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# TOWARD THE QUANTITATIVE THEORY OF THE «INSTANTON LIQUID» IV. TUNNELING IN THE DOUBLE-WELL POTENTIAL

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Toward the Quantitative Theory
of the «Instanton Liquid» IV.
Tunneling in the Double-Well Potential

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ABSTRACT

This paper deals with a quantum mechanical motion in two potential wells separated by a barrier. We illustrate in this simple context the ideas used in the previous papers of this series, e. g. explicitely find the «streamline» set of paths and the instanton—anti-instanton interaction law. We also obtain high-quality «large lattice» numerical data for the path ensemble, and make their comparison with the theory. Finally, we describe a set of new numerical methods using «small lattices», which may turn helpful for the lattice studies of the gauge theories as well.



## 1. INTRODUCTION

This is the forth paper in the series, and in it we jump from such complicated subject as the quantum gauge theories to just quantum mechanics. There are essentially two different reasons for it.

The first is the pedagogical one: presenting the works [1] I came across the necessity to illustrate their ideas in some simple context. And indeed, as we show below with this «toy model» it is possible e.g. find the *«streamline»* set of configuration and to determine the «instanton—anti-instanton interaction law» explicitely. In contrast to the gauge theory context, we can in this case easily check which trial functions are good or bad, etc. Thus, this paper definitely may help to understand the previous three.

Another reason is practical: this toy model is nice object for testing these ideas, confronting them to the «experimental facts» in form of the computer-generated ensemble of configurations. It is similar to the comparison done previously for the gauge theories, but now it is possible to perform calculations with the accuracy not so far available for the gauge theories.

Another important aim of this paper is the development of new calculational methods. In particular, we suggest *the «small lattice» approach*, aiming to give more economic description of the tunneling phenomena. We hope that these ideas may turn to be useful for gauge theories as well, keeping in mind how severe are technical limitations in that case.

And finally, in this paper we have discussed some new concepts.

In the previous works we have concentrated only on the topological fluctuations, but in this paper we also have paid attention to some strong but nontopological fluctuations. In the quantum mechanical toy model under consideration they are just an ocasion in which the particle moves far into the classically forbidden region of coordinates and then returns back. Following the name suggested in different although related context by A.M. Baldin, we call them «*fluctons*». We show that they are in fact important ingredient of the path ensemble, and that both their semiclassical theory and numerical studies can be developed quite analogously to that for the instantons. Moreover, it turns to be impossible even to separate a close instanton—anti-intanton pairs from a fluctons, for they are just two different ends of the same «valley» in the configuration space.

This paper is structured as follows. In Section 2 we introduce known facts concerning the instantons in the double-well system and their semiclassical theory. The «flucton» concept is introduced in Section 3, where we also are trying to develop their semiclassical theory. Section 4 is probably the central one in this paper: it deals with the valley connecting instanton pairs with fluctons, here we have studied several trial functions and compare them to the «streamline» set of configuration found numerically. In Section 5 we report the results of the «large lattice» numerical calculations, while in Section 6 we present another possible approach, the «small lattice» one, dealing with the «constrained» paths ensuring the presence of the fluctuation we are interested in. Similar method but for the studies of the nongaussian effects around instantons and modification of their density we study in Section 7. Finally, in Section 8 we address the issue of the instanton interaction, confronting the «large lattice» data to the theory developed in Section 3.

## 2. THE INSTANTONS

Tunneling through some classically impenetrable barrier is one of the most striking quantum phenomena, and its discussion is made in any text book on quantum mechanics. However, it is usually based on the traditional Schrödinger formulation, dealing with the Schrödinger equation. Unfortunately, its application for complicated multi-dimensional barriers is difficult (and for the quantum field problems it is hopeless), so we use instead the path integral formulation due to Feynman.



The particular problem to be discussed is the motion in the potential with two wells separated by a barrier. Its particular action (transformed to the Euclidean time $\tau = it$) is as follows

$$S^{(E)} = \int d\tau \left[\frac{m\dot{x}^2}{2} + K(x^2 - f^2)^2\right] \qquad (1)$$

and below we use unites $\hbar = K = 2m = 1$. The only free parameter is then $f$, half of the distance between the well bottoms. Large $f$ means wide barriers, for which the semiclassical theory should work. (In order to see how the deviation looks like we have made calculations mostly for $f = 1.4$, which is at the boundary of the semiclassical region, see below).

Our interest in the particular system (1) is related to the fact that it has in fact two different correlation lengths: $\tau_{osc}$, the oscillation time near the well bottom, and the tunneling time $\tau_{tun}$. Relation between them can be written as

$$\tau_{tun} = \tau_{osc}/P \qquad (2)$$

where $P$ is small tunneling probability. Another feature of this system is the symmetry in respect to the coordinate reflection $(x \to -x)$. At time periods $\tau \sim \tau_{osc}$ coordinates are strongly correlated in sign, but at larger time scale $\tau > \tau_{tun}$ the tunneling mix them, restoring the symmetry of the ground state [2]. This manifests in the behaviour of the correlation function

$$K(\tau) \stackrel{def}{=} \langle x(\tau)\, x(0) \rangle \to \exp(-\Delta E \cdot \tau) \qquad (3)$$

connected with finite «mass gap» $\Delta E = E_1 - E_0$. 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.

As emphasized by A.M. Polyakov [2], the «instanton» of this problem is the path, leading from one well to another and possessing the minimal possible action:

$$x_{cl}(\tau) = f \cdot \tanh[2f(\tau - \tau_c)]; \qquad S[x_{cl}] \equiv S_0 = \frac{4}{3} f^3. \qquad (4)$$

Gaussian fluctuation around this path were treated in Ref. [3] (see also a pedagogical presentation in [4]). Let me mentioned few key points here. Writing the path in the form

$$x(\tau)=x_{cl}(\tau)+\delta x(\tau) \tag{5}$$

and expanding the action in powers of the «deviation» $\delta x$ one has

$$S[x(\tau)]=S_0+\frac{1}{2}\int \delta x(\tau)\,\Box\,\delta x(\tau)d\tau+\dots$$
$$\Box=-\frac{1}{4}\frac{\partial^2}{\partial\tau^2}+V''(x)=-\frac{1}{4}\frac{\partial^2}{\partial\tau^2}+12x^2-4f^2. \tag{6}$$

The next standard step the diagonalization of the arizing quadratic form:

$$\Box x_n(\tau)=\lambda_n x_n(\tau),$$
$$\int Dx(\tau)\exp(-S[x(\tau)])\sim\exp(-S_0)\cdot\prod_n(1/\sqrt{\lambda_n}). \tag{7}$$

However, the differential operator entering this expansion has one zero mode

$$\Box x_0=0;\quad x_0(\tau)\sim\frac{dx_{cl}(\tau)}{d\tau}\sim\frac{1}{\cosh^2[2f(\tau-\tau_c)]} \tag{8}$$

related to a shift of the instanton as a whole in the (Euclidean) time. Thus, there is one direction in the functional space in which the integral is nongaussian, and the integral over it can be rewritten as the integral over the instanton position $\tau_c$. Therefore we in fact evaluate the «instanton density» $dn/d\tau_c=d$.

The product of the nonzero eigenvalues corresponding to the «transverse» coordinates is divergent, but it can be «regularized» by comparison to some problem for which the exact Green function is known (e. g. that for linear oscillator).

