions $f(r)$ defined as

$$\langle f \rangle \equiv \frac{\int f(r) W(r)\, dr}{\int W(r)\, dr} \qquad (3)$$

by the direct ariphmetic average over $\{r\}$. If the functions

$f(r)$ are much simpler than $W(r)$, and we have many of them, such way of calculations becomes reasonable.

The next point is the crucial one, for it is connected with the main difficulty of the problem under consideration. In (N·d)-dimensional space of paths nearly all volume is occupied by some insignificant ones, for which the weight $\exp(-\frac{S}{\hbar})$ is small. Therefore, random generation of paths is not effective: nearly all of them will be rejected.

The main point is that only rather small <u>variations</u> of paths are randomly generated, so that the probability never decrease more than by factor of the order one.

For example, the Metropolis [7] algorithm used is formulated as follows. For one time moment $t_k = k \cdot a$ and one coordinate $x_\alpha(t_k)$ we generate the random shift Δx and calculate the change of action ΔS. If $\Delta S < 0$, the shift is accepted*). If $\Delta S > 0$, we compare $\exp(-\frac{\Delta S}{\hbar})$ with random $\xi \in [0,1]$ and accept it only if $\exp(-\Delta S/\hbar) > \xi$. Repeating this for each α and each k we have the so called iteration of the system. Repeating such iteration, starting from some arbitrary path, we observe the relaxation phenomenon: average values of all path parameters tend to some definite limits.

Two more technical comments [6], which can help the readers to write down their own programs for path generation. First, during the small time a the motion is of diffusion type so that $\langle(\Delta x)^2\rangle$ is proportional to a. Therefore, it is reasonable to make shifts to $|\Delta x| \lesssim const \cdot \sqrt{a}$. Second, if the shift Δx is not accepted, it is reasonable to try again several times [6], we have used $\overline{n} = 5 \div 30$.

Now, suppose the ensemble of paths $\{x(t)\}$ is ready. What it can be used for?

First, let us consider the limit of large imaginary time $\tau \to \infty$. From the standard decomposition of the Green function (1) over stationary states one finds

*) Note that it only cases with $\Delta S < 0$ be accepted, it will be the evident algorithm looking for the minimal action.

$$G(x_i, x_f, \tau) \underset{\tau \to \infty}{\simeq} \psi_0(x_f)\, \psi_0^*(x_i) \exp\left(-\frac{E_0 \tau}{\hbar}\right) \qquad (4)$$

where ψ_0 and E_0 the wave function and energy of the grownd state. The correction to (4) is $\exp(-\frac{\Delta E \cdot \tau}{\hbar})$, where ΔE is the energy gap up to the first excitation, and this explains how large τ should really be.

This consideration shows, that at large enough τ <u>our ensemble $\{x(\tau)\}$ is equivalent to grownd state wave function.</u> For example, the probability to find the particle between x and $x+dx$ in ensemble is $|\psi_0|^2 dx$, etc. All correlations fall as $\exp(-\frac{\Delta E \cdot \tau}{\hbar})$ along the system, so for large τ the end values x_i, x_f are rather insignificant.

Attempts to calculate the average energy over $\{x(\tau)\}$, or E_0, met [6] rather unexpected difficulty: the average value $\langle \dot{x}^2 \rangle = \langle \frac{(\Delta x)^2}{a^2} \rangle \simeq 1/a$ and it diverges at $a \to 0$. In [6] it is suggested to use another definition of kinetic energy, which is finite at $a \to 0$, but, according to our experience, incorrect. The most useful way of measuring energy is provided by the *Virial* theorem, so that

$$\langle E \rangle = \left\langle \left(\sum_{\alpha=1}^{d} \frac{1}{2} x_i \frac{\partial V}{\partial x_i} + V \right) \right\rangle \underset{\tau \to \infty}{\longrightarrow} E_0 \qquad (5)$$

The next point is that ensemble $\{x(\tau)\}$ allows to obtain information about lowest excited states as well. The method is completely identical to the widely known sum rule method [8] used in QCD. Let us consider some operators O_i and, for simplicity, assume their average value over grownd state be zero. Then their correlator at different time moments

$$K_{ij}(\tau) = \langle O_i(\tau)\, O_j(0) \rangle \qquad (6)$$

(by zero we mean here <u>any</u> time moment, using the homogeneity of time). It is easy to see that at large τ

$$K_{ij}(\tau) \to \langle 0|O_i|1\rangle \langle 1|O_j|0\rangle \exp(-\frac{\Delta E \cdot \tau}{\hbar}) \qquad (7)$$

so by measurements of correlators of different operators (say, with different angular momentum) we may find the lowest state energies and transition matrix elements.

The final point is the following comment. Using periodic boundary conditions $X_i = X_f$ and integrating over X_i one has

$$\int dx\, G(x,x;\tau) = \sum_n \exp\left(-\frac{E_n \tau}{\hbar}\right) \qquad (8)$$

which is the statistical sum of the system at temperature $T = \hbar/\tau$. Therefore, we can also obtain characteristics at finite T, and even simpler than at T = 0 because the corresponding τ interval is in such case reduced.

3. The nonlinear oscillator

The simplest problem of quantum mechanics is that of linear oscillator and in this case the related path integral is Gaussian and can be computed analytically. The Monte-Carlo simulations for this case are discussed in Ref. [6].

Another problem, being the subject of applications of quite different theoretical methods, is that of nonlinear oscillator. Especially interesting is the system with the action

$$S = \int d\tau \left[\frac{m x^2}{2} + c\cdot(x^2 - f^2)^2\right] \qquad (9)$$

which for $f^2 > 0$ have two wells, separated by some barrier. Penetration through such barrier, being studied from the early days of quantum mechanics, recently was often discussed in connection with similar phenomena in quantum field theory.

