ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

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QUANTITATIVE STUDIES OF TOPOLOGICAL EFFECTS IN QUANTUM FIELD THEORIES

1. TUNNELING IN QUANTUM MECHANICS

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Quantitative Studies of Topological Effects in Quantum Field Theories

1. Tunneling in Quantum Mechanics

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ABSTRACT

This paper starts a series of works devoted to topological fluctuations in quantum field theories. Main idea of the methods developed is the introduction of some effective theory for such fluctuations in terms of their collective coordinates. Introduction of such coordinates into functional integrals and methods for their evaluation in «small lattice» numerical experiments are explained using the simplest problem of the kind, one-dimensional static potential with two wells separated by a barrier.

1. INTRODUCTION

Nowdays «numerical experiments» with computers are widely used for studies of complicated systems in various branches of science. However, for a long time quantum physics was an exception because with traditional methods based on Schredinger equation even quantum systems with several nonseparable degrees of freedom (to say nothing on quantum fields) were considered as too complicated for practical computations, if no simplifying approximations are made.

The situation has rapidly changed few years ago, when more efficient methods of calculations were found, based on direct simulation of functional integrals. Even the particular results [1, 2] obtained so far for lattice gauge theories [3] have provided much more interesting information than it could be anticipated few years ago. The story just begins, existing algorithms are rather straightforward and there are general hopes that with further work one can develop much more effective numerical models for quantum fields. It has also became clear that field of applications of such methods can be essentially extended (see e. g. first calculations in quantum mechanics, including applications to simplest atoms and nuclei [4]).

Nevertheless, the primary goal of this program—to obtain quantitative description of four-dimensional gauge theories—is not reached so far, and in order to do this more ingenious methods are badly needed. There exist two main reasons for it. First, nonabelian theories in four dimensions are indeed too complicated for available computers, if one use straightforward lattice parametrization of the fields. As we demonstrate below, in order to obtain accurate values of local observables (to say nothing about correlation functions) the number of lattice sites N should be taken to be of the order of few hundreds, or even thousends even for simplest quantum-mechanical problems. Obviously, it is technically impossible to do so in four dimensions. The situation in QCD is especially difficult in this respect, because nonperturbative effects here range from scale of about 1 fermi (confinement length) to about 0.2—0.3 fermi (power corrections, presumably of instanton nature), see e. g. review [5]. In cal-

culations with available lattices of size about 10^4 one assumes from the start that there is only one scale of the correlation length and that, say, a factor 3 is large parameter. Thus, the results obtained are qualitative at best, and they can not be used but for exploratory investigations.

Another problem is even deeper. Suppose one day technical limitations are overcomed and one finds, say, the desired quantitative agreement with experimental hadronic masses. This will be triumph of science, of course, but we need not only numbers but also some insight into the underlying physics. It is true that computer data are much richer than experimental ones, but the standard way toward understanding based on development of some approximate simplified models can hardly be avoided in any branch of science.

Both reasons mentioned force us to reduce a number of parameters describing field configurations. The problem is how to do this. One (widely discussed) possibility is to use renormalization group methods [6]. Such approach has proved very useful in perturbative context, as well as in the theory of critical phenomena. In both these problems the fluctuations are rather similar at all scales, therefore «effective theory» differs with the original one only in some «renormalized» coupling constants. Nevertheless, it is clear on general grounds that such method can not work if the underlying physics rapidly changes at some fixed scale, so that effective theory at larger scale may look completely different from the original one.

In this series of works we study the possibility to construct some effective theory based on completely different principles. Main variables are now not the «block spins» or some other local field, but rather positions and parameters of some strong and «essential» fluctuations, for brevity called «fluctons». (This word was picked up from some different but related context. A.M. Baldin suggested it for configurations in which two or more nucleons in nuclei are very close together.) It is assumed that fixing parametrers of such fluctuations one can approximately reconstruct individual field configurations, at least its «most essential» features. This idea has many roots, in particular in solid state physics. For example, inelastic deformation, melting and other properties of crystals are attributed to dynamics of dislocations. Another obvious example of the kind is the domain walls: fixing their positions one in fact fixes field configuration in all space.

Such fluctuations happen in random places and, generally speaking, they are correlated. Therefore, an effective theory proposed reminds that for some liquid. Although numerical models in such case

are somewhat more difficult to put into efficient code (compared to «spin crystals» in lattice formulation), the economy in number of parameters is usually so great that it more than compensate for it. In particular, considering QCD applications for «instanton liquid» [7] (see also [8] and later papers of this series) one may compare them to nowdays lattice studies and find that the number of parameters (per unite four-dimensional volume) is reduced by huge factor about $10^4 - 10^5$. Even in the simplest problem considered in this work, about a thousend parameters describing the individual path is substituted by positions of just few instantons, again with essential computational economy.

In the present series of works we concentrate mainly on topological fluctuations, but, in principle, methods developed can be used in more general context and we sometimes consider it. The simplest example of nontopological fluctuation in quantum mechanical framework is just an occasion in which particle moves far into classically forbidden region and then returns. Such simplest «fluctons» are also studied below.

Topologically nontrivial fluctuations, or instantons, were first discovered for a number of theories in the framework of semiclassical theory by A.M. Polyakov with collaborators [9]. It was demonstrated that barriers separating topologically different configurations of the field (the so called «classical vacua») are penetrable. We postpone detailed description of these problems till next papers of this series, and now only outline the fundamental shortcoming of semiclassical approach. It is applicable if the action for classical configuration is sufficiently large

$$S_{class} \gg 1 . \tag{1}$$

This in turn means that tunneling probability P is very small

$$P \sim \exp(-S_{class}) << < 1 \tag{2}$$

so that it is not easy to confront it with any observable effects.

The main aim of the present work is to develop methods capable to describe tunneling phenomena outside the semiclassical context. The remaining condition is as follows

$$P \ll 1 \tag{3}$$

and it appears just because one should be able to tell tunneling event from «ordinary» quantum fluctuations. Although conditions (2) and (3) look similar, they are completely different from more

practical point of view. In particular, below we show, using the simplest example, that semiclassical theory is not reliable for P larger than, say, 1% level. Considering P in the range 1/3—1/30, we show that our methods work here reasonably well.

Two different approaches toward understanding of fluctons are possible. The most straightforward possibility is direct generation of configuration ensemble and its subsequent studies. Unfortunately, such «large lattice» calculations are not easy to perform because of technical limitations. Therefore we develop alternative approach, which, up to our knowledge, was not used before. Its main idea is to introduce certain auxilliary condition, ensuring existence of one (or more) «fluctons» with given parameters. For example, paths of some particle moving in the potential well comes via some distant point very rarely, but if one is interested in such fluctuation he may integrate only over paths with pass throgh it. The problem is to develop methods capable to estimate how often such events happen in real case, for the unbiased ensemble, and they are described and tested in the present work. Such methodical improvement may turn to be extremely useful in field theory context.

Because of technical reasons this work is split into several papers. First pair of them are devoted to topological effects in double-well system and the two-dimensional O(3) sigma model. Later we are going to consider four-dimensional SU(2) Yang—Mills theory without and with light quarks. (Some preliminary results on «instanton liquid» for pure gauge SU(2) theory are already published [8].)

2. TUNNELING IN THE DOUBLE-WELL POTENTIAL

From the very first days of quantum field theory it was obvious that traditional Schredinger formulation of quantum mechanics is hopeless in this context, so some other language was needed. Heisenberg operator formalism suits better, but only few problems can be solved on this way. After Feynman formulation was discovered it was for a long time limited to gaussian integrals, nevertheless it has produced such useful methods as Feynman rules, semiclassical theory etc. Nevertheless, for quantum mechanical problems this method was considered as some curious way of presenting known results, rather than a tool for practical computations.

The main aim of the present work is purely methodical, we are trying to develop a language natural for this formulation of quantum mechanics. Therefore we consider the simplest and well known example, the nonlinear oscillator with two wells. Its action (in Euclidean time $\tau=-it$) looks as

$$S^{(Euclidean)}=\int d\tau\left[\frac{m\dot{x}^2}{2}+K(x^2-f^2)^2\right]. \tag{4}$$

In what follows we use unites $\hbar=K=2m=1$.