Resulting density of the topological fluctuations (the sum for instantons and anti-instantons) is equal to

$$d=8(2/\pi)^{1/2}f^{5/2}\exp\left(-\frac{4}{3}f^3\right)(1-0.97/f^3+\dots) \tag{9}$$

where the former term corresponds to the Gaussian approximation outlined above and the correction term in brackets corresponds to the nongaussian effects, recently calculated by Alejnikov and myself [5].

Concluding this Section we note, that although the theory outli-



ned above is technically compicated, it has important advantages over the WKB theory. In particular, it can be directly generalized to arbitrary number of variables. Also it has absolute normalization, while the WKB «tunneling rate» contains a constant which shuld be defined by rather tedious consideration of the vicinity of the «stopping point». (Advantage of the WKB expression, in turn, is as follows: it can be used for any state, not only the ground one.)

Our more general comment is that all semiclassical results are applicable if the classical action for the instanton is large

$$S(\text{classical})\gg 1 \tag{10}$$

(say, it exceeds 6, see below). This condition in turn, implies that the tunneling probability $P$ is exponentially small

$$P\sim\exp(-S(\text{classical}))\ll 1 \tag{11}$$

(say, $\exp(-6)=0.002$).

However, the idea that quantum paths can be considered as Gaussian oscillations near the well bottom plus some tuneling events is meaningful if

$$P\ll 1 \tag{12}$$

(where $P$ is the ratio of the oscillation period to the tunneling time): one can tell «tunneling» from «ordinary oscillations». Although conditions (11) and (12) look similar, they are rather different from a practical point of view. Thus, one of our aims is to developed the methods capable to treat «deformed instantons» which happen with small, *but not exponentially small* rate (say, in the range 1/3—1/30).

### 3. THE «FLUCTONS»

In this Section we introduce new type of objects, the «*fluctons*». Like instantons, they are some strong fluctuations of the system, being well localized in the (Euclidean) time. However, they are not related with topology or symmetries, so we do not actually need a barrier to introduce them, but just the classically forbidden coordinate region. Unlike instantons, they do not contribute much to the long-range correlation function for the double-well system, but are important for the understanding of the ground state wave function. As far as we know, such type of objects were not discussed in the quantum field theory context.

It is convenient to start with the familiar methods based on the Schredinger equation. The small «tails» of the ground state wave function $\Psi_0(x)$ in the classically forbidden region are described by the well known WKB formula

$$\Psi_0(x) \simeq \text{const} \cdot \exp\left( - \int_{x_{\text{stopping}}}^{x} p(x')\,dx' \right). \qquad (13)$$

The quantum field theory language we use in this work deals with the ensemble of the paths $[x(\tau)]$ rather with the wave functions. (Of course, this ensemble describes not only the coordinate distribution in the ground state but also many other dynamical properties of the system). One may ask which paths are responsible for this «tail» and what is the analog to the semiclassical WKB theory.

Let me remind how the path ensemble is related to the ground state wave function. For this we have to compare two general expressions for the Green function, the one due to Feynman and the standard decomposition over the stationary states:

$$G(x_i, x_f, \tau) = \int_{x_i}^{x_f} Dx(\tau)\, \exp(-S[x(\tau)]) = \sum_n \Psi_n^*(x_i)\, \Psi_n(x_f)\, \exp(-E_n \tau). \qquad (14)$$

Thus, large Euclidean time limit corresponds to the ground state term , and in principle the corresponding wave function can be read from the large-time Green function dependence on its end points.

For a number of reasons it is not convenient to do so, and we prefer to consider some arbitrarily long paths and take the «observation point» $\tau_0$ somewhere inside it. If we ask for the amplitude to have at this point some given coordinate value $x_0$, it is described by the product of two Green functions and therefore to the ground state wave function squared:

$$P(x_0) \sim G(x_i, x_0, \tau_+)\, G(x_0, x_f, \tau_-) \xrightarrow[\tau_\pm \to \infty]{} |\Psi_0(x_0)|^2. \qquad (15)$$

(We are not interested in the remoted end points, so we may well integrate over them.)

Now, suppose the point $x_0$ in a classically forbidden region is fixed and we ask how the paths which managed to reach it looks like. This question can of course be answered straightforwardly, by looking at the path ensemble generated numerically (we do it in Section 6). However, if $x_0$ is deep enough in the forbidden region, the question can be answered semiclassically. As usual, the idea is that in this case such paths should be close to that possessing the minimal possible action.

For simplisity we start with the linear oscillator

$$S^{osc} = \int d\tau \left[ \frac{m\dot{x}^2}{2} + \frac{m\omega^2 x^2}{2} \right] \qquad (16)$$

The minimal action path which goes through $x_0$ has the form

$$x_{cl}(x_0, \tau_0, \tau) = \begin{cases} x_0 \exp[-\omega(\tau - \tau_0)] & \tau > \tau_0 \\ x_0 \exp[\omega(\tau - \tau_0)] & \tau < \tau_0 \end{cases} \qquad (17)$$

and this is the «flucton» shape for this problem. The corresponding classical action is $S_{cl} = m\omega^2 x_0^2$, and therefore the probability to meet it in the ensemble is proportional to $\exp(-S_{cl})$. From this we conclude that asymptotics of the ground state wave function is as follows:

$$\Psi_0(x_0) \xrightarrow[x_0 \to \infty]{} \exp\left( -\frac{m\omega}{2} x_0^2 \right). \qquad (18)$$

(For this particular system all semiclassical results including this one are in fact exact because the path integral is Gaussian exactly.)

For the double-well system (1) it is also easy to find the classical path corresponding to the same conditions, say for $|x_0| < f$ it looks as

$$x_{cl}(x_0, \tau_0, \tau) = \begin{cases} f \cdot \tanh[-2f(\tau - \tau_0)] & \tau > \tau_0 \\ f \cdot \tanh[2f(\tau - \tau_0)] & \tau < \tau_0 \end{cases} \qquad (19)$$

and the corresponding action is equal to

$$S_{cl} = \frac{2}{3} x_0^3 f - 2 x_0 f^2 + \frac{4}{3} f^3. \qquad (20)$$

Under the barrier fluctons contribute to the wave function on equal footing with the instantons. Consider for example the point $x_0$ (see Fig. 1). Using the wave function language one may say that here the wave function tails from both wells are added, therefore the wave function is nearly doubled and the probability is about four times larger than if there would be just one single well. The same consideration in the path integral language looks as follows: there are four different paths (instanton, anti-instanton and two fluctons, see Fig. 1) which all are present with comparable probability.

Now we will try to connect the ground state wave function with the flucton density. Let us consider some classically forbidden region (e. g. $|x_0| > f$ for our toy model) in which fluctons can be characterized by the maximum distance from the bottom $x_{max}$ and position in time $\tau_0$. Their density is defined as follows

$$dN_{\text{fluctons}} = P(x_{\max})\, d\tau_0 dx_{\max} \tag{21}$$

The probability to find particle at some coordinate $x$ is the integrated density of sufficiently strong fluctuations divided by the velocity $\dot{x}$ at which the particle passes this point

$$|\Psi_0(x)|^2 \sim \int_x^\infty dx_{max} \;\; P(x_{max})/\dot{x}_{cl}(x_{max}). \tag{22}$$

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

$$P(x_{max}) \sim \exp\{-S[x_{cl}(x_{max})]\}. \tag{23}$$

and expanding the classical action

$$S_{cl}(x_{max})\; S_{cl}(x = x_{max}) + m\dot{x}\,(x - x_{max}) \tag{24}$$

one can integrate over $x_{max}$ and to write the final result in a compact form

$$P(x_{max}) \simeq V(x_{max})\, |\Psi_0(x_{max})|^2. \tag{25}$$

where $V(x)$ is the potential. (We have used the energy conservation at the classical path and have assumed that the potential well bottom is taken at zero energy value).