Note, that the action (9) contains parameters m,c,f and, together with the Plank constant $\hbar$ it becomes 4. The choice of mass, length and time units remains only one dimensionaless combination which is really relevant, let it be

$$\varkappa = \frac{4\sqrt{2}}{3}\,\frac{\sqrt{m}}{c\hbar}\,f^3 \qquad (10)$$

Numerical coefficient will be explained later, and now we only comment that large $\varkappa$ corresponds to classical limit. In what follows we put $\hbar = c = 2m = 1$.

The first set of our calculations refers to ground state

energy dependence on $\varkappa$, and the results are displayed at Fig. 1. We have also shown results of other calculations, such as numerical diagonalization of the Hamiltonian [13] and previous MC simulations [6]. All results are in reasonable agreement.

Using this set of calculations, for which the results were known beforehand, let us consider the questions concerning the accuracy of MC method. The main parameter in this case is obviously the number of points N needed. At one hand, $a = \tau/N$ should be much smaller than the typical time of oscillation; $a \ll 1$; on the other, τ should be large compared to it: $\tau \gg 1$. Therefore, N should be about 10^2–10^3 or more.

The calculation consists of two different phases: relaxation and measurements. During the former phase all averages tend to some limiting values, while during the latter one they fluctuate around them. With a big enough statistical ensemble such fluctuations are averaged out.

Therefore, the question concerning accuracy can be split into three distinct ones:

1. How many iterations are needed in order to reach reasonable equilibrium?
2. How long one should continue the measurements?
3. What is the remaining systematical error, introduced by the discrete time approximation?

It is clear, that with the total computer time fixed the optimal strategy is such that all three types of errors should be comparable.

Using a varying from 0.05 to 1 with similar number of points we did not find significant variations of the relaxation time*). In all cases 200 of iterations was sufficient to start measurements.

The second question concerning statistical accuracy is simple in principle: with K independent trajectories the relative statistical error is $K^{-1/2}$. The question is then how many iterations are needed in order to obtain independent trajectory. Note, that each coordinate moves randomly with average

*) Unless the initial conditions are too bad, when small a case is in obvious disadvantage: it can not produce big alterations from one iteration to another one.

square shift $\langle(\Delta X)^2\rangle \sim a$ per step. Clear, that with about $1/a$ steps $\langle(\Delta X)^2\rangle$ will be $\mathcal{O}(1)$ and therefore trajectories become independent.

The last point, concerning the systematical error, is most difficult, and it was studied "experimentally". Surprisingly, we find the situation completely different for small and large $\varkappa$ values (small and large barrier, respectively). The results, shown at Fig. 2, represent the values of the ground state energy $E_0(\varkappa)$ versus the step length a. It is seen, that the low $\varkappa = 1.3$ case is connected with relatively small errors even for $a = 0.5-1$, while for $\varkappa = 5.4$ the values obtained with so large a are completely wrong!

The suggested explanation is as follows. Large $\varkappa$ means large barrier with very low penetration probability. However, if a is a large enough the system can penetrate through the barrier by one step, so that there are no points of the descretized trajectory which are under the barrier. As a result, the barrier is somehow lost and, instead of going through it, the particle just "jumps over" it. Respectively, the energy is strongly reduced.

This unwanted phenomenon can well happen also in QCD calculations on the lattice. As it is shown in the phenomenological analysis [9] of instanton-type fluctuations, their typical size is about 0,3 fm which is just of the order of step values used in calculations. Therefore, the real accuracy of these calculations should be questioned. Unfortunately, in this case it is not technically possible to reduce a by an order of magnitude, as it is done at Fig. 2.

One can check that such "jumps" over the barrier is indeed the main source of the errors, displayed in Fig. 2, proceeding in the following way. Let us make the path to be continuous, approximated by straight lines between neighbouring X_k. Evidently it makes the algorithm to be more complicated: instead of $a(V(x'_k)-V(x_k))$ one has some integrals depending not only on old and new values, X_k and X'_k, but on X_{k+1}, X_{k-1} as well. However, the continuous path exclude "jumping" over the barrier discussed above.

In Fig. 2 we demonstrate our results of such a calculation, shown by triangles. It turns out that no dependence on a is seen in this case up to $a = 0.5$. The ground state energy agrees with the exact one up to several percent.

Now we proceed to more detailed discussion of the barrier penetration in nonlinear oscillator. As it was shown in [10], it can be described in the semiclassical approximation by the trajectory with minimal action, leading from the bottom of one well to another. Such trajectory, the so called "instanton" (or "kink"), is then the solution of (imaginary time!) equations of motion and can easily be found

$$X_{cl}(\tau) = f\,\mathrm{th}[2f(\tau-\tau_0)] \tag{11}$$

as well as the corresponding action

$$S[X_{cl}] = \frac{4}{3}f^3 = \varkappa \tag{12}$$

Now, the numerical factor in (10) becomes clear.

The qualitative picture of the trajectory at large $\varkappa$ looks as follows: it consists of long periods of oscillations near the bottom of one of the wells, and rare instantons separated by distances proportional to $exp(\varkappa)$. In order to find the instanton density explicitly, one should integrate over quantum fluctuations about the classical solution (11). This integration is nontrivial because of zero translational mode and the interested reader should consult to papers [10-12]. The result looks as follows

$$\frac{dn}{d\tau_0} = 8\left(\frac{6}{\pi}\right)^{1/2}\left(\frac{3}{4}\right)^{5/6} e^{-\varkappa} \tag{13}$$

where we have included both instantons and "antiinstantons" i.e. the backward transitions.