Familiar methods based on Schredinger equation suggest that the ground state wave function has two maxima at $x=\pm f$ of about gaussian shape (harmonic approximation). Small «tails» of the wave function in classically forbidden region are described by familiar WKB formula

$$\Psi^{WKB}(x)=\text{const}\cdot\exp\left[-\int P_E(x)\,dx\right],\quad P_0(x)=(x^2-f^2). \tag{5}$$

What we are going to do below is closely related to these methods. We also separate small and large fluctuations, also consider gaussian approximation and test its accuracy in a number of ways. However, an object of our discussion is not the ground state wave function but the path ensemble $\{x(\tau)\}$. It describes not only the coordinate distribution in the ground state but also many other dynamical properties of the system. Let us remind that such ensemble is generated according to famous Dirak—Feynman expression for the Green function (or transition amplitude)

$$G(x_i 0|x_f \tau)=\int_{x(0)=x_i}^{x(\tau)=x_f} Dx(\tau)\exp\{-S^{(Euclidean)}[x(\tau)]\}. \tag{6}$$

Writing standard decomposition over stationary states

$$G(x_i 0|x_f \tau)=\sum_n \Psi_n^*(x_i)\Psi_n(x_f)\,e^{-E_n\tau} \tag{7}$$

one can see that at large enough $\tau\gg 1/\Delta E$ the ground state dominates ($\Delta E=E_1-E_0$, it is the so called mass gap).

It is instructive to say the same thing also in terms of one-dimensional discretized «lattice» model with «spins» x_k at sites. Kinetic energy term is now the interaction of neighbouring «spins». «Large τ» means lattice long enough compared to spin correlation length, so that particular boundary conditions become irrelevant.

Our interest in the particular system (4) is related to the fact that it has in fact two different correlation lengths: τ_{osc}, the oscilla-

tion frequency, and τ_{tun}, the tunneling time. Relation between them can be written as

$$(P \ll 1) \qquad \tau_{osc} = P \cdot \tau_{tun} \ll \tau_{tun} \tag{8}$$

where P is the tunneling probability.

Special feature of this system is the symmetry in respect to coordinate reflection ($x \to -x$). At time periods $\tau \ll \tau_{tun}$ coordinates are strongly correlated in sign, but at larger time scale $\tau \gtrsim \tau_{tun}$ the tunneling mix them, restoring the symmetry of the ground state [10]. This manifests in the behaviour of the correlation function

$$K(\tau) = \langle x(\tau)\, x(0) \rangle \to \text{const} \cdot \exp(-\Delta E \cdot \tau) \tag{9}$$

connected with finite **«mass gap»** ΔE. Evaluation of such correlation functions, especially at large times, is the central point of numerical experiments with quantum field theories, therefore we pay special attention to this quantity in our calculations.

3. EXPERIMENTS WITH «LARGE LATTICES»

In order to define parameters of the discretized system to be studied in our numerical experiment one should write down the following sequence of conditions

$$a \ll \tau_{osc} \ll \tau_{tun} \ll T = Na\,. \tag{10}$$

Assuming that each strong inequality corresponds to one order of magnitude, one should take the lattice with the number of sites not smaller than a thousend! So, although we now deal with one-dimensional (mechanical) system, its straightforward numerical studies need rather large lattice. (Fortunately, for such simple system such conditions can really be satisfied, but not for field theories in more dimensions!)

Generation of path ensemble is done by standard Metropolis algorithm, its introductory presentation in this context is contained e. g. in refs [4]. We only mention that measurements of the correlation functions and other details to be considered below make it necessary to have much better ensemble than, say, for measurements of the ground state energy or the wave function. So, instead of hundreds of iterations as done in refs [4], we had to make up to 10^5 ones. (Again, it is technically difficult to do the same for field theories!)

In our studies reported in ref. [4 b] we have found some artifact, the «lattice instantons», being the instantaneous jump from one potential well to another, without a point under the barrier. For lattice step of the order 0.2 or so this phenomenon produce significant systematical errors, therefore in this work we both use smaller step and compare results for the following two lattice actions

$$S^{standard} = \sum_i [(x_i - x_{i+1})^2/4 + (x_i^2 - f^2)^2]\,,$$

$$S^{improved} = \sum_i [(x_i - x_{i+1})^2/4 + \int_{t_i}^{t_{i+1}} V(x)\,dt]\,. \tag{11}$$

(The latter corresponds to paths consistent in some set of straight segments, as shown in [4 b] it effectively kills «lattice instantons».)

Traditional question no.1 is the time-averaged distribution over coordinates in our ensemble, corresponding to the ground state wave function squared. Our «large lattice» results are shown at Fig.5 where they are confronted with other calculations to be specified below.

The nontraditional questions which are difficult to ask in ordinary stationary state formalism is how the fluctuations are developing in time. «Experimental» approach to it is based on selection of events in which, say, the particle reaches $|x|$ larger than some fixed value x(bound). Superimposing maxima of these fluctuations we obtain the average «flucton profile», examplified at Fig.1. Note that such fluctons are well localised in time and have typical «triangular» shape.

Fluctuations under the barrier ($|x| < f$) are specific for double-well system because there are in general four topologically distinct paths coming via some fixed point (see Fig.2). Two last cases are known as instanton and antiinstanton, two other cases in which the particle returns to the same well we call «fluctons». Unfortunately, with finite density of fluctuations (per unite time) it is not possible to make clear separation of these possibilities. For example, close instanton-antiinstanton pair can be called a flucton as well.

In order to give some meaningful definition of the instantons one should make use of the idea of two separate time scales (8). It simultaneously helps to get rid of «zitterbewegung» phenomenon, of very irregular and complicated behaviour of individual quantum paths (see Fig.3,*a*). In order to describe some gross features of the path it is tempting to make them more smooth. Let the averaging width τ_{av} is taken somewhere in between of the two scales

$$\tau_{osc} \ll \tau_{av} \ll \tau_{tun} \qquad (12)$$

ensuring that the results are practically independent on τ_{av} and the particular procedure used. (We have used gaussian expression

$$\bar{x}_i = \sum_k \exp[-(\tau_k - \tau_i)^2/2\tau_{av}^2]\, a/\sqrt{2\pi}\,\tau_{av} \qquad (13)$$

but it is not important.) For smoothed paths tunneling events are clearly seen (see Fig.3,*b*), while the unwanted narrow «spikes» which cross zero x are suppressed. Guiding by the «smoothed» paths we may locate positions of «true» instantons and measure their characteristics. As soon as condition (12) is satisfied they are reasonably stable, with uncertainty due only to unprobable configurations with too close fluctuations.

The most obvious question is the average instanton shape, shown in Fig.1. (To avoid misunderstanding we emphasize that it corresponds to original, not the «smoothed» paths.) One may also find the instanton density and consider their relative distribution in time. All these data should be explained by the theory to be considered below.

In our discussion above the existence of two scales was connected with the specific behaviour of correlation function (9), an analog of Green functions interesting in field theory context. Now we present relevant data and discuss this point in greater details. It is convenient to plot not the correlators by themselves, but their logarithmic derivative

$$F(\tau) = -\frac{d}{d\tau} \log \langle x(\tau)\, x(0) \rangle \,. \qquad (14)$$

Our results for $f = 1.4$ and 1.6 are shown at Fig.4. At small $\tau \sim \tau_{osc} = 1/\omega_{osc} = 1/4f$ this quantity is rather large: correlation is affected by «ordinary» oscillations. At intermediate τ it decreases: here the correlator is nearly constant, close to $\langle x \rangle_{one\,well}$ (averaged only over motion in one well). At large τ tunneling effects come into play and «mix » the correlation completely. Here $F(\tau)$ tends to constant, the energy gap, as is very clearly seen from these data. (Again, let me note that so clean exponential asymptotics was never observed in lattice data for field theories.)

Particular values of the parameter f used above correspond to tunneling probability P about 1/10 and 1/30, respectively. As we are going to show below, semiclassical theory is not capable to describe tunneling through so transparent barriers. Nevertheless, as it

follows from discussion above, the two time scales tunneling effects can clearly be separated from «ordinary» oscillations.

The last point we demonstrate in this section is the following statement: the «smoothed» paths correctly reproduce the long-range correlations, see points shown by stars at Fig.4. It is important for us because it is the «smoothed» paths which are parametrized by collective coordinates, positions of the instantons, and they are the basis of our effective theory.