#### 4. THE TRIAL FUNCTIONS AND THE «STREAMLINE»

The tunneling through the barrier and penetration into it to some depth are, of course, strongly related. Similarly, the instantons are in fact connected with the fluctons, which becomes evident if we consider the annihilation process of a instanton (I) with an anti-instanton (A). In the paper I of this series [1] we have already mentioned that a IA pair can continuously be transformed to the trivial $x = \pm f$ paths via a kind of a «valley» in the functional space. Unfortunately, that was rather complicated construction for the Yang—Mills theory, but now we are going to study this valley for the double-well system.

It is clear that any IA-type configuration is not the action minimum: these «pseudoparticles» attract each other. Therefore, for a long time it was unclear how to select a set of configurations, interpolating between the well separated IA pair and the fluctons.

At first sight, any interpolation can well be used, and one may consider some arbitrarily taken «trial functions». For example, one may take the one suggested by Bogomolny [6], which satisfies the equations of motion at all points but one

$$x^{|B|}(\tau) = \begin{cases} f \cdot \tanh[2f(\tau - \tau_I)] & \tau < 0 \\ -f \cdot \tanh[2f(\tau - \tau_A)] & \tau > 0 \end{cases} \tag{26}$$

We will call it «B» ansatz (from «break» or Bogomolny).

Another possible suggestions are, say, the «S» and «P» trial functions (from the «sum» and the «product», respectively):

$$\begin{aligned} x^{|S|}(\tau) &= f\{\tanh[2f(\tau - \tau_I)] - 1 - \tanh[2f(\tau - \tau_A)]\}, \\ x^{|P|}(\tau) &= -f\, \tanh[2f(\tau - \tau_I)]\, \tanh[2f(\tau - \tau_A)]. \end{aligned} \tag{27}$$

However, for an interpolating function taken at random the semiclassical calculations become complicated at later stages. In particular, let us write an arbitrary path in the form of the ansatz one plus the «deviation»

$$x(\tau) = x^{\text{ansatz}}(z, \tau) + \delta x(\tau) \tag{28}$$

where $z$ is some parameter marking the ansatz configurations. The «deviation» can be expanded into the «longitudinal» and «transverse» part in respect to the ansatz:

$$\begin{aligned} \delta x_{\parallel}(\tau) &= \frac{\partial x^{\text{ansatz}}}{\partial z}(z, \tau) \frac{\int d\tau\, \delta x(\tau) \frac{dx^{\text{ansatz}}}{\partial z}(z, \tau)}{\int d\tau \left| \frac{dx^{\text{ansatz}}}{dz} \right|^2} \\ \delta x_{\perp} &= \delta x - \delta x_{\parallel} \end{aligned} \tag{29}$$

The «longitudinal» part of the deviation is not interesting now: integration over it can be absorbed by the integral over z. The integral over the transverse one in Gaussian approximation looks as follows:

$$\int D\delta x_\perp \exp\left[-S(x^{\text{ansatz}})-\int d\tau f_\perp(\tau)\delta x_\perp(\tau)-\frac{1}{2}\int d\tau\delta x_\perp \Box_\perp \delta x_\perp+\ldots\right]\simeq$$
$$\simeq \exp\left[-S(x^{\text{ansatz}})-\frac{1}{2}\int f_\perp(\tau)(\Box_\perp^{-1})_{\tau\tau'} f_\perp(\tau')\,d\tau d\tau'\right] \qquad (30)$$

where $f(\tau)\equiv\frac{\delta S}{\delta x}$ is the «force» (for the Yang—Mills fields in I it was naturally «the current»).

The key point is that the «transverse force» term in the effective action is parametrically as large as the former «classical» one. It is not easy to evaluate it in practice: the main difficulty is, of course, the inverse operator $\Box_\perp^{-1}$ (or the corresponding Green function in the non-uniform «background field» $x^{\text{ansatz}}(z,\tau)$)

Some time ago the way out was suggested by Balitsky and Young [7] and myself [8], it was based on the particular choice of the interpolating set of configurations called the *«streamline»* [7]. We have discussed its qualitative properties in I, but now we find it explicitely. Its main property is that the force $f(\tau)$ has *no «transverse» part*, so the annoying «force term» in (30) is absent.

In order to find it numerically [8] one should do exactly what he does coming back from the mountains: to start at the remoted initial point (well separated IA pair) and then just follow the direction of the «force» . It is done iteratively, calculating the force and making small steps in its direction

$$x_{n+1}(\tau)=x_n(\tau)-\varepsilon f_n(\tau) \qquad (31)$$

where $\varepsilon$ is some small numerical parameter (we have taken it to be 0.001). An example of the results is shown in Figs 2, 3 in the form of the paths themselves and the corresponding action distribution. (Note that the force is growing rapidly as the pseudoparticles approach each other, so convergence of (31) is at first very slow and then becomes more rapid.)

It is instructive to compare the «streamline» found to the trial functions mentioned above, but for doing this one should introduce some common parameterization. Of course, any parametrization of these configurations can be used. The simplest one would be the action itself, ranging from twice the instanton action to zero. However, we use other parametrization which is simpler to use in «lattice experiments» to be discussed below.

Our parametrization (chosen rather arbitrarily) splits the «valley» into two parts, the «IA pair» and the «flucton» one, depending on whether the path crosses the barrier center $x=0$ or not. In the former case it is called the IA pair, and the parameter $D$ (called the IA separation) is the time distance between two crossing of the $x=0$ line. In the latter case it is considered as a flucton, which we map by the maximal deviation from the well bottom $x_{\max}$ (ranging from 0 to $f$). (In particular, the $D=0$ pair and the $x_{\max}=f$ flucton is in fact the same configuration.)

Wondering whether the simple trial functions suggested above are similar to the «streamline» one may introduce the so called «cos Ф» combination

$$\cos\Phi=\frac{\int d\tau f(z,\tau)\frac{\partial x^{\text{ansatz}}}{\partial z}(z,\tau)}{\left[\int f^2 d\tau\cdot\int d\tau f(z,\tau)(\partial x^{\text{ansatz}}/\partial z)^2\right]^{1/2}} \qquad (32)$$

where $f(z,\tau)$ is the force and $x^{(\text{ansatz})}(z,\tau)$ is the trial function. Roughly speaking, the angle $\Phi$ is between the force and the tangent to the ansatz line. By definition, for the streamline $\cos\Phi=1$. For the $B$ ansatz $\cos\Phi=0$, for in this case the force is the delta-function and its norm is infinite. For «S» and «P» trial function its dependence on $D$ is shown in Fig. 4 . From these numbers one may have an impression that these trial functions are reasonably good approximations to the «streamline» .