The main effect caused by the instantons is evidently the splitting of energy levels, otherwise being doubly degenerate: The instructive way to look at this problem, suggested by Polyakov [10], is to connect it with coordinates correlator

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

Without the instantons it tends to f^2 at $\tau \to \infty$, but instantons destroy correlations and $K(\tau)$ behaves as $exp(-\Delta E \cdot \tau)$ where ΔE is the splitting between symmetric and antisymmetric states.

Assuming the positions of the instantons to be random (the so called dilute gas approximation, DGA) one can easily calculate $K(\tau)$ and find that

$$K(\tau) = f \exp\left(-\frac{dn}{d\tau_0}\cdot\tau\right) \qquad (15)$$

Therefore, the energy splitting is just equal to the instanton density:

$$\Delta E = \frac{dn}{d\tau_0} \qquad (16)$$

Since in our calculation below we discuss the accuracy of (13,15), it is reasonable to compare these relations with those obtained from "standard" WKB solution of Schrödinger equation

$$\Delta E = \frac{\omega}{\pi}\exp\left(-\int_{-x_0}^{x_0}(2m|E-V(x)|)^{1/2}\,dx\right)$$
$$\omega^{-1} = \frac{1}{2\pi}\left(\frac{m}{2}\right)^{1/2}\int_{x_0}^{x_1}\frac{dx}{(|E-V(x)|)^{1/2}} \qquad (17)$$

It turns out that at $x_0 \to \infty$ this agrees with (13), but only if quadratic interpolation formulae are used near the turning point. The ordinary linear ones, connected with Airy function, are wrong by the factor $\sqrt{\frac{\pi}{8}}$ [11]. At the same time, (17) contains the nontrivial dependence on x due to modification of instantons by the nongaussian fluctuations around them, so (17) works up to much smaller x than (13,16).

Our MC calculations of the correlator $K(\tau)$ allows to check the relation (15). Some results, shown at Fig. 3, clearly demonstrate that exponential behaviour is in fact valid only at large $\tau > 1$. The fitted values of the slope at large τ, identified with ΔE, is shown at Fig. 4 together with theoretical expressions (13,16 and 17); and also with the very accurate

numerical calculation [13]. We have used $\alpha = 0.1$, $N = 150$ and about 10^3 iterations*). The accuracy is certainly not worst than several percent over the whole region.

We have also measured directly the instanton density, calculated from the number of times when X changes sign. The results are also shown at Fig. 4. They follow closely the trend of $\Delta E(x)$, but are about 20-30% higher. The reason for it can best be demonstrated by the distribution of the relative instanton spacing D, shown at Fig. 5. For random instanton position such distribution should be

$$\frac{dn}{d\mathcal{D}} \propto \exp\left(-\mathcal{D}\frac{dn}{d\tau_0}\right)$$

While experimentally we observe significant enhancement over the exponential tail. We have also observed other manifestations of such instanton attraction, in the form of clusters containing several close instantons at the probability level well above any statistical fluctuations. Note also similar behaviour of the correlator shown at Fig. 3.

The physical nature for such attraction is evident: if the trajectory do not reach the bottom of the second well and soon returns to the first one the action is smaller than $2x$. We did not find any repulsive core for the instanton interactions, on which there are speculations in the literature.

The closely bound instanton-antiinstanton pair is not effective in breaking of correlations, therefore ΔE is somehow smaller than $\frac{dn}{d\tau_0}$. Such deviations from the DGA relation (16) are present even at large enough x, but they do not spoil the whole approach based on instantons. As it is demonstrated by Fig. 4, the gaussian relations (13),(16) have accuracy of several percent only at $x \gtrsim 5$–6, while the picture of modified instantons (the WKB estimates 17) holds up to

*) This is several times larger than needed for the measurements of the ground state energy. The reason is that at large τ the correlator is small and sensitive to small "islands" on the trajectory where the instanton density is still below the equilibrium value.

$\varkappa \sim 3$. Presumably, proper account of the instanton interaction discussed above can lead to reasonable results up to $\varkappa \sim$ 1÷2.

Better understanding of these questions is important, for they are analogous to those in QCD. Although we do not have any external parameter (like $\varkappa$) beforehand, phenomenology tells us that due to some reason instantons with action equal to several unites are really important, therefore, we have to develop appropriate methods to treat them. Unfortunately, the instanton interaction is much stronger in 4 dimensions than in the one-dimensional example of nonlinear oscillator.

4. Atomic systems

As we have emphasized in the Introduction, the advantage of the method considered is connected essentially with its applicability to multidimensional systems. Quite naturally then to apply it to atomic systems, in which the interaction low is simple and well known

$$V = -\sum_i \frac{Z}{R_i} + \sum_{i>j} \frac{1}{R_{ij}} \qquad (18)$$

Here Z is the charge of nuclei, R_i and R_{ij} are distances of the i-th electron from the nuclei and the j-th one, respectively. In this section we use atomic unites in which $\hbar = e = m = 1$.

In MC calculations of atomic systems we have found some phenomena, looking rather puzzling from the start.

First, we have observed the falling of trajectory into the Coulomb center. The reason can, however, be simply explained. Imagine some discrete trajectory (or sequence of $\vec{X}(t=\kappa a)$) going near the centre. The shift of one of the points $\vec{X}_k \to 0$ results in greater probability: the integral $\int d^3 x_k \exp(+\frac{Z}{|\vec{X}_k|})$ evidently diverges at $\vec{X}_k \to 0$. So, the potential should be made smooth at small enough distances in order to make the integral convergent. Note, that the error due to such cut off vanishes together with $a \to 0$.

Besides, we have found that after the relaxation to correct values of energy, radii etc. seems to be reached, and we start measurements, the system suddenly can got to arbitrary large R, and such phenomenon persists in all (long enough) runs.