4. SEMICLASSICAL THEORY

It is instructive to start with simplest fluctons in the simplest problem imaginable, the motion in some potential well in which fluctuations are just occasions when particle moves far into classically forbidden region. It seems very natural that in order to study them one may consider only paths which go through some fixed point. Being more definite, let us consider ensemble of paths satisfying the following three conditions

$$x(\tau_i) = x_i \qquad x(\tau_c) = x_c \qquad x(\tau_f) = x_f \,. \qquad (15)$$

The corresponding three-point amplitude $G(x_i|\, x_c|\, x_f)$ satisfies the following normalization condition

$$\int dx_c\, G(x_i|\, x_c|\, x_f) = G(x_i|\, x_f) \,. \qquad (16)$$

where $G(x_i|\, x_f)$ is ordinary two-point propagator. We are not interested in dependence of $G(x_i|\, x_c|\, x_f)$ on its ends: assuming that they are at distance much larger than the correlation length we forget about them and concentrate on the dependence on our constraint parameter, x_c. Note that under conditions $|\tau_c - \tau_i|\,, |\tau_c - \tau_f| > \tau_{tun}$ this dependence is proportional to the ground state wave function

$$\int dx\, G(x|\, x_c|\, x) \to |\Psi_0(x_c)|^2 \exp[-E_0(\tau_f - \tau_i)] \,. \qquad (17)$$

As always, semiclassical theory is based on the idea that most important paths are close to some «classical» one, providing extremum of the action. Starting with the simplest example, we show that such conditional extreme path for linear oscillator is just

$$x_{cl}(\tau) = \begin{cases} x_c \exp[-\omega(\tau - \tau_c)] & \tau > \tau_c \\ x_c \exp[+\omega(\tau - \tau_c)] & \tau < \tau_c \end{cases} \qquad (18)$$

The corresponding classical action is $S_{cl}=m\omega x_c^2$, and therefore we conclude that asymptotics of the ground state wave function is as follows:

$$|\Psi_0(x_c)|^2 \sim \exp(-m\omega x_c^2)\,. \tag{19}$$

Obviously, for this particular system this result is in fact exact, and (19) holds at all x.

For our double-well system it is also easy to find classical paths corresponding to the same conditions, say for $|x|<f$ it looks as ($f\,\mathrm{th}\,\tau_0=x_c$)

$$x_{cl}(\tau)=\begin{cases} f\,\mathrm{th}[-4f(\tau-\tau_0)] & \tau<\tau_0 \\ f\,\mathrm{th}[4f(\tau-\tau_0)] & \tau>\tau_0 \end{cases} \tag{20}$$

(see also Fig.2,*a*). The corresponding action is equal to

$$S_{cl}(x_c)=\frac{2}{3}x_c^2-2x_cf^2+\frac{4}{3}f^3\,. \tag{21}$$

Important particular solution is the instanton

$$x_{cl}(\tau)=f\,\mathrm{th}\,(4f\tau)\,. \tag{22}$$

Comparison of these configurations with flucton and instanton average shapes extracted from numerical data will be made below, see Figs 6, 7, and at Fig.5 we compare results following from (21) to data for the ground state wave function. An obvious conclusion about accuracy of these analytic results (in the region of parameters under investigation) is that they are qualitatively correct, but not very precise.

The next standard step is evaluation of quantum corrections in gaussian approximation, based on diagonalization of the arising quadratic form

$$x(\tau)=x_{cl}(\tau)+\delta x(\tau)\,,$$

$$S[x(\tau)]=S[x_{cl}(\tau)]+\int d\tau\,\delta x_i\,W_{ij}\,\delta x_j+\ldots \tag{23}$$

by standard decomposition into its eigenfunctions

$$x(\tau)=\sum_n C_n x_n(\tau)\,,$$

$$Wx_n(\tau)=\lambda_n x_n(\tau)\,. \tag{24}$$

Thus the so called functional determinant appears:

$$\int Dx(\tau)\exp\{-S[x(\tau)]\}=\exp(-S_{cl})\cdot(\det W)^{-1/2} \tag{25}$$

which is divergent and usually normalized to some other problem, for which the exact result is known. Taking the ratio of the corresponding Green function to that for linear oscillator one finds

$$G(x_i|x_c|x_f)=G_0(x_i|x_f)\,G_0(x_c|x_f)\exp(-S_{cl})\det\left(-\frac{\partial^2}{4\partial\tau^2}+\omega^2\right)(\det{}^c W)^{-1/2}, \tag{26}$$

where G_0 is Green function for harmonic oscillator

$$G_0(x_i|x_f)=\sqrt{\frac{m\omega}{2\pi\,\mathrm{sh}\,\omega\tau}}\exp\left\{-\frac{m\omega}{2\pi\,\mathrm{sh}\,\omega\tau}[(x_i^2+x_f^2)\,\mathrm{ch}\,\omega\tau-2x_ix_f]\right\}. \tag{27}$$

Note the subscript c (which means «constrained»): only paths satisfying (15) should be included in determinant calculation. Let us write down the constraint explicitly and show that it can be integrated away with the help of «zero mode», existing due to translational invariance

$$\int\prod_n dC_n\exp(-\lambda_nC_n^2)\delta(\textstyle\sum C_n x_n(\tau_c)-x_c)=\dfrac{1}{x_0(\tau_c)\sqrt{\det' W}} \tag{28}$$

the remaining «primed» determinant contains only nonzero modes. Not going into its calculation in general case we note that for instantons such determinant was calculated in ref. [11], renormalized by means of linear oscillator it leads to the following answer:

$$\det' W=1/12\,. \tag{29}$$

Resulting density of instantons (together with antiinstantons) is equal to [11]

$$d_G=8\sqrt{\frac{2}{\pi}}f^{5/2}\exp\left(-\frac{4}{3}f^3\right). \tag{30}$$

This theory is more complicated than WKB semiclassical theory, but it can be used for arbitrary number of variables. Second, it has absolute normalization, while (5) contains a constants which is defined by rather tedious consideration of the vicinity of «stopping point». (Advantage of the WKB expression, in its turn, is as follows: it can be used for any state, not only the ground one.)

So far we have used the constrained paths for determination of time-averaged x distribution, or the ground state wave function, but

now we address the question concerning the flucton density. For example, for simplest nontopological fluctons (at $|x|>f$) characterized by the maximum value x_{max} and position in time τ_c one may define it as follows

$$dn^{fluct} = P(x_{max})\, d\tau_c\, dx_{max}\,. \tag{31}$$

It is clear that at large enough $|x|$ where fluctons can be reasonably well identified some integral over their density is related with the ground state wave function considered above. Indeed, the probability to find particle at some coordinate x is the integrated density of sufficiently strong fluctuations divided by velocity $\dot{x}$ at which particle passes this point

$$|\Psi_0(x)|^2 = \frac{1}{\tau}\int_0^{\tau} d\tau_c \int_x^{\infty} dx_{max}\, P(x_{max})/\dot{x}(x_{max})\,. \tag{32}$$

This relation can be further simplified in the semiclassical limit. Writing the probability as

$$P(x_{max}) \sim \exp\left[-S_{cl}(x_{max})\right] \tag{33}$$

and expanding the classical action

$$S_{cl}(x_{max}) = S_{cl}(x) + m\dot{x}\,(x - x_{max}) \tag{34}$$

one can integrate over x_{max} and to write the final result in a compact form containing potential $V(x)$

$$P(x_{max}) \simeq 2V(x_{max})\,|\Psi_0(x_{max})|^2\,. \tag{35}$$

(We have used that energy is conserved at the classical path and that potential well bottom was taken at zero energy.)

5. THE GROUND STATE WAVE FUNCTION AND CONSTRAINED PATHS ON «SMALL LATTICE»

In this section we continue discussion of constrained paths, made in the preceeding section in gaussian approximation, with the account for nongaussian effects. Obviously, they are treated by some numerical methods, but now it is done in more economic way compared to straightforward «large lattice» calculations reported above. The reason for this is that we now study only the vicinity of one individual flucton, fixed by constraint, and therefore one strong

inequality (in fact, the most severe one) in (8) is not needed. This is what we call «small lattice» calculations.

The first natural thing to do is to generate path ensemble under the same conditions as done in the preceeding section and to check to what extent their average behaviour follows the classical prescriptions. Some examples of corresponding data for flucton and instanton shapes are shown at Fig.6, 7. Deviations are clearly seen, and they are due to nongaussian effects ignored in semiclassical approximation. In particular, $\langle x\rangle_{one\ well}$ is shifted by $(\delta x)^3$ term.

The next obvious step is to compare actions for these two calculations, numerical and semiclassical ones. Here one comes across two kind of problems, so to say ultraviolet and infrared ones. The former is connected with the fact that actions (11) contain kinetic energy which diverges at time step $a\to 0$, while the latter means that the action attributed to some localized fluctons should be separated from that of «ordinary» fluctuations, occuring all the time. Both problems is easier to handle if one evaluate not the total action but rather distribution of its density (or Lagrangian) distribution in time. The corresponding data are shown at Fig.8. The constant level corresponds to «ordinary» fluctuations, while the noticeable excess is due to constraint and is qualitatively similar to Lagrangian for classical trajectories (shown in lower part of the figure).