This idea is also supported by the action dependence (see Figs 5, 6 for the «IA pairs» and fluctons, respectively): all trial functions follow the «streamline» reasonably well. It means that the «transverse force term» in action which is so difficult to calculate is in fact only a 10% correction. (Hopefully, something similar takes place in field theory context as well.) The resulting «IA interaction law» given in Fig. 5 will be compared with the «large lattice» data in Section 8.

### 5. NUMERICAL EXPERIMENTS ON THE «LARGE LATTICE»

Studies of the double-well system on the lattice have already been made in Refs [9, 10], so we do not discuss any details of the method. We just remind that 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

$$a \ll \tau_{osc} \ll \tau_{tun} \ll T = Na . \qquad (33)$$

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! Thus, although we now deal with one-dimensional (mechanical) system, its straightforward numerical stadies need rather large lattice. (Fortunately, for such simple system such conditions can really be satisfied, but not for the field theories in more dimensions.)

Generation of the path ensemble is done by the standard Metropolis algorithm. We only mention that the measurements of the correlation functions and other details to be considered below make it necessary to have much better ensemble than, say, for the measurements of the ground state energy or the corresponding wave function. Therefore, instead of hundreds of iterations as in Refs [9, 10], we had to make up to $10^5$ ones.

In our studies reported in Ref. [10] 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 the lattice step of the order 0.2 or so this phenomenon produces significant systematical errors, therefore in this work we both use smaller step and compare results for the following two lattice actions

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

$$S^{(improved)} = \sum_i [x_i - x_{i+1})^2/4a + \int_i^{i+1} d\tau \, (x^2 - f^2)^2] , \qquad (34)$$

(The latter corresponds to the paths made of a set of straight segments. As shown in [10]', by makng the path continuous one can effectively kill the «lattice instantons» .)

As discussed above, the time-averaged distribution over coordinates in our ensemble corresponds to the ground state wave function squared. Our «large lattice» results are shown at Fig. 7 where they are confronted with other calculations to be specified below.

New type of questions is how the strong fluctuations are developing in time. «Hunting for the fluctons» one may select all events in which, say, the particle reaches some fixed distance from the well bottom. Superimposing maxima of such fluctuations we obtain the average «flucton profile», examplified at fig.11. Note that such fluctons are well localised in time and have typical «triangular» shape (as those suggested by the semiclassical arguments).



Although it is generally impossible to make clear separation of the IA pairs from the fluctons, one may make use of the existence of two separate time scales $\tau_{osc}$, $\tau_{tun}$ and ignore this problem for a while. While trying to describe some gross features of the paths it is desirable to make them «more smooth». More precizely, let the averaging width (av) is taken somewhere in between of the two scales

$$\tau_{osc} \ll \tau_{av} \ll \tau_{tun} . \qquad (35)$$

It helps to get rid of «quantum noise» at scales from $a$ to $\tau_{av}$. Relation (35) ensures that the results are practically independent on $\tau_{av}$ and the particular procedure used. (We have used Gaussian expression

$$\bar{x}_i = \sum_{k=-\infty}^{\infty} \exp[-(\tau_{k+i} - \tau_i)^2/2\tau_{av}^2] \, \frac{a}{\sqrt{2\pi}} \, \frac{1}{\tau_{av}} \qquad (36)$$

but it is not important.) For the smoothed paths the tunneling events are clearly seen (see Fig. 8 ), and for them it is easy to locate positions of the instantons. Superimposing them we have found the average instanton shape, see Fig. 9. (To avoid misunderstanding we emphasize that it corresponds to original, not the «smoothed» paths.) One may also find the instanton density and consider their distribution in time. These data will be discussed in Section 7. Lattice calculations for QCD tends to present measurements of the correlation function, being the basis of the «hadronic spectroscopy» . We have also made such measurements for this toy model and have found that the existence of two scales leads to some spectacular behaviour of the correlation functions. It is convenient to plot not the correlators by themselves, but their logarithmic derivative $F(\tau)$

$$F(\tau) \stackrel{def}{=} -\frac{d}{d\tau} \log \langle x(\tau) x(0) \rangle . \qquad (37)$$

Our results for $f = 1.4$ and 1.6 are shown in Fig. 10. At small

$\tau \sim \tau_{osc} = 1/4f$ this quantity is rather large: correlation is affected by the «ordinary» oscillations. At intermediate $\tau$ it decreases: here the correlator is nearly constant, close to $\langle x \rangle$ (averaged only over the motion in one well). At large $t$ tunneling effects come into play and «mix» the correlation. Here $F(t)$ tends to constant, the energy gap, as is very clearly seen from these data. (Again, let us note that so clean exponential behaviour is impossible to observe in the lattice data for a field theory.)

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 in this Section is the following statement: the «smoothed» paths correctly reproduce the long-range correlations, see points shown by stars at Fig. 10. It is important because the «smoothed» paths can be parametrized by the collective coordinates, positions of the instantons. Thus, the long-range correlations are insensitive to the «quantum noise»!

## 6. EXPERIMENTS ON THE «SMALL LATTICE». THE GROUND STATE WAVE FUNCTIONS AND FLUCTONS

The previous Section has started with the formulation of rather strong conditions for the lattice numerical experiments devoted to studies of the instantons (or fluctons). Besides the general conditions for any lattice calculations, our case is even more difficult because strong fluctuations happen rarely and one needs especially long lattice for their observation.

The «small lattice» approach is the method to generate paths constrained by some condition, ensuring the presence of the instanton or the flucton of interest. Thus, the calculations become much more effective compared to the straightforward «large lattice» ones. Let us start with the case of fluctons. The first natural thing to do is to generate paths coming through some fixed point $x_0$. We have done the same in Section 3 in the semiclassical context, so one may wonder to what extent the average path behaviour follow the minimal action one. An example of the kind for fluctons are shown in



Fig. 11. Deviations are clearly seen, and they are due to the nongaussian effects ignored in the semiclassical approximation.

It is more delicate thing to «pin down» an instanton. It is straightforward to generate only «transverse» deviations from the classical instanton path, satisfying the orthogonality condition

$$\int d\tau \, [x(\tau) - x_{cl}(\tau)] \frac{dx_{cl}(\tau, \tau_c)}{d\tau_c} = 0 . \qquad (38)$$

It can be done by «updating» points in pairs, holding the integral (38) to be strictly conserved. However, it is simpler to use another condition $x(\tau_c) = 0$. (In both cases, one should of course add the corresponding Jacobian factor into the weight function.)

It is instructive to compare action distribution for the «small lattice» constrained paths and the classical ones. Here one comes across a problem of, so to say, ultraviolet type: the mean kinetic energy diverges at time step $a \to 0$, and this large «quantum noise» part should be subtracted. The corresponding data are shown at Fig. 12. Large time-independent level corresponds to «ordinary» fluctuations, while the excess is due to the constraint and is qualitatively similar to action distributions for classical trajectories (shown in lower part of the figure).

Our main quantity of interest is the fluctuation probability. In order to find it one may, in principle, directly compare probabilities of the individual paths for our problem (e. g. the double-well system) with that for some «reference point» (e. g. for the linear oscillator). Generating path ensemble for the «reference point» system one may try to average the following factor

$$F_{\text{weighted}} = \langle \exp[-\int d\tau \Delta V(\tau)] \rangle \qquad (39)$$

where $\Delta V = V_{DW} - V_{osc}$ is just the difference of the potential energies. Note, that the problems connected with the divergent kinetic energy are gone. Unfortunately, this factor fluctuates too much, so it turns to be impossible to use such averaging and one has to use more ingenious methods.