The explanation is as follows. Choosing the time interval τ to be finite, we work at some small but finite temperature $T = 1/\tau$. As far as the electron happen to be at R as large as $Z/R \sim T$, in the case of periodic trajectory boundary conditions it has good chances to leave the system. In other terms, the statistical sum (8) is divergent untill we put the system in a box. In the particular case of Coulomb forces, this happens even with discrete spectrum, which contains infinite number of states. The obvious cure is to reduce T by large τ , to make a box big enough in order not to disturb the ground state wave function. It is also helpful is to get rid of periodicity, fixing the initial and final points near the nuclei, so that the ground state is mainly excited.

The first example, as usual, is the hydrogen atom. Of course, it is separable problem and angular variables can generally be singled out. However, we are interested in three-dimensional simulations of path, and we did it accordingly. The typical results are shown in Fig. 6 as the bound energy versus iteration number. The convergence to the correct value ($-1/2$) needs about 10^3 of iterations for $a = 0.2$, $N = 50$. The typical computer time at ES-1040 is about 10 min.

Similarly we have studied atoms with two electrons, or 6-dimensional system. Again, in principle 3 Euler angles can be singled out, but we did not do it. The results are also shown at Fig. 6 together with experimental values

$$E_H = -0.5\,, \quad E_{He} = -2.904\,, \quad E_{Be^{++}} = -13.656 \qquad (19)$$

For next atoms we have to consider two identical fermions, with proper antisymmetrization of paths. We did not attempt to develop an algorithm for such calculations.

5. Nuclear systems

Being interested in the test of the method for as many degrees of freedom as possible, we have also considered the nuclear systems. In such case spin and isospin of nucleons allows one to go up to He^4 nuclei without problems related with identical fermions. Note, that out of 12 variables describing the motion of four nucleons only 6 are really relevant, the other being the c.m. coordinates and angles of rotation of the system as a whole. However, we did not make these simplifications.

The evident problem with nuclear systems is the ambiguity of the nuclear potentials, which also are known to depend on total spin and isospin of the nucleon pair, spin orientation relative to position (tensor forces) and angular momentum (spin-orbit forces) etc. We did not included all such complications in our calculations and have used one common central potential

$$V_0(r) = 0.5\left[(R^2+0.1)^{-1} - 5\right]\cdot\left[R^4+0.18\right]^{-1} \qquad (20)$$

This expression was choosen rather randomly for its simplicity, for it is similar to Reid soft core potential. Writing the total potential $V = V_0 + V'$ (where V' is spin dependent, etc.) one can measure $\langle \exp(-\int V' dt)\rangle$ over the ensemble obtained without significant increase of computer time. We hope to return to this elsewhere.

The nuclear systems have their own particular features as far as MC calculations are concerned. This can best be explained by the introduction of some natural nuclear units, e.g. $\hbar = m_N = 1$, $\ell_0 = 1$ fermi. In this case the units of time is $\tau_0 \simeq 1.7\cdot10^{-23}$ сек and that of the energy is $E_0 = \hbar/\tau_0$ = 41 MeV, so that potential at distances of the order of ℓ_0 is of the order of unity. However, nuclear systems (especially H^2, H^3, He^3) are very loosely bound, with only few MeV of the binding energy or several percent of E_0.

Therefore, taking the value of τ about 10 units, as made in all calculations above, is not possible: this means temperature about 4 MeV which evidently is high enough to break

the nuclei in question. This is what really was observed, when we started the calculations: the nucleons were "Evaporated". Of course, the phenomenon have disappeared when τ was essentially increases up to τ = 50÷100.

Because of this, the total number of integrated variables for α particles (the values of $X_\alpha(\tau_k)$) have reached several thousends. Still the method was capable to handle them and, with about 1 hour computer time (at ES-1040) we have obtained reasonable relaxation. Some examples for He^4 are shown at Fig. 7.

6. Green functions

In this chapter we discuss the possibility to calculate the path integrals in absolute normalization, which is not directly given by the algorithm described in section 2 and applied above.

However, the average of some operators are the logarithmic derivatives of the statistical sums, therefore one can try to integrate them back. What is then needed is the integration constant, or the value of I in some particular case.

Let us consider such trick in the case of Green function, defined by the path integral (1). The Green function of the free motion is known.

$$G_0(\tau; x_i = 0, x_f = 0) = \left(\frac{1}{2\pi m\tau}\right)^{1/2} \qquad (21)$$

and the problem is to calculate such quantity G in some nontrivial potential. Let us introduce the new parameter η in the action

$$S_\eta = \int\left[\frac{m\dot{x}^2}{2} + \eta V(x)\right] d\tau \qquad (22)$$

It is to see that

$$\langle V\rangle_\eta = -\frac{\partial}{\partial\eta}\ln\int\mathcal{D}x\, e^{-S_\eta} \qquad (23)$$

where $\langle \dots \rangle_\eta$ is the average with the action (22). Integrating (24), one has

$$G = G_0 \exp\left(-\int_0^1 d\eta \langle V \rangle_\eta\right) \qquad (24')$$

As far as $\langle V \rangle_\eta$ is calculated as described above, the value of G is found. In such calculation it is useful to change slightly η from one iteration to another, so that new value of η practically does not need the relaxation process. So to say, we prefer to switch the potential adiabatically.

As the example of such calculation let us mention the Green function of the harmonic oscillator, which is explicitely known

$$G(\tau) = \left(\frac{\omega}{2\pi m \operatorname{sh} \omega\tau}\right)^{1/2} \qquad (25)$$

At the same time, it differs strongly from G_0 at sufficiently large values of τ. At Fig. 8 we have plotted (25) and (21) together with our calculations. The value of N = 25 was used, which is rather small, but even in this case the agreement is reasonable. Note, that the correction factor in (25) which is really calculated reach the values of the order of $10\text{-}10^2$. We have also tryed to calculate three-dimensional Green function. e.g. too Coulomb potential, and the results are reasonable as well.