Data analysis reported so far is sufficient for conclusion that the semiclassical theory is not very accurate in the case under consideration. However, it does not provide any estimate for the main quantity of interest, the fluctuation probability. In order to do so one may, in principle, directly compare probabilities of the individual paths for our problem (the double-well system) with some «reference point», say the linear oscillator. Generating path ensemble for the latter system one may try to average the following factor

$$F_{path} = \exp\left(-\int d\tau\, \Delta V\right), \tag{36}$$

where ΔV is just the difference of potential energies. Note, that problems connected with divergent kinetic energy are gone, but, unfortunately, this factor fluctuates from path to path so strongly that it is practically impossible to make this averaging for system parameters under investigation, and one needs mone ingenious method.

This is a point where «adiabatic switching method» [4 b] comes into play, for it includes averaging of much less fluctuating quantity. Let us introduce a set of actions with some parameter alfa, interpolating between the two actions S_{osc} for linear oscillator and

S_{DW} for double-well potential.

$$S_\alpha = S_{osc}(1-\alpha) + \alpha S_{DW} = S_{osc} + \alpha \cdot \Delta V \,. \tag{37}$$

The average value of ΔV can be written as the logarithmic derivative of the statistical sum

$$\langle \int d\tau \, \Delta V \rangle_\alpha = -\frac{\partial}{\partial \alpha} \log \int Dx(\tau) \exp(-S_\alpha) \,. \tag{38}$$

Integrating this relation back one has

$$G_{DW} = G_{osc} \exp[-\int_0^1 d\alpha \, \langle \int \Delta V \, d\tau \rangle_\alpha] \,. \tag{39}$$

Evaluation of the integral in exponent of (39) can be done with (rather standard) trick: alfa value is gradually increasing and then decreasing again. The measured «histeresis cycles» (see examples at Fig.9) provide estimates of the magnitude of nonequilibrium effects. (Note, that using such method we get rid of them in first order.)

Application of (39) to calculation of wave function is straightforward:

$$|\Psi_{DW}(x_c)|^2 = |\Psi_{osc}(x_c)|^2 \exp[(-E_{osc} + E_{DW})\tau - \int d\alpha \, \langle \int d\tau \, \Delta V \rangle_\alpha] \tag{40}$$

Even simpler is to consider the ratio of probabilities to find particle at different coordinates

$$\left| \frac{\Psi_{DW}(x_1)}{\Psi_{DW}(x_2)} \right|^2 = e^{-m\omega(x_1^2 - x_2^2)} \exp[-\int d\alpha \, (\langle \int d\tau \, \Delta V \rangle_\alpha^{(1)} - \langle \int d\tau \, \Delta V \rangle_\alpha^{(2)})] \,. \tag{41}$$

(Note that in order to reproduce the wave function under the barrier one should include all types of paths shown at Fig.2. Using the language of wave function it means that two exponentials are added, for example in the center this effect increases the probability by the factor 4. In our statistical formulation the same result is due to existence of four topologically distinct «fluctons» (with equal probability at the center). This consideration is used for further reduction of the lattice size needed for wave function calculation, and our «little lattice» length can now be taken smaller than τ_{tun}. It was typically taken to be about 2 unites, therefore we were able to use very small lattice step $a = 0.05 - 0.01$ and to study relevant fluctuations with good accuracy.)

Combining expression (41) and our data for $\langle \int d\tau \Delta V \rangle_\alpha$ we have found results for the ground state wave function shown at Fig.5 by stars, to be compared to those found in «large lattice» numerical experiment. Although calculations correspond to completely different methods, different lattices etc., results reasonably agree.

6. NONGAUSSIAN EFFECTS AND THE INSTANTON DENSITY

In the present section we address the question of accuracy of semiclassical (gaussian) approximation for the instanton density (30). Again we use «adiabatic switching» of nongaussian effects, and the «reference system» is now chosen to be semiclassical (Gaussian) approximation. So, our interpolating action looks as follows

$$S_\alpha = S_G + \alpha G_{NG} \,;$$

$$S_{NG} = \int (4x_{cl}(\tau) \, \delta x^3 + \delta x^4) \, d\tau \tag{42}$$

and with its help we are able to evaluate corrections due to nongaussian effects to some amplitude, say to

$$G(x = -f, \tau | x = f, 0) \equiv \exp(-E_{DW}\tau) \, d_{NG} \, 4f \,. \tag{43}$$

Here the quantity d is, by definition, the instanton density (the lattice length, as usual, is assumed to be much longer than τ_{osc}). Combining this expression with similar one in gaussian approximation one may express the quantity d_{NG} to be

$$d_{NG} = d_G \exp(-\int_0^1 d\alpha \, \langle S_{NG} \rangle_\alpha) \,. \tag{44}$$

Note, that apart from correction to tunneling amplitude, the nongaussian effects also modify ordinary oscillations, making the contribution proportional to lattice length. In other terms, the ground state energy is shifted, and this effect should be accurately taken into account. In practice, calculations were done as follows. The presence of instantons was ensured by antiperiodic boundary conditions, and the measured integral effect of nongaussian effects was subtracted from results of similar «control» measurements with periodic paths. Our results for instanton density are given at Fig.10. In order to see more clearly the effect of nongaussian corrections we have plotted them as the ratio to predictions of gaussian approxima-

tion (30). It can be concluded from this figure that such corrections are really large enough for barriers considered, and, contrary to general belief, semiclassical approximation is not very reliable, unless the barrier penetrability is at 1% level.

It is important, that such method can be generalized to field theories in several dimensions, for which the role of nongaussian effects may be even greater than for the simple example considered in this work.

In calculation reported above the presence of the instanton was forced by antiperiodic boundary condition, but now we are going to discuss how one can locate them by some constraint, introducing a kind of collective variable—the instanton position. The simplest constraint possible (similar to that used in the preceeding section) just fixes the point at which paths cross zero. Formally it looks as the following trick: one introduces unity in functional integral

$$1 = \int d\tau_c \, \delta(x(\tau_c)) \, \dot{x}(\tau_c) \tag{45}$$

and then put the integral over τ_c outside. Note, that jacobian is now simply velocity at constrained point, and in discretized lattice approximation it is relevant for updating of only «spins» next to the fixed one at $\tau = \tau_c$. Such collective variable is much more convenient for numerical calculations than the one following from ortogonality to zero modes usually considered, because it is local in time. Another advantage is that jacobian contribution to the action $S = -\log(\dot{x}(\tau_c))$ is not very fluctuating from path to path: in the instanton center the motion is more close to classical one than in other places.

7. INSTANTON INTERACTIONS AND THE «INSTANTON GAS»

As usual, we start with «large lattice» unbiased data and consider some «experimental facts». Considering instanton interactions it is most reasonable to study their relative positions along the time axis. We remind that our definition of the instantons depends on existence of two distinct scales, so for close enough pairs such definition can not be unique. Respectively, the question of the instanton interaction at small distances can not have some absolute meaning.

For example, we compare two definitions. The first «naive» one calls the instanton each crossing of $x=0$ line, another does the

same but using instead of the original quantum path its «smoothed» versions (defined in section 3). The corresponding distribution over instanton separations are given at Fig.11. At small distances behaviour is indeed different. However, at larger separation $D \gtrsim 1$ both set of data are similar, producing good exponential behaviour

$$dn/dD \sim \exp(-D/\langle D \rangle) \tag{46}$$

typical for «ideal gas» of instantons with density $d = 1/\langle D \rangle$. This means that no long-range interaction is present, whatever is the instanton definition. This conclusion is easy to explain. Even in semiclassical framework the interaction at large distances is in this model exponentially small. (Note that it is not the case for field theories: here interaction is of power type and more important.) At intermediate distances one finds evidences for instanton-antiinstanton attraction (which is also quite clear theoretically, and even in agreement with simple estimates coming from evaluation of action for classical path with two points fixed), while at small D one observes some repulsion.

Is the ambiguity in the instanton interaction at small distances a serious defect? We have to remind that our main goal is to construct some effective theory dealing with parameters of fluctuations, say the positions of instantons. So, this ambiguity just means that such theory is not unique: one may obviously calculate functional integral introducing different sets of coordinates. (It is another question which one is more natural and leads to simpler calculations.)

Whatever is the definition of collective coordinate, one can fix their values and study constrained configurations. For example, the «zero crossing» prescription considered at the end of the preceeding section can well be used for arbitrary number of instantons, fixed at given places.

So, we may now formulate our final «effective theory» for long-range effects in the double-well oscillator. It is a gas of instantons with the following partition function

$$Z = \sum_n \int_{(\tau_1 < \ldots < \tau_n)} d\tau_1 \ldots d\tau_n (d_{NG}\tau)^n \exp\left[-\sum_i V_{int}(\tau_{i+1} - \tau_i)\right]. \tag{47}$$

Its main ingredients are the instanton density d_{NG}, considered above, and the instanton interaction $V_{int}(D)$.