As a practical method we use the «adiabatic switching» one [10], including less fluctuating quantities. Let us introduce a set of actions with some parameter alfa, interpolating between the action $S_{osc}$ (for the linear oscillator) and $S_{DW}$ (the double-well potential).

$$S_\alpha = S_{osc}(1-\alpha) + \alpha S_{DW} = S_{osc} + \alpha \Delta V. \qquad (40)$$

The average value of $\Delta V$ can be written as the logarithmic derivative of the statistical sum

$$\langle \int d\tau \Delta V \rangle_\alpha = -\frac{\partial}{\partial \alpha} \log \int Dx(\tau) \exp(-S_\alpha). \qquad (41)$$

Integrating this relation back one has

$$G_{DW} = G_{osc} \exp\left[-\int_0^1 d\alpha \langle \int d\tau \Delta V \rangle_\alpha \right]. \qquad (42)$$

Evaluation of the integral in exponent of (42) can be done with (rather standard) trick: alfa value is gradually increasing and then decreasing again. The measured «histeresis cycles» provide estimates of the nonequilibrium effects.

Application of (42) to the calculation of the probablity distribution (the wave function squared) is straightforward. Most simple is to look for the probability ratio for two coordinate values

$$\left|\frac{\Psi_{DV}(x_1)}{\Psi_{DV}(x_2)}\right|^2 = \left|\frac{\Psi_{osc}(x_1)}{\Psi_{osc}(x_2)}\right|^2 \exp[-\int d\alpha(\langle \int d\tau \Delta V\rangle_{\alpha,1}\rangle - \langle \int d\tau \Delta V\rangle_{\alpha,2})]. \quad (43)$$

(We remind that

$$|\Psi_{osc}(x_1)/\Psi_{osc}(x_2)|^2 = \exp[-m\omega(x_1^2 - x_2^2)]. \qquad (44)$$

Note also that in order to reproduce the wave function under the barrieir one should include all types of paths shown at Fig. 1.) Using this expression we have found results shown at Fig. 7 by stars, which are close to those found in the straightforward «large lattice» calculations.

### 7. THE INSTANTON DENSITY AND THE NONGAUSSIAN EFFECTS

We continue presentation of the «small lattice» calculations, demonstrating how one can use it for the estimates of the instanton density. Again we use the «adiabatic switching» method, accounting



for the nongaussian effects, while the «reference system» is now the formulae obtained in the semiclassical (Gaussian) approximation. Thus, our interpolating action looks as follows

$$S_\alpha = S_G + \alpha S_{NG},$$
$$S_{NG} = \int d\tau [4x_{cl}(\tau)\delta x^3 + \delta x^4] \qquad (45)$$

We evaluate corrections due to the nongaussian effects to the transition amplitude

$$G(x_i = -f, x_f = f, \tau) = \exp[-E_{DW}\tau] \cdot 4f \cdot d \qquad (46)$$

where the quantity $d$ is, by definition, the instanton density. Combining this expression with that in the Gaussian approximation one may express the quantity $d$

$$d = d_G \exp\left(-\int_0^1 d\alpha \langle S_{NG}\rangle_\alpha\right). \qquad (47)$$

Apart of the correction to the tunneling amplitude, the nongaussian effects also modify oscillations in the wells, shifting the ground state energy. In practice, the calculations were done as follows. The presence of the (odd number of) instantons was ensured by the antiperiodic boundary conditions. The measured effect due to the nongaussian terms in action were subtracted from the results of the «control» measurements made for the periodic paths. The results for the instanton density are given at Fig. 13 plotted as the ratio to predictions of gaussian approximation (29). The results agree with analytic estimates [5] (which actually were obtained later than these data).

As already discussed above, the presence of the instanton can also be forced by some constraints. The simplest one possible just fixes the point at which the paths cross zero. Formally it looks as the following trick: one introduces unity in functional integral

$$1 = \int d\tau \delta(x(\tau_c))\, \dot{x}(\tau_c) \quad , \qquad (48)$$
$$Z = \int Dx \exp(-S) = \int d\tau_c \int Dx(\tau)\, \delta(x(\tau_c))\, \dot{x}(\tau_c) \exp(-S)$$

and then put the integral over $d\tau_c$ outside. Note, that the Jacobian is now simply a velocity at the constrained point, and on the lattice it is relevant only for the points next to the fixed one. (Such collective variable is simpler than that following from the ortogonality to the zero modes: it leads to additional action which is local in time. Another advantage is that Jacobian-induced action $S=\log(\dot{x}(t))$ is not very fluctuating from path to path: in the instanton center the motion is most close to the classical one.) We have done such simulations too, and the results agree with those obtained by the «antiperiodic path» method.

Our conclusion is that the nongaussian corrections to the semiclassical theory are noticeable, unless the barrier penetrability is at 1% level, while the methods developed above can well be used in the case when deviations from its prediction is of the order of one.

## 8. INSTANTON INTERACTIONS

The issue of the interaction of the pseudoparticles was the main concern in the theory of the «instantonic liquid» discussed in the previous papers of this series. For the double-well system it does not play so important role as for the gauge theories: the interaction decays exponentially instead of some power law.

We start with the «large lattice» data and first present some «experimental facts». In particular, we have studied correlation in the instantons positions, defined as the time moments when the paths cross the $x=0$ line (we have in fact use the «smoothed» paths defined above). The distribution over the instanton separations $D$ are given at Fig. 14. For $D>1$ the data demonstrate very good exponential behaviour

$$\frac{dN}{dD}\sim\exp(-D/\bar{D}) \tag{49}$$

typical for the «ideal gas» of instantons, showing that the interaction is only short-range. At intermediate distances we have evidences for the instanton—antiinstanton attraction. This effect is compared to the following correction

$$\frac{dN}{dD}\sim\exp[-D/\bar{D}-\Delta S^{interaction}(D)] \tag{50}$$

where $\Delta S^{\text{interaction}}$ is that for the «streamline» set of configurations. It reproduces well enough the IA attraction at small distances.

Thus, we have quantitatively described the IA interaction, which



is the main conclusion for this section.

It is just simple exercise to make a program generating ensemble of points, the instanton positions, separated according to this interaction law. Instead of the «streamlines» or any trial functions one may use even the simplest step-function parametrization for the paths

$$x(\tau)=f\cdot\prod_i \varepsilon(\tau-\tau_i);\qquad \varepsilon=\begin{cases} 1 & \tau<0 \\ -1 & \tau>0 \end{cases} \tag{51}$$

Such simple description for the «instanton liquid» (which is in this case only slightly deviating from an ideal gas) can reproduces the «mass gap» of the theory and other details of the correlation functions at large time scale.

## 9. CONCLUSIONS

The main goal of the present work was development of some new methods for studies of the strong fluctuations in quantum systems. Together with the well-known «instantons», related to tunneling through the barrier, we have also introduced the «fluctons». We have shown that they also are important ingredient of the path ensemble, in particular affecting its ground state wave function in classically forbidden region. Moreover, we have explicitely found the best set of configurations (called the «streamline» ), continuously connecting the separated instanton—anti-instanton pairs with the flucton sector.