7. Conclusions and discussion

In the course of the present work we have found the method of Monte-Carlo simulations with Metropolis algorithm to be indeed simple and effective. It is rather general (no restrictions for the potential type), very transparent and use nothing but first principles of the theory. We did not attempted to reach very high accuracy, but already with computer time 15-30 min at mediate power computer ES-1040 (about $5 \cdot 10^{6}$ op/sec) we have estimated the energies of atomic and nuclear systems with up to 12 degrees of freedom. It is quite

clear that such calculations based directly on Schrödinger equation are completely unrealistic.

Evidently, one can invent much wider applications of the method. To give an example not mentioned above, one may calculate probabilities of chemical reactions between complicated molecules, involving penetration through multidimensional barrier.

At the same time, we have found some unexpected features of this approach, showing that its application needs great care and should be well tested. Such situation is natural because the method is relatively new and not well understood so far.

As an example, let us mention those displayed in Fig. 2 and related with the simplest system considered, the nonlinear oscillator. At the values of $\alpha \sim 0.5 \div 1$ the relaxation takes place etc, but to completely wrong value of the energy! (See our explanation of this phenomenon as being due to "jumping" over the barrier in § 3). We think that even this observation alone is sufficient to raise question on the real accuracy of the results obtained by the lattice QCD. There are many barriers in the field configuration space and it was never demonstrated that their penetration is treated correctly, even in the case when the semiclassical methods are applicable.

And finally, there are also some limitations of the method, which are not so far overcomed. In particular, one should try to include identical particles, fermions or bosons, in order to start calculations for more complex systems. Another problem is the motion of relativistic particle, which contains the product of γ-matrices along the path which is not positively defined. Effective algorithm for such a case is not so far developed. We hope to return to these questions elsewhere.

In conclusion, we emphasize once more the simplicity and the great power of the method, especially for multidimensional quantum systems. We are sure that its wider practical applications are possible.

References

1. R.P.Feynman. Rev. Mod. Phys., 20, 367 (1948).
   R.P.Feynman, A.R.Hibbs. "Quantum mechanics and path integrals", McCraw-Hill, N.Y., 1965.
2. A.A.Belavin, A.M.Polyakov, A.S.Schwartz, Yu.S.Tyupkin. Phys. Lett., 59B (1975) 85.
3. K.Wilson. Phys. Rev. D10 (1974) 2445.
4. M.Creutz. Phys. Rev. Lett. 43 (1979) 533.
5. Yu.M.Makeenko, ITEP preprints N124-126, Moscow, 1982, P.Hasenfratz, CERN Preprint, TH, 3187, 1981.
6. M.Creutz, B.Freedman, Ann. Phys., 132, (1981) 427.
7. N.Metropolis, A.Rosenbluth, M.Rosenbluth, A.Teller, E.Teller. J. Chem. Phys., 21 (1953) 1087.
8. M.A.Shifman, A.I.Vainshtein, V.I.Zakharov. Nucl. Phys. B147, (1979) 385, 447.
9. E.V.Shuryak. Nucl. Phys. B203 (1982) 93, 116, 140.
10. A.M.Polyakov. Nucl. Phys. B120 (1977) 429.
11. E.Gildener, A.Patrascioiu. Phys. Rev. D16 (1977) 423.
12. A.I.Vainstein, V.I.Zakharov, M.A.Shifman. Uspekhi Fiz. Nauk 136 (1982) 554.
13. K.Banerjee, S.P.Bhatnagar. Phys. Rev. D18 (1978) 4767.

Figure captions

Fig. 1. The dependence of ground state energy of nonlinear oscillator on the parameter $\varkappa$. The solid line is the exact result [13], the circles are our results, and the crosses are taken from Ref. 6.

Fig. 2. The dependence of ground state energy of nonlinear oscillator on the time step a at $\varkappa$ = 5.46 and 1.33. Data O, ● are obtained by discrete point approximation of trajectory, while ∇ correspond to the continuous approximation between the neighbouring points (see text).

Fig. 3. The normalized correlator $\langle x(\tau)x(0)\rangle/\langle x^2\rangle$ versus the time difference τ. The points ● and O correspond to values of $\varkappa$ = 5.46 and 3.66, respectively, the straight lines are the corresponding exponential parametrization at $\tau > 0.7$.

Fig. 4. The energy splitting ΔE between the ground and first exited state versus parameter $\varkappa$. The upper curve corresponds to dilute instanton gas approximation, see eqs. (13,16) and the lower one presents the exact results, obtained in [6, 13]. The dashed curve is the "modified" WKB [13], given by eq. (17). The points ● and × show our Monte Carlo results for ΔE and the instanton density, respectively.

Fig. 5. The distribution of spacing D between the neighbouring instantons. The upper and lower plots correspond to $\varkappa$ = 1.33 and 5.46, respectively. The straight lines are the exponential parametrization at $D > 1$.

Fig. 6. The average energy of atomic system versus the iteration number.

Fig. 7. The calculated properties of nucleus He^4 versus the iteration number; K and U are the kinetic and potential energy, respectively.

Fig. 8. The linear oscillator Green function the lower curve is exact analitical result (25), while the upper one is the Green function for free particle. The points are our Monte Carlo results.