It is just simple exercise to make a program generating ensemble of points τ_i, the instanton positions, according to (47). With simple step-function parametrization of the paths

$$x(\tau)=f\prod_{i=1}^{n}\bar{\theta}(\tau-\tau_i),$$

$$\bar{\theta}(\tau)=\begin{cases}1 & \tau>0\\ -1 & \tau<0\end{cases} \qquad (48)$$

one can indeed mimic correlation function at large times, provided that instanton density was correct. Introducing mediate-range attraction and short-range repulsion one may also obtain «more realistic» behaviour, similar to what is shown at Fig.11. We do not present here all these data because such questions are much more important in field theory context, for which we consider them in great details elsewhere.

9. CONCLUSIONS AND DISCUSSION

The main goal of the present work was development of theoretical methods for studies of fluctuations in various quantum systems. More precisely, we have tested these methods considering tunneling via one dimensional barrier.

The main conclusion of our investigation is that (contrary to some statements in literature and initial hopes) semiclassical theory is not sufficiently accurate unless tunneling probability P is at one per cent level. Otherwise, the tunneling paths have noticeably modified shape, and even much stronger modified probabilities. If it is the case for simplest imaginable problem, it can be so for instantons in field theories as well.

Positive methodical result of our investigation can be formulated as follows. Using special constraints ensuring the presence of fluctuations of interest we were able to pass from straightforward («large lattice») calculations to much more economic and simultaneously more precise «small lattice» ones. Properties of such fluctuations, their interaction etc. can be measured in such way, providing a basis for some «effective theory», the simplified model of the theory we have looked for. Its test is produced by measurements of various correlation functions, with subsequent comparison to other data.

This work may have also applications in many other fields, where penetration through some multidimensional barriers is of interest: say, in quantum chemistry, nuclear reactions etc. Some work in this direction is in progress.

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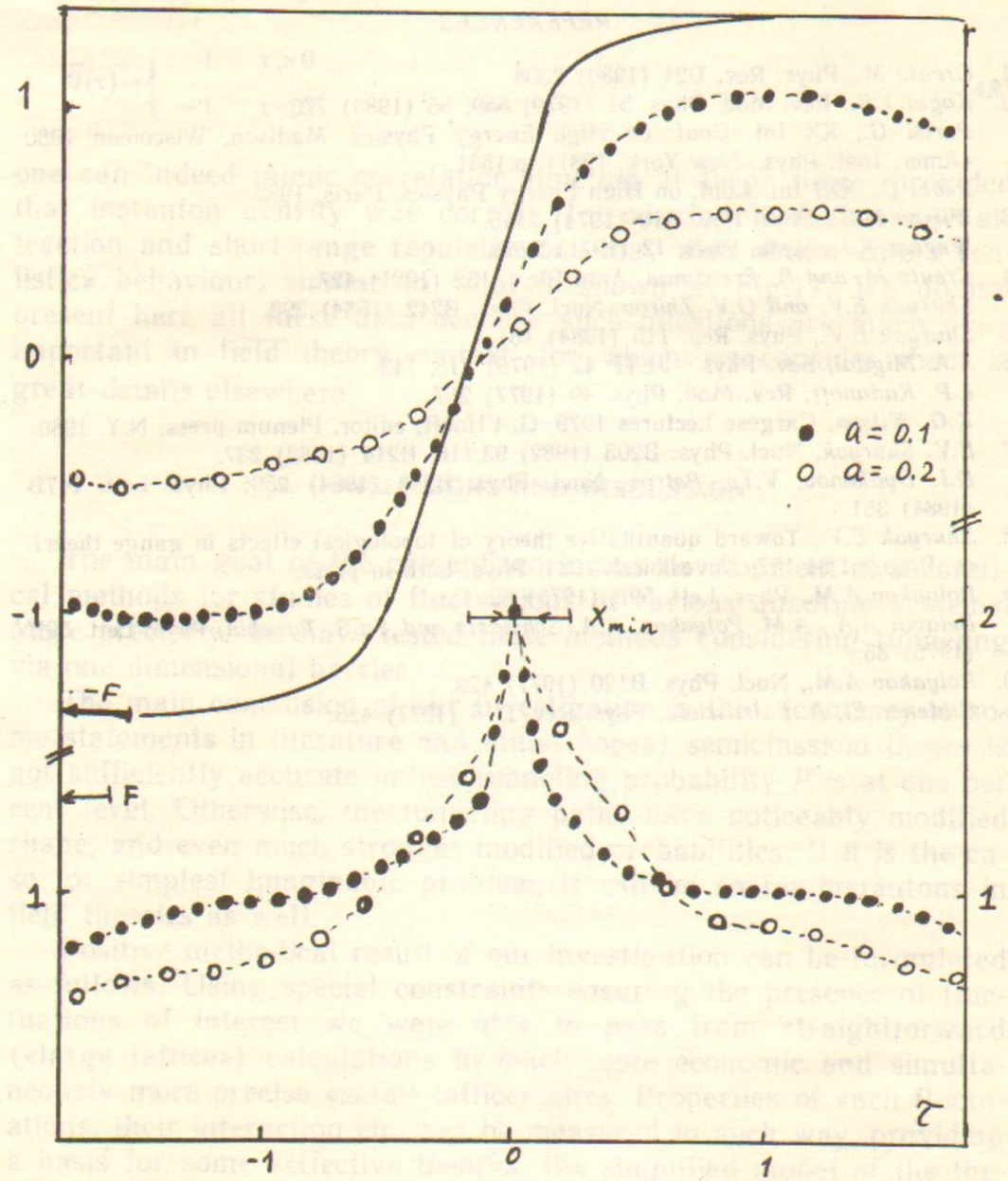

Fig.1. The average profile of instantons (upper part of the figure) and nontopological fluctons extracted from «large lattice» numerical experiment. The particular criteria for observing the instantons are discussed in the text. Fluctons are determined by the condition that at least one point of the path is at $x>2$. Calculation corresponds to lattice of length 40 with step 0.1 (closed points) and 0.2 (open points). The solid line corresponds to classical instanton configuration.

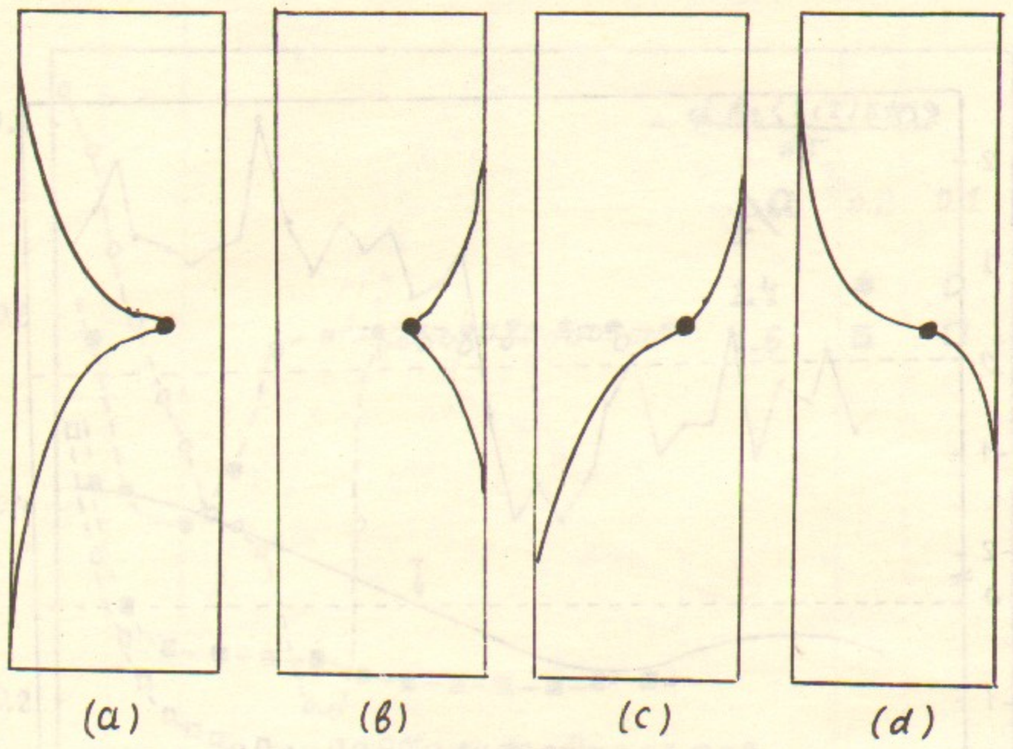

Fig.2. Four topologically different paths coming via the same point x under the barrier.