This «streamline» is a generalization to the «classical paths» as used in ordinary semiclassical theory. Indeed, in the latter case one deals with the «action minima», while we study a (one parameter) set of configurations being the minima in respect to «tranverse» deviations from this set. We have shown that such «streamline» have correctly reproduced the instanton—anti-instanton interaction law. One may also hope that this generalization of the semiclassical theory will find many other applications in the quantum physics.

Second, in this paper we repoted results of the «large lattice» calculations, capable to provide high quality data on the path ensemble. In particular, we have measured some correlation functions and studied the distribution of the pseudoparticles in time.

Third, new technical methods are suggested, based on the simulation of the paths on the «small latttices». These paths are subject to some constraints, ensuring the presence of the fluctuations of interest. With their help we have successfully studied the role of the «nongaussian» effects (deviations from the semiclassical theory) for the instanton density.

Of course, it would be desirable to repeat at least part of this program for the quantum field theories. The most interesting points are the analogs of our «fluctons» and the «streamline», as well as the studies of the nongaussian effects on the instanton density. We hape to report them in further works of this series. We again underline, that using the «small lattice» approach one may get rid of one strong inequality, which may open completely new perspectives.

Finally, this work may also have applications in realistic quantum mechanical calculations related with a penetration through some multidimensional barriers: say, in quantum chemistry, nuclear fusion etc.

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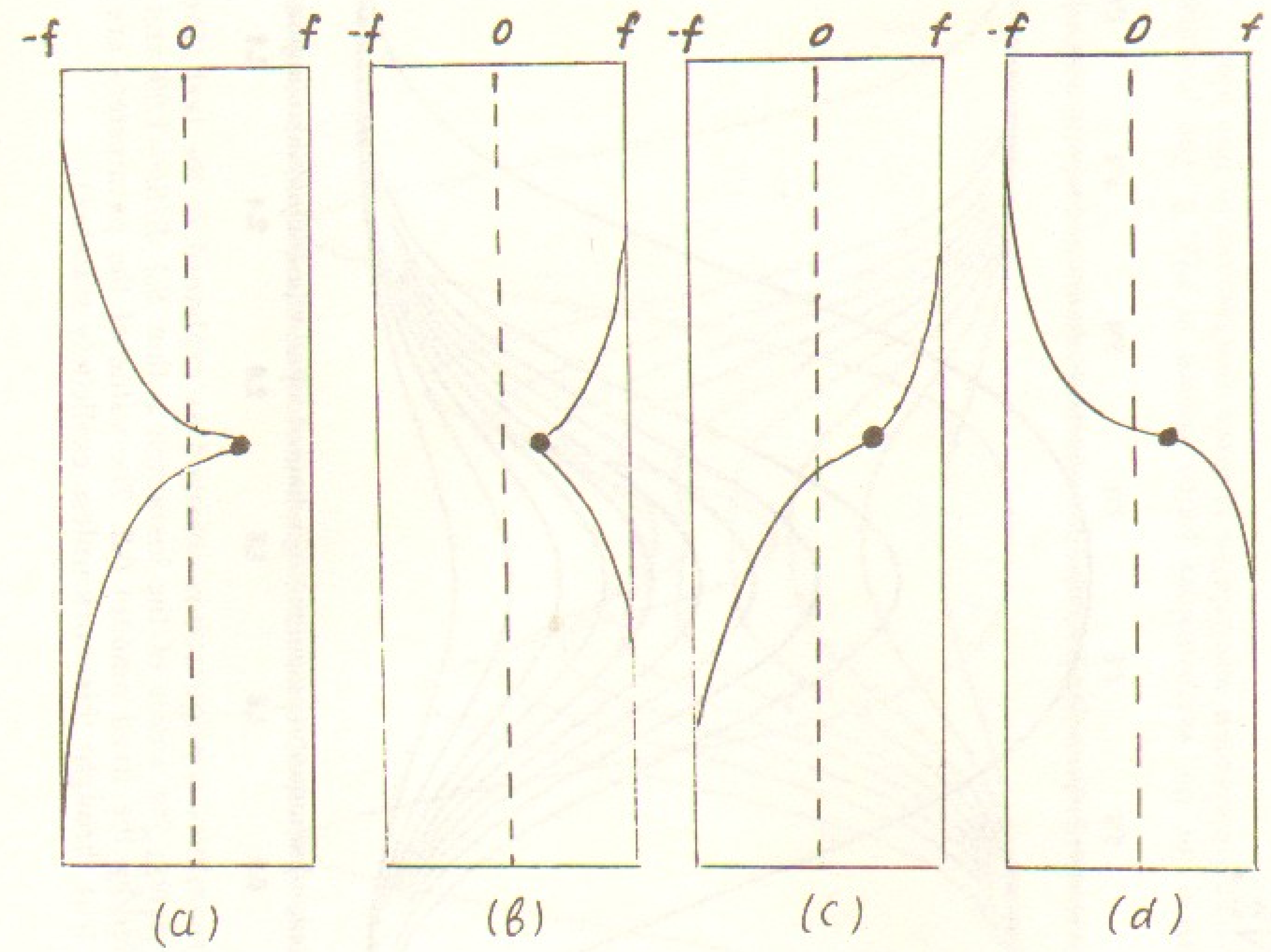


*Fig. 1.* Four topologically different paths coming via the same point $x$ under the barrier. The vertical axis corresponds to Euclidean time, the horisontal one to particle coordinate. The dashed lines are the barrier center and the solid lines at $x=\pm f$ are the well bottoms.