Fig.1

Fig.2

Fig.3

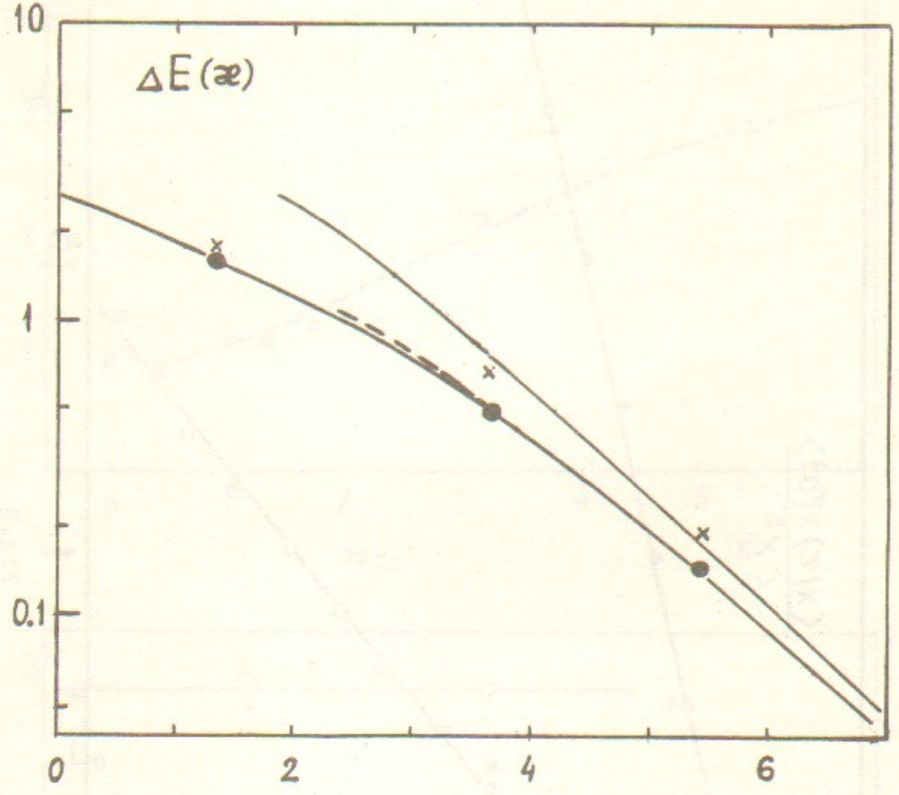

Fig.4

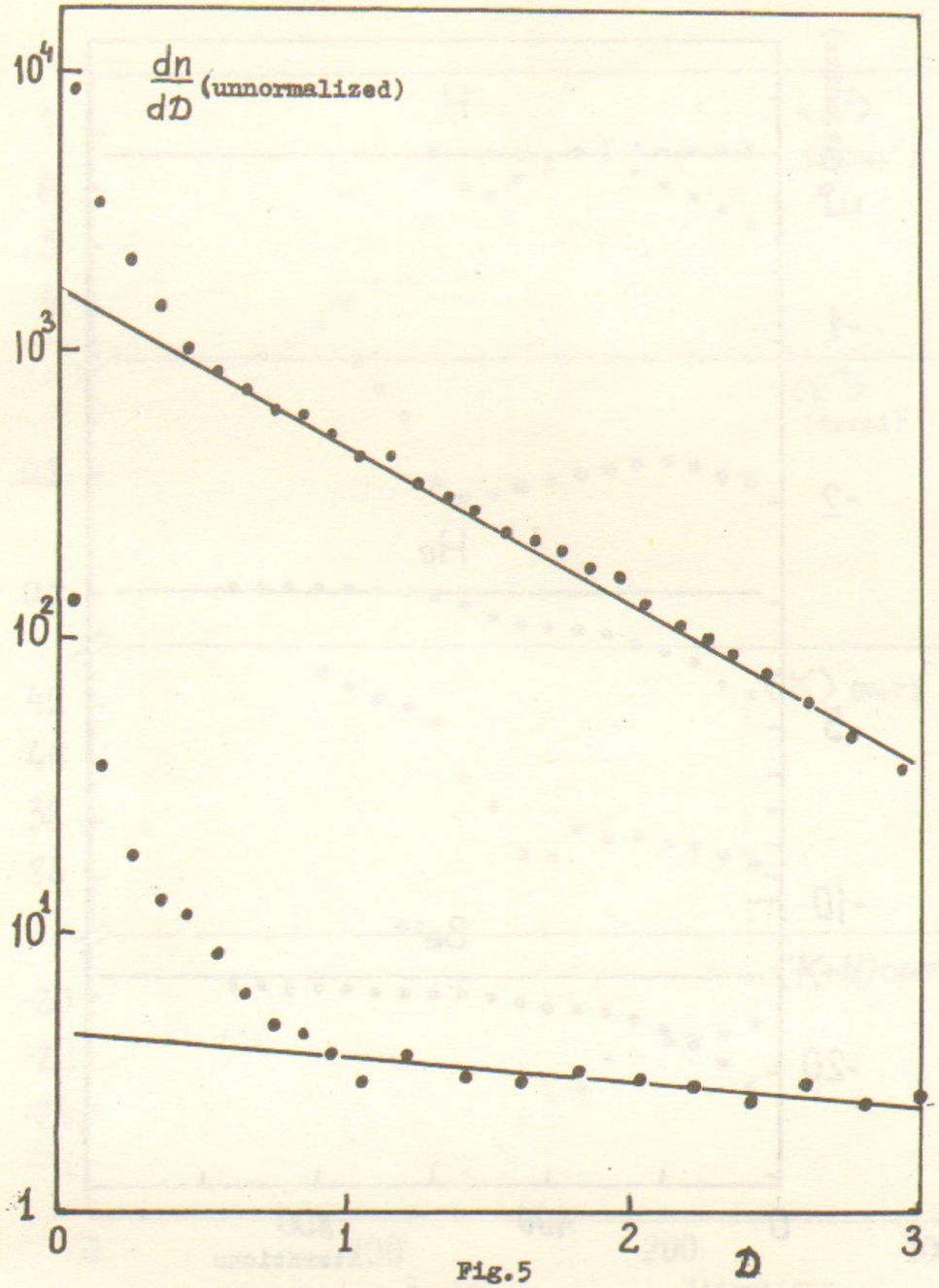