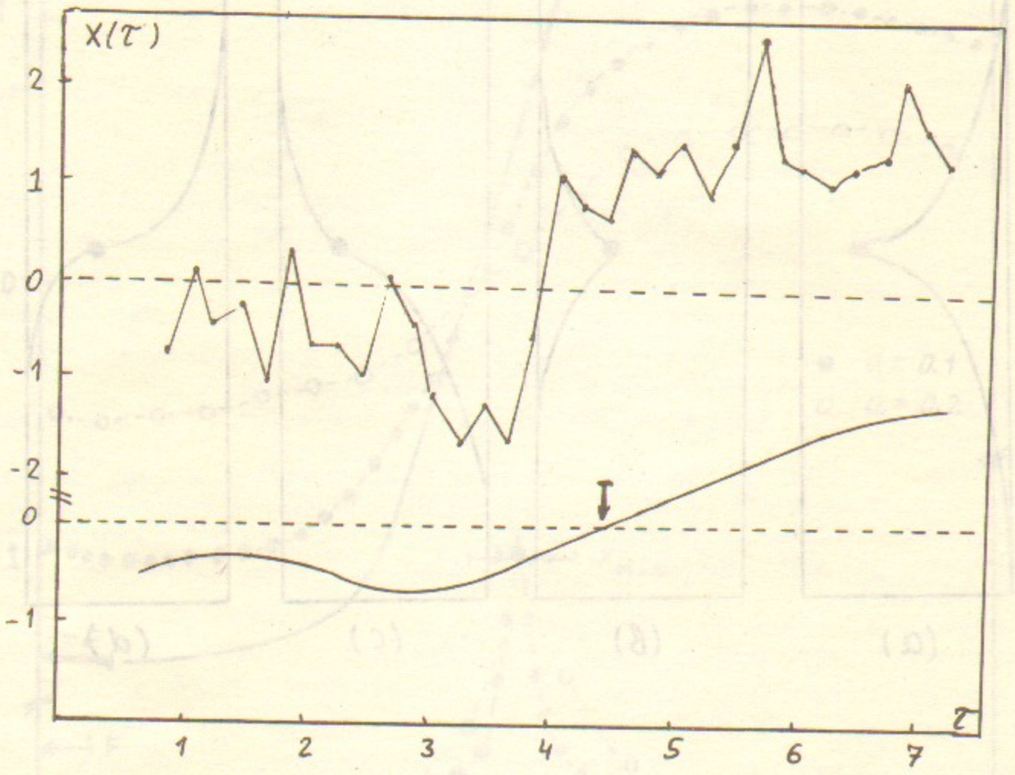

Fig.3. Some quantum path (*a*) and its «smoothed» version (*b*). An arrow shows the position of the instanton found with the help of smoothening, while auxilliary zero crossing at one-point level are disregarded.

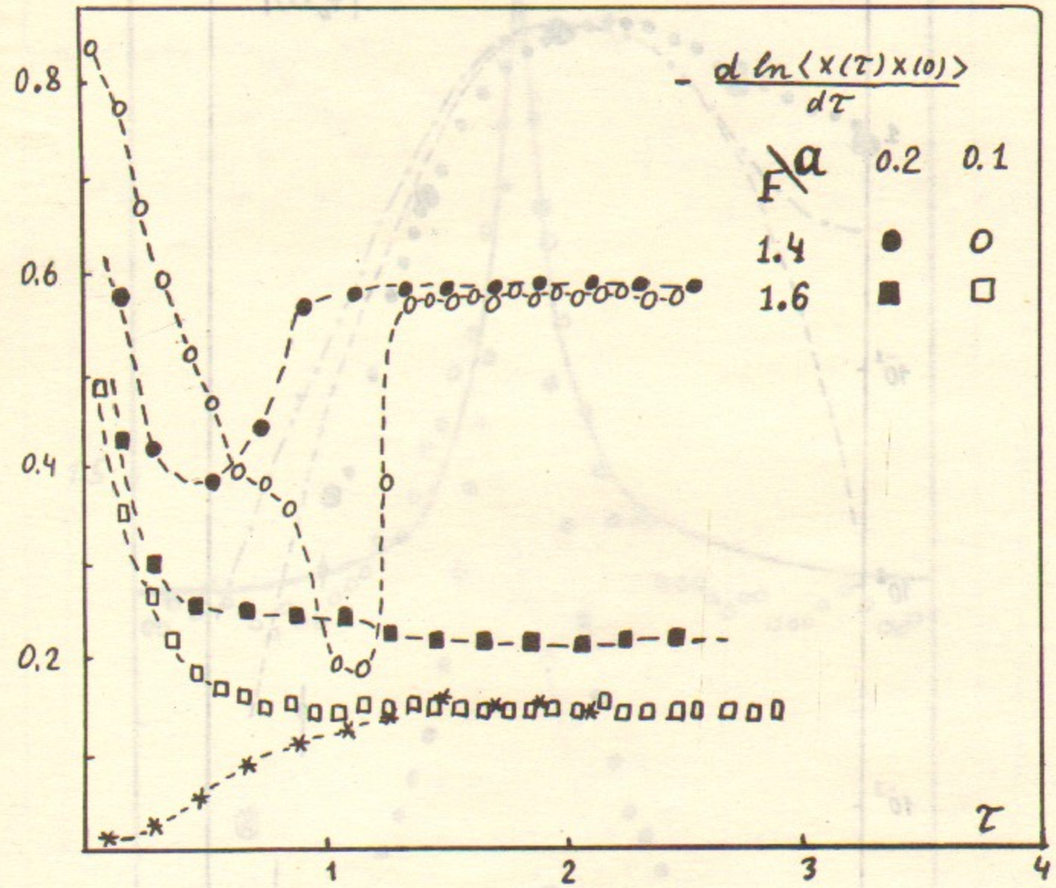

Fig.4. The logarithmic derivatives of the coordinate correlator. Parameter of the potential *f* and lattice step *a* are given at the figure. The dashed lines are only to guide the eye. Points shown by stars correspond to correlation of smoothed paths with width equal to 1.5.

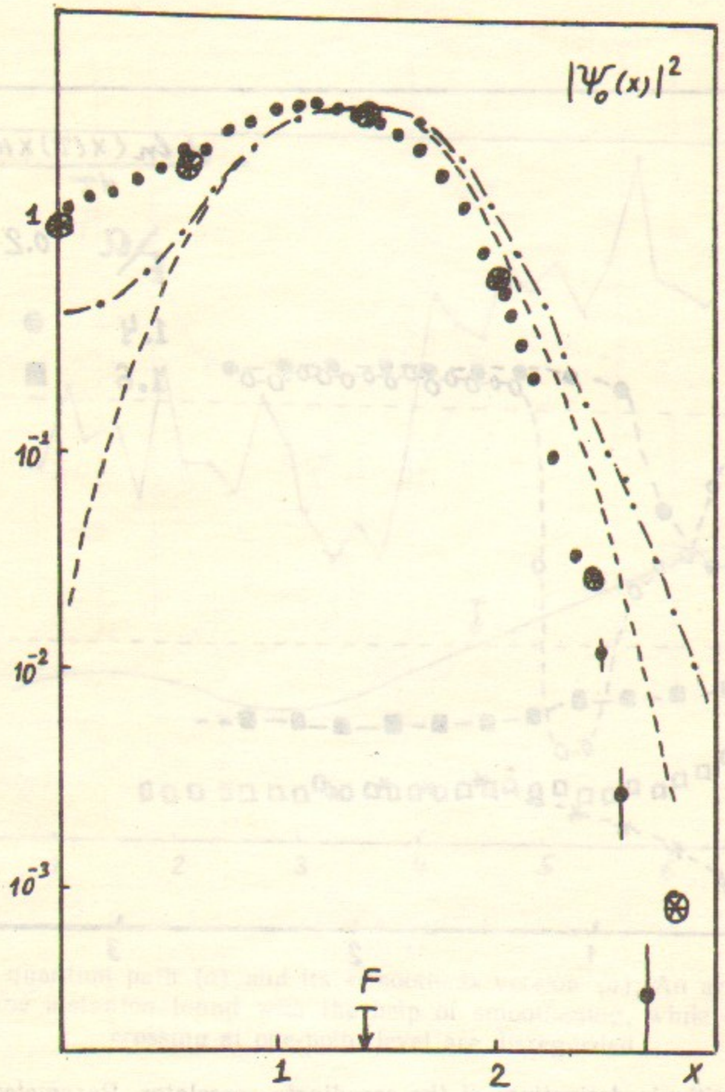

Fig.5. Time averaged probability to find the particle in some coordinate bin (or the ground state wave function squared) at $f=1.4$. The dashed and dash-dotted lines correspond to linear oscillator and to the sum of $\exp(-S_{class})$ for double-well potential for all types of the paths shown at Fig.2. Points shown by stars correspond to «adiabatic switching» method described in the text.