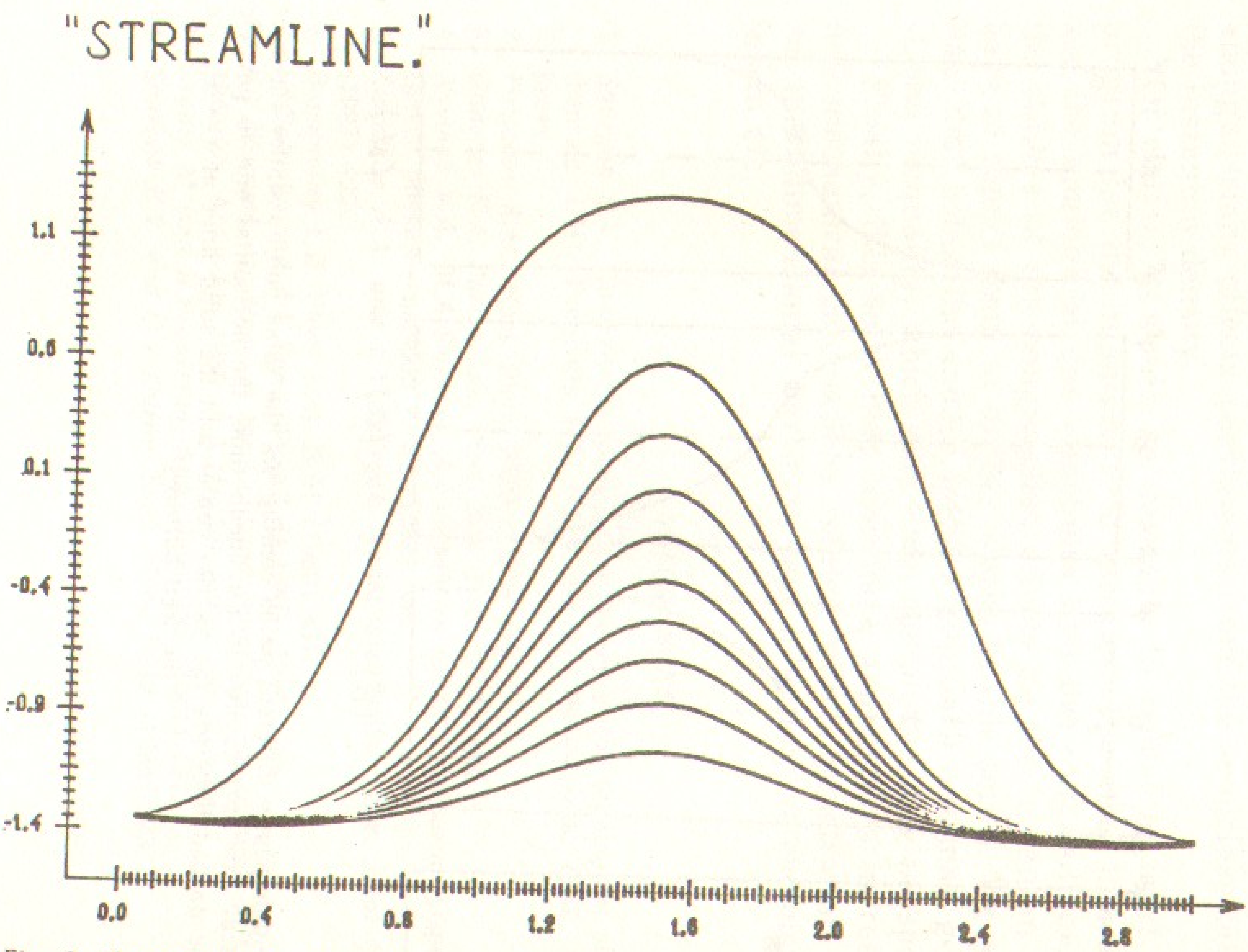


*Fig. 2.* The set of the «streamline» configurations obtained as explained in the text. The upper curve corresponds to the action (in unites of the instanton action $S_0$) $S/S_0=1.99$ and others correspond to $S/S_0$ smaller by the fixed amount 0.2. The value of the parameters are $f=1.4$ (this is true throught this work unless explicitely stateted).



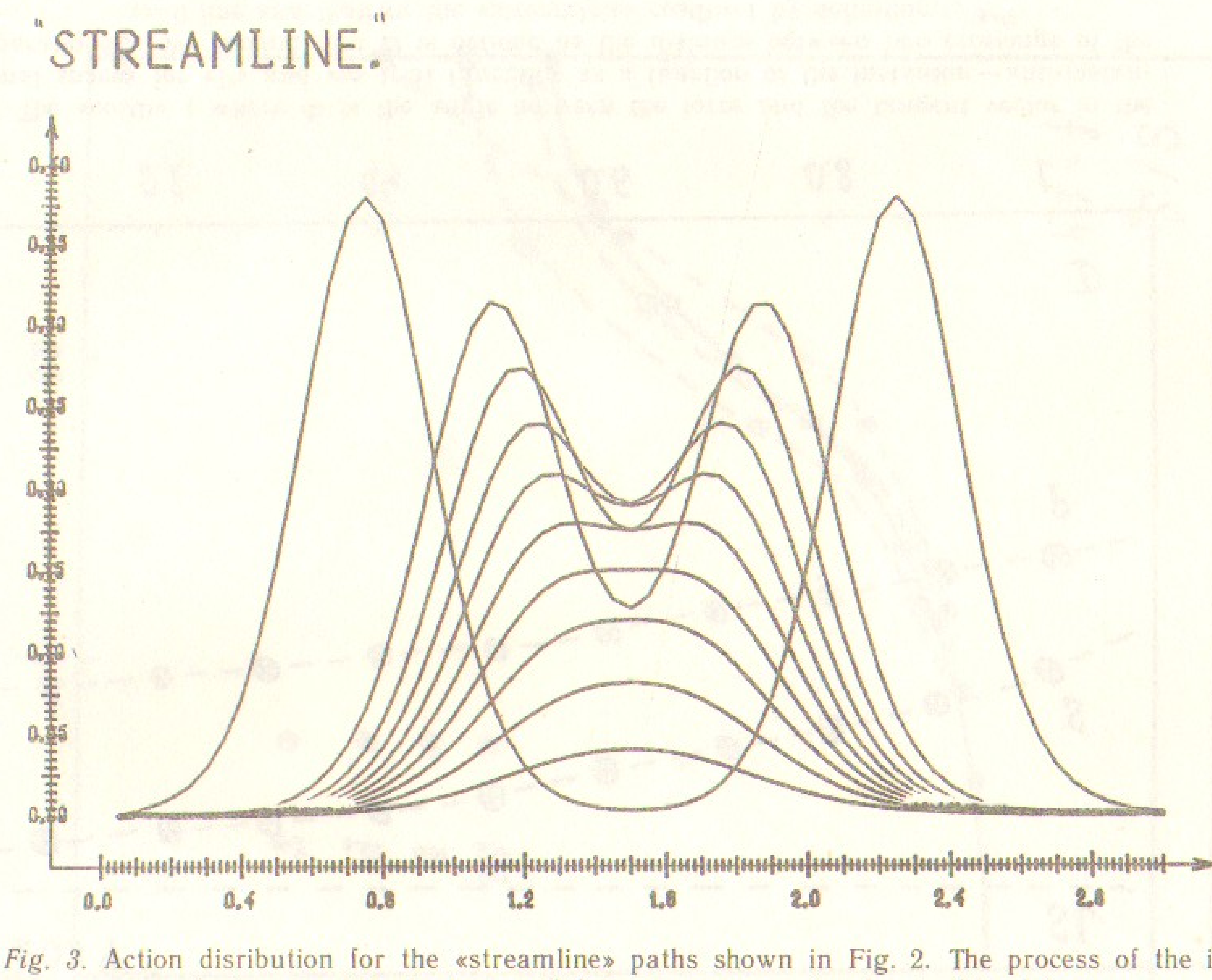


*Fig. 3.* Action disribution for the «streamline» paths shown in Fig. 2. The process of the instanton — anti-instanton annihilaion is more spectacular in this plot.