Fig.5

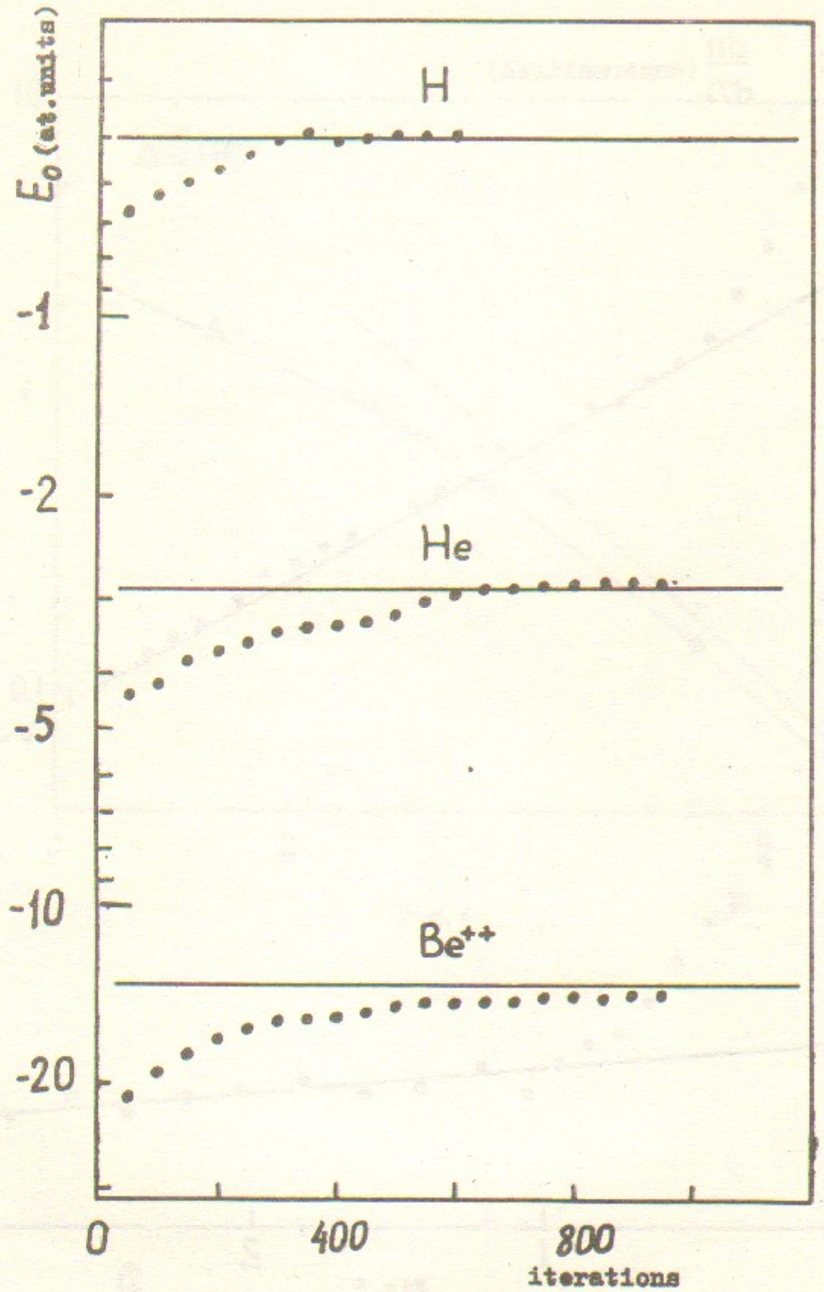
E_0 (at.units)
H
He
Be^{++}
-1
-2
-5
-10
-20
0
400
800
iterations