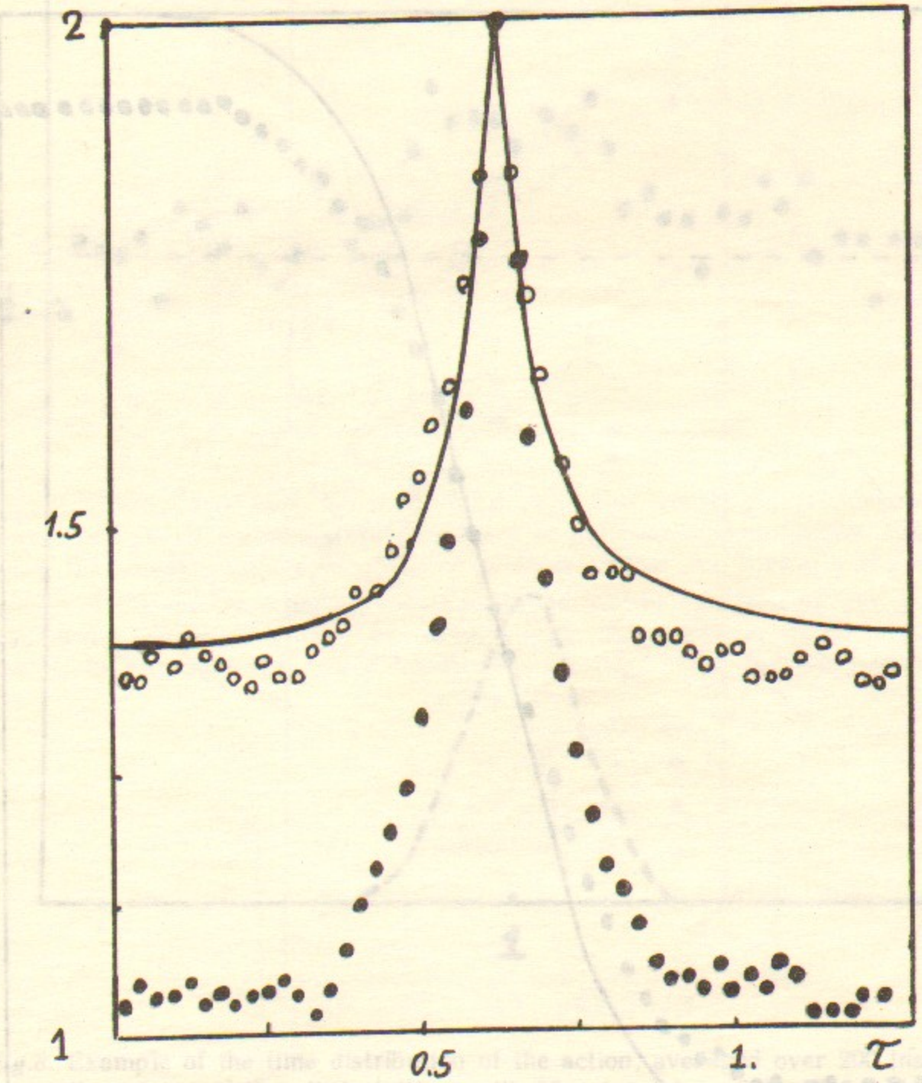

Fig.6. Example of the flucton profile at $f=1.4$ resulting from «small lattice» calculation with constraint at some point $x=2$. The curve corresponds to classical path, open and closed points are for linear and double-well oscillators, respectively. Calculation reported has very small lattice step $a=0.025$ and, unlike the data given at Fig.1, it is no more sensitive to it.

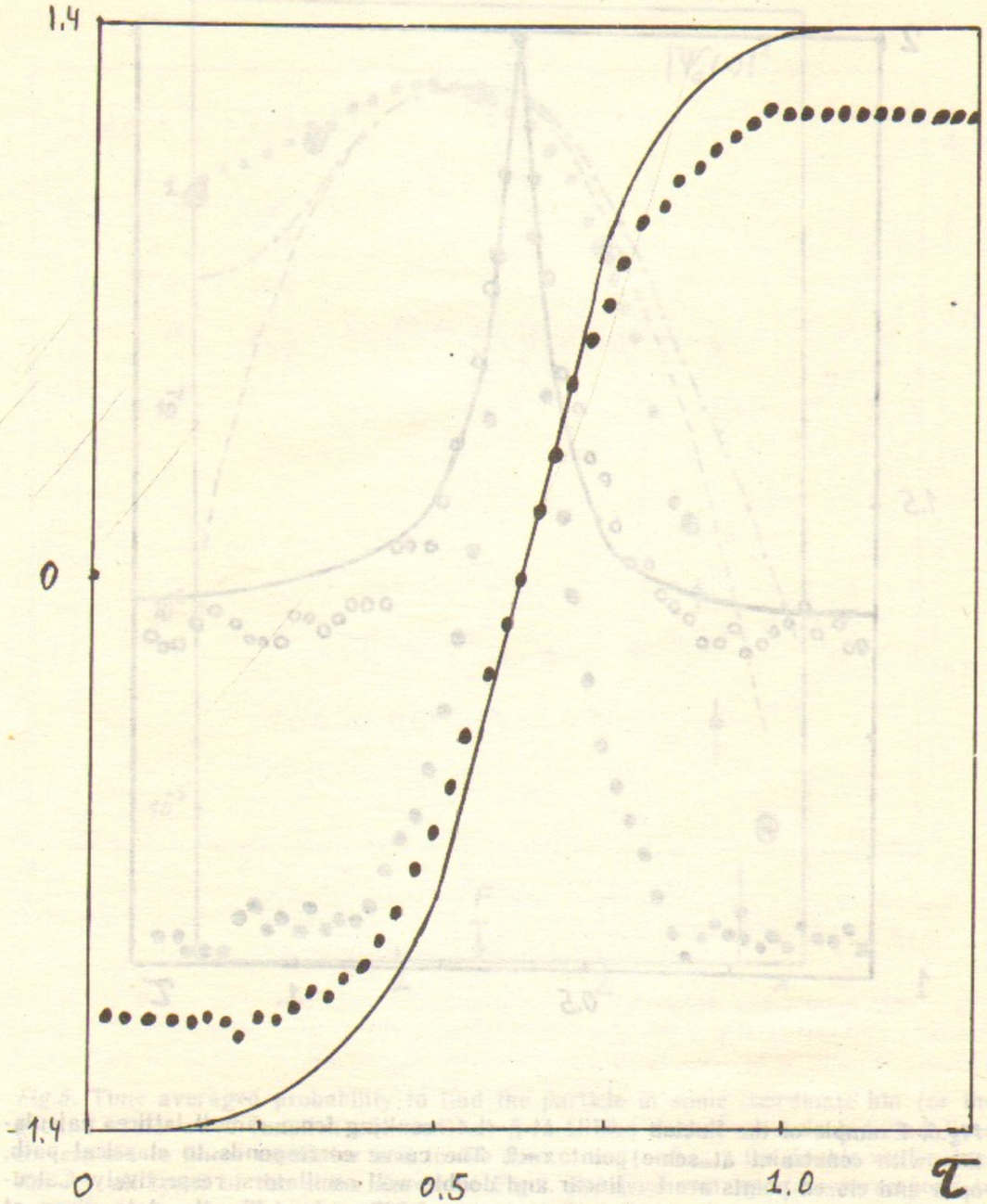

Fig.7. The instanton profile resulting from «small lattice» calculations. All notations and parameters are as for Fig.6.