Fig.6

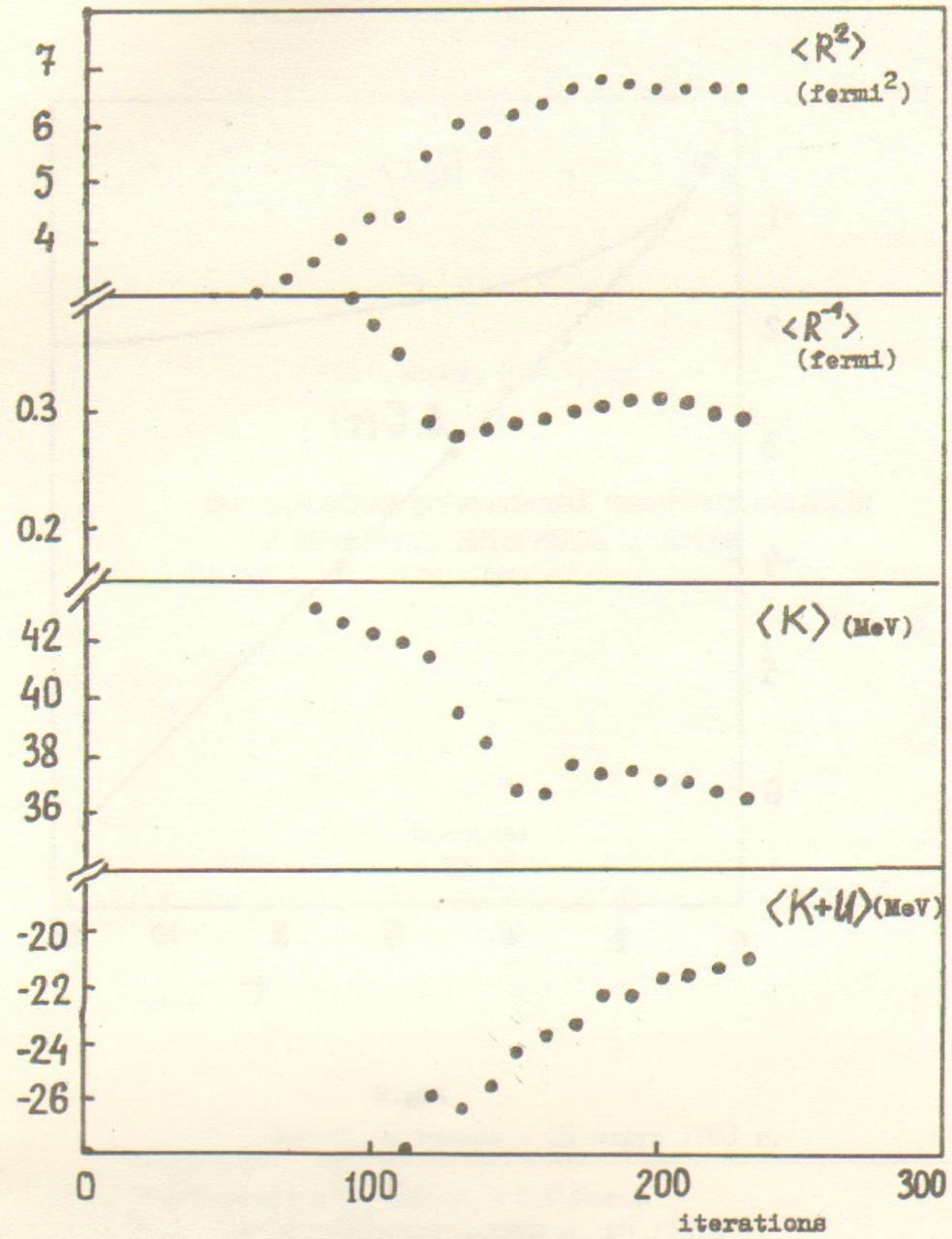
$\langle R^2 \rangle$ (fermi^2)
$\langle R^{-1} \rangle$ (fermi)
$\langle K \rangle$ (MeV)
$\langle K+U \rangle$ (MeV)
7
6
5
4
0.3
0.2
42
40
38
36
-20
-22
-24
-26
0
100
200
300
iterations

Fig.7

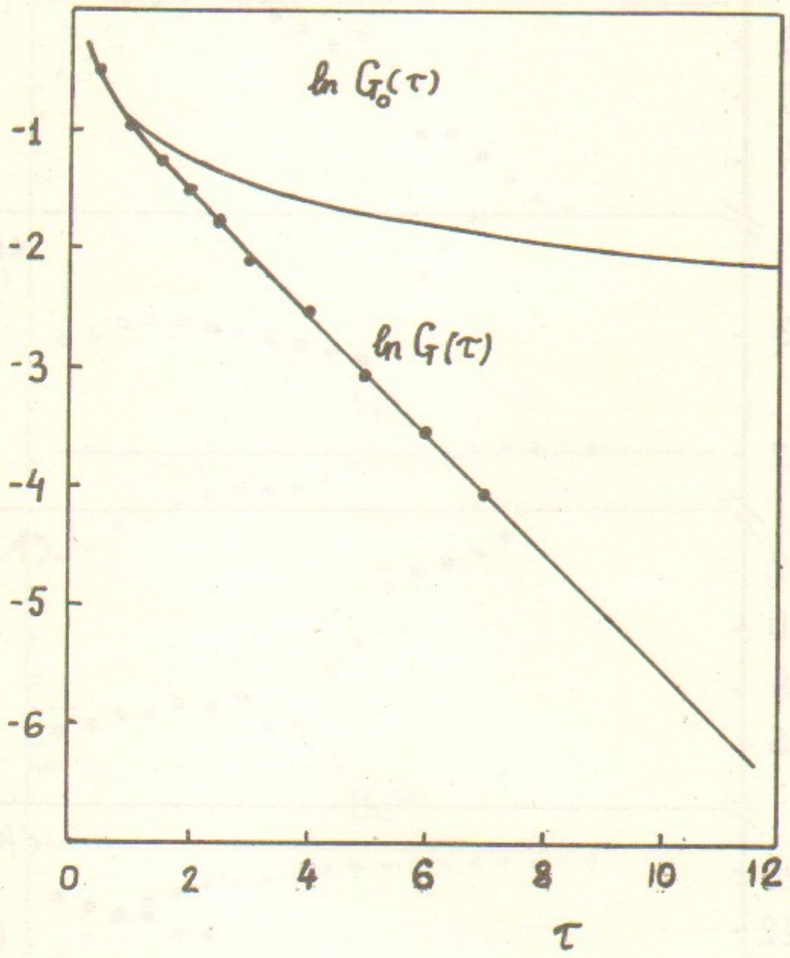

Fig.8

О.В.Жиров, Э.В.Шуряк

ФЕЙНМАНОВСКАЯ ФОРМУЛИРОВКА КВАНТОВОЙ МЕХАНИКИ И ВЫЧИСЛЕНИЕ ИНТЕГРАЛОВ ПО ПУТЯМ НА ЭВМ

Препринт
№ 83-47

Работа поступила - 25 марта 1983 г.

Ответственный за выпуск - С.Г.Попов
Подписано к печати 13.4-1983 г. МН 17515
Формат бумаги 60x90 1/16 Усл.2,3 печ.л., 1,8 учетно-изд.л.
Тираж 290 экз. Бесплатно. Заказ № 47.

Ротапринт ИЯФ СО АН СССР, г.Новосибирск, 90