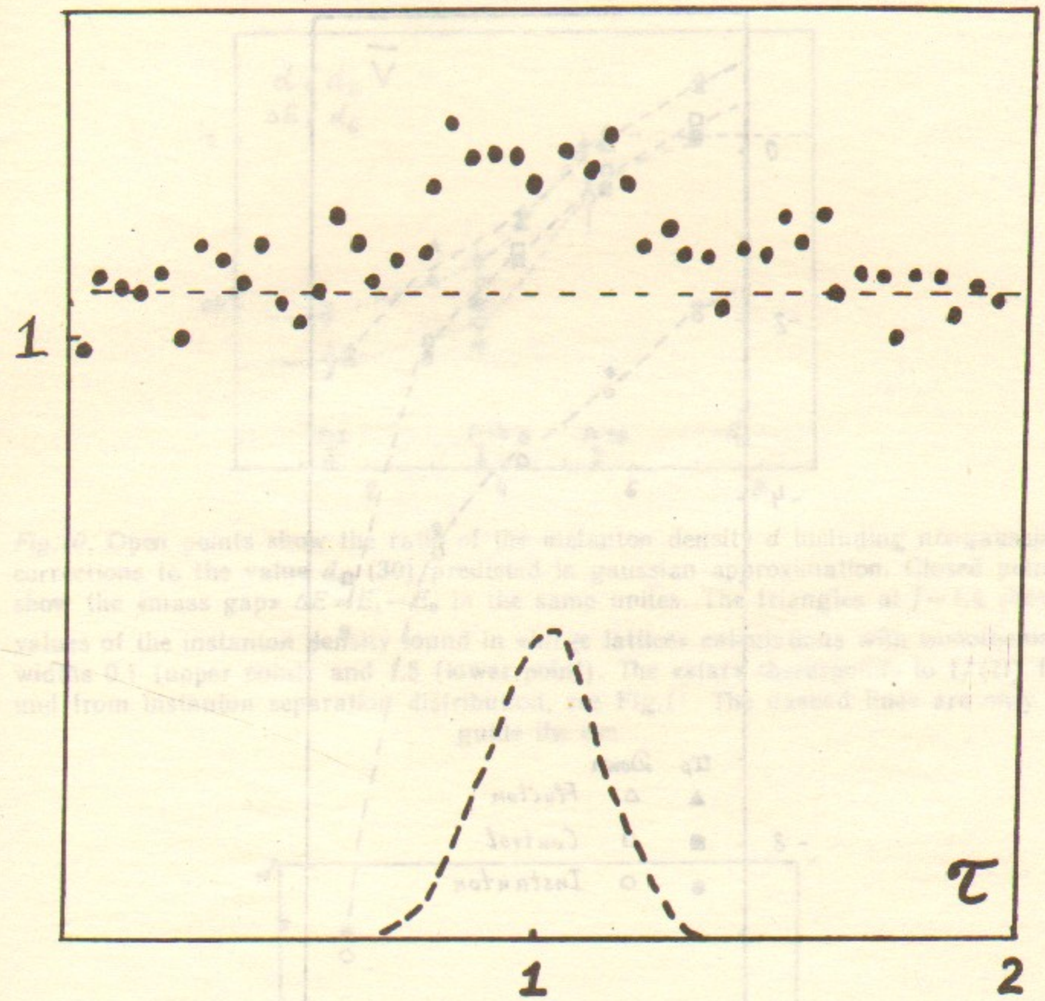

Fig.8. Example of the time distribution of the action, averaged over 200 instanton-type configurations of the «little lattice» with 50 points at $a=0.04$. The dashed line below corresponds to classical instanton solution, the dashed straight line above shows the average level of «quantum noise» in control configurations without instantons. (Note, that at $a\to 0$ such noise becomes more significant.) Although a trace of instanton is definitely seen, quantitative measurements are not possible to do with such data.

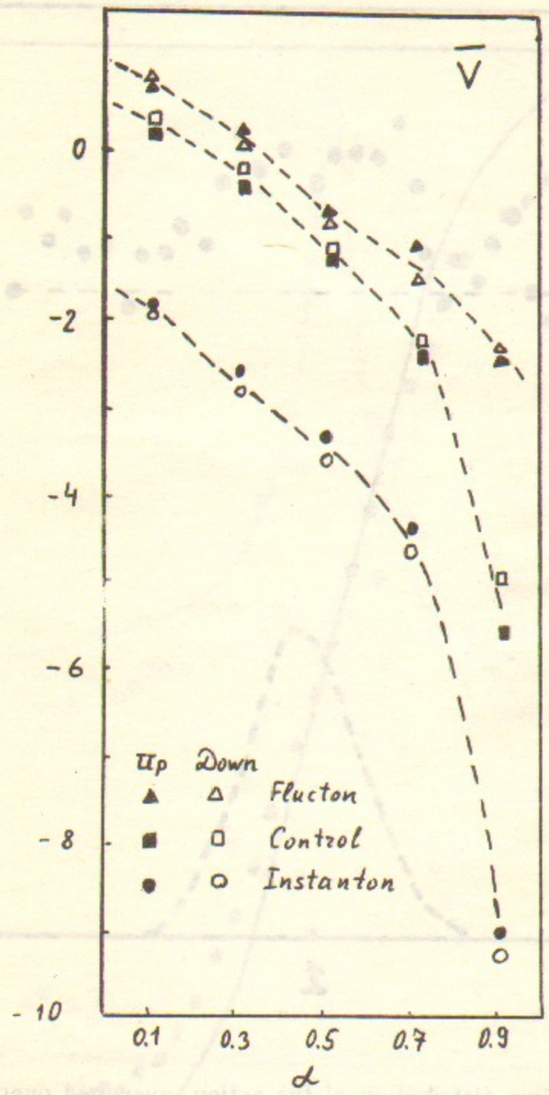

Fig.9 «Histeresis cycles» for dependence of $\langle \Delta V \rangle_\alpha$ on parameter alfa, for three different constraints. The points marked «up» («down») corresponds to increase (decrease) of alfa. Constraint marked «flucton» corresponds to a point fixed at $x=2$, the «instanton» one corresponds to antiperiodic boundary conditions, the «control» calculation are made without constraints. The dashed lines are only to guide the eye.

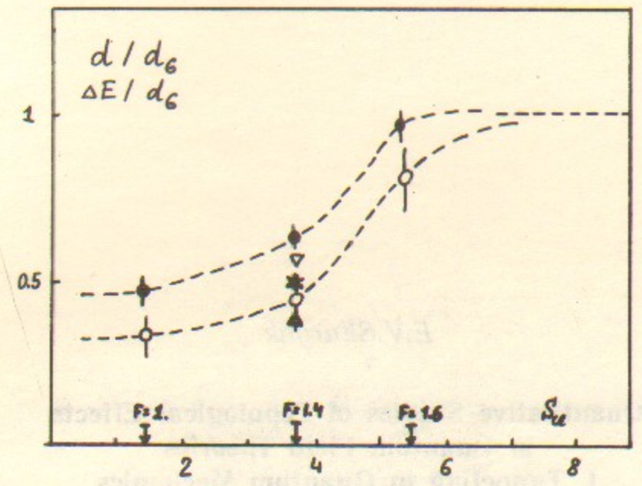

Fig.10. Open points show the ratio of the instanton density d including nongaussian corrections to the value d_G (30) predicted in gaussian approximation. Closed points show the «mass gap» $\Delta E = E_1 - E_0$ in the same unites. The triangles at $f=1.4$ shows values of the instanton density found in «large lattice» calculations with smoothening widths 0.1 (upper point) and 1.5 (lower point). The «star» corresponds to $1/\langle D \rangle$ found from instanton separation distribution, see Fig.11. The dashed lines are only to guide the eye.

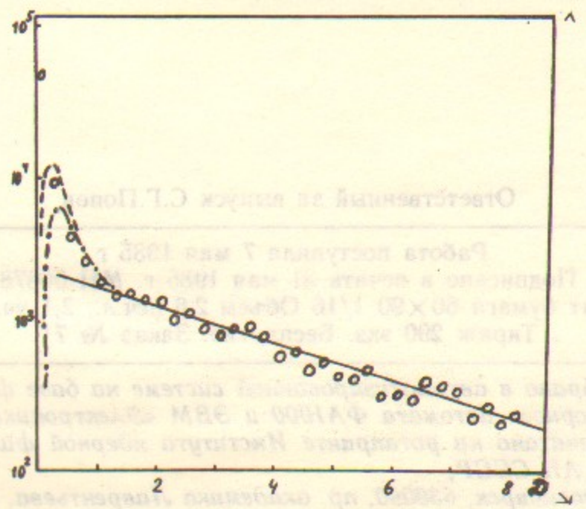

Fig.11. Distribution over instanton time separation D (in arbitrary unites read from experimental hystogramm). The open points corresponds to «large lattice» data with $T=40$, $a=0.2$ and most «naive» definition of the instanton as any zero crossing. The dashed and dash-dooted lines are for definitions of the instanton including smoothening with widths 0.1 and 1.5, respectively. In all cases behaviour at large D is well fitted by exponential $\exp(-0.29 \cdot D)$, shown by solid line.

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Quantitative Studies of Topological Effects in Quantum Field Theories 1. Tunneling in Quantum Mechanics

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