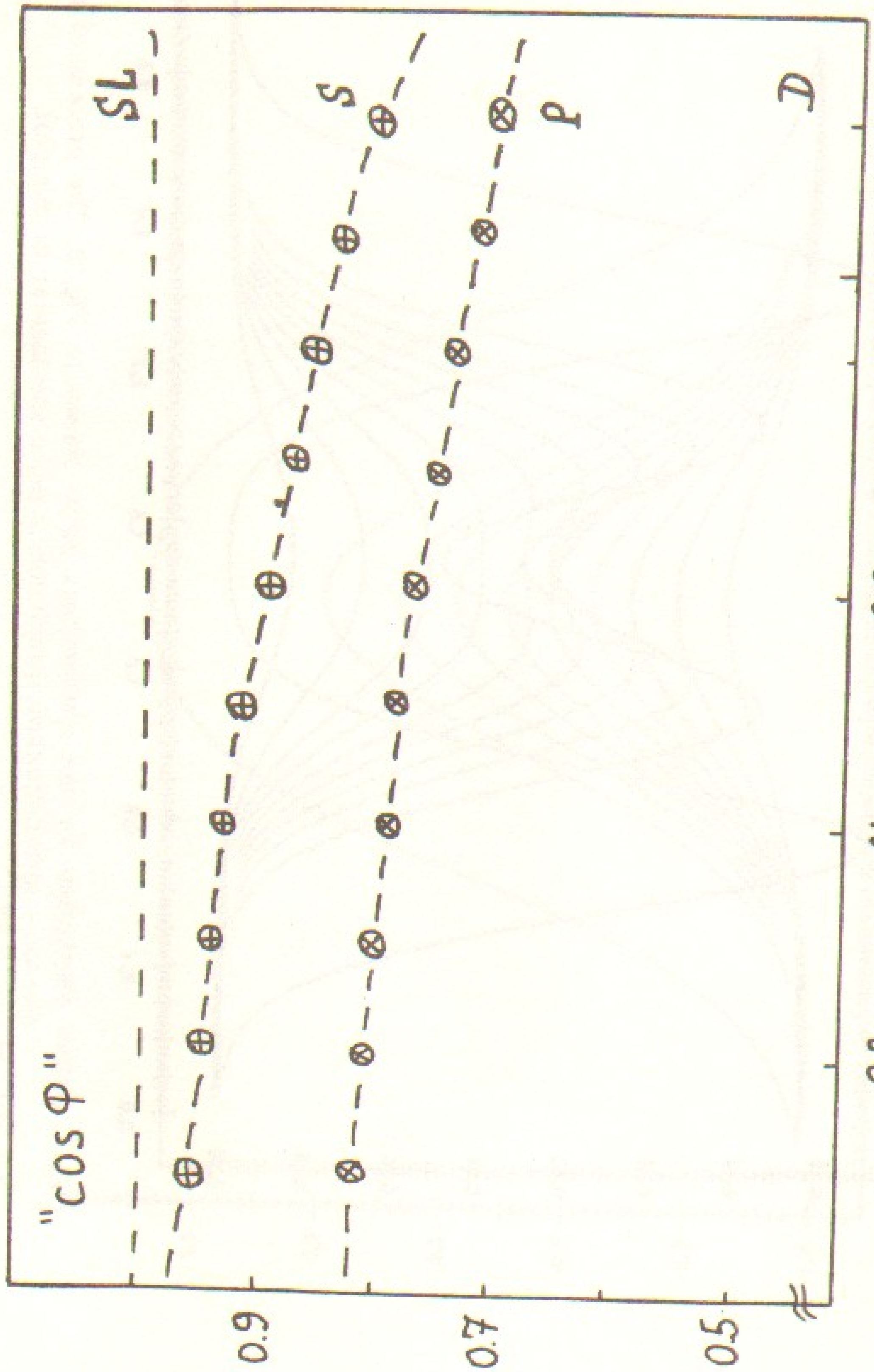


*Fig. 4.* The «cosΦ» ( where Φ is the angle between the force and the tangent vector in the functional space) for «P» and «s» trial functions as a function of the instanton — anti-instanton separation *D*. We remind that *D* is defined as the distance between two crossings of the $x=0$ line and that for the «streamline» $\cos\Phi=1$ by definition.



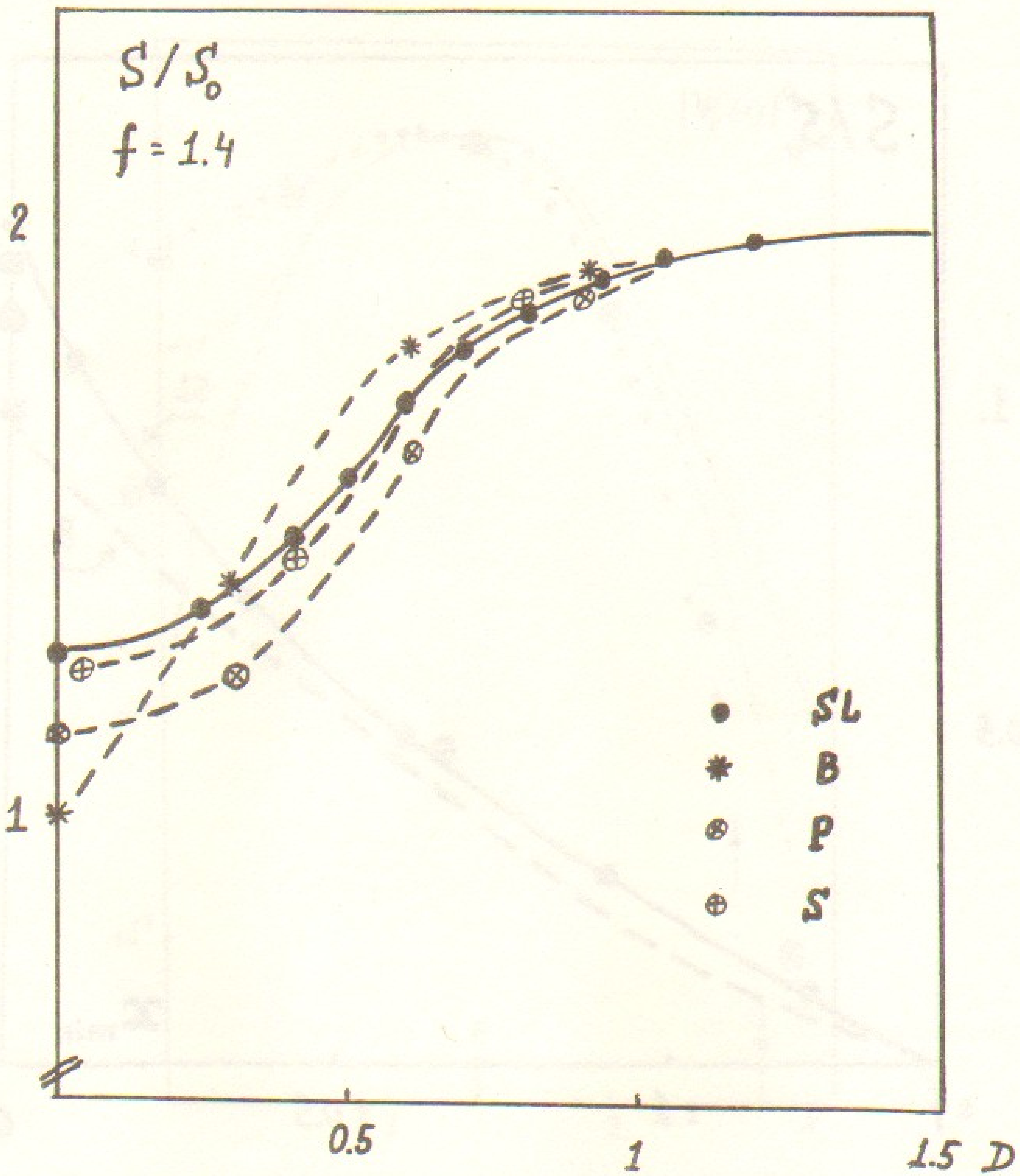


*Fig. 5.* The action *S* (in unites of the instanton action *S*) versus the instanton — anti-instanton separation *D* for the «streamline» set (the closed points and the solid line) as well as for the trial functions (other type of points as indicated in the figure, the dashed lines are for guiding the eye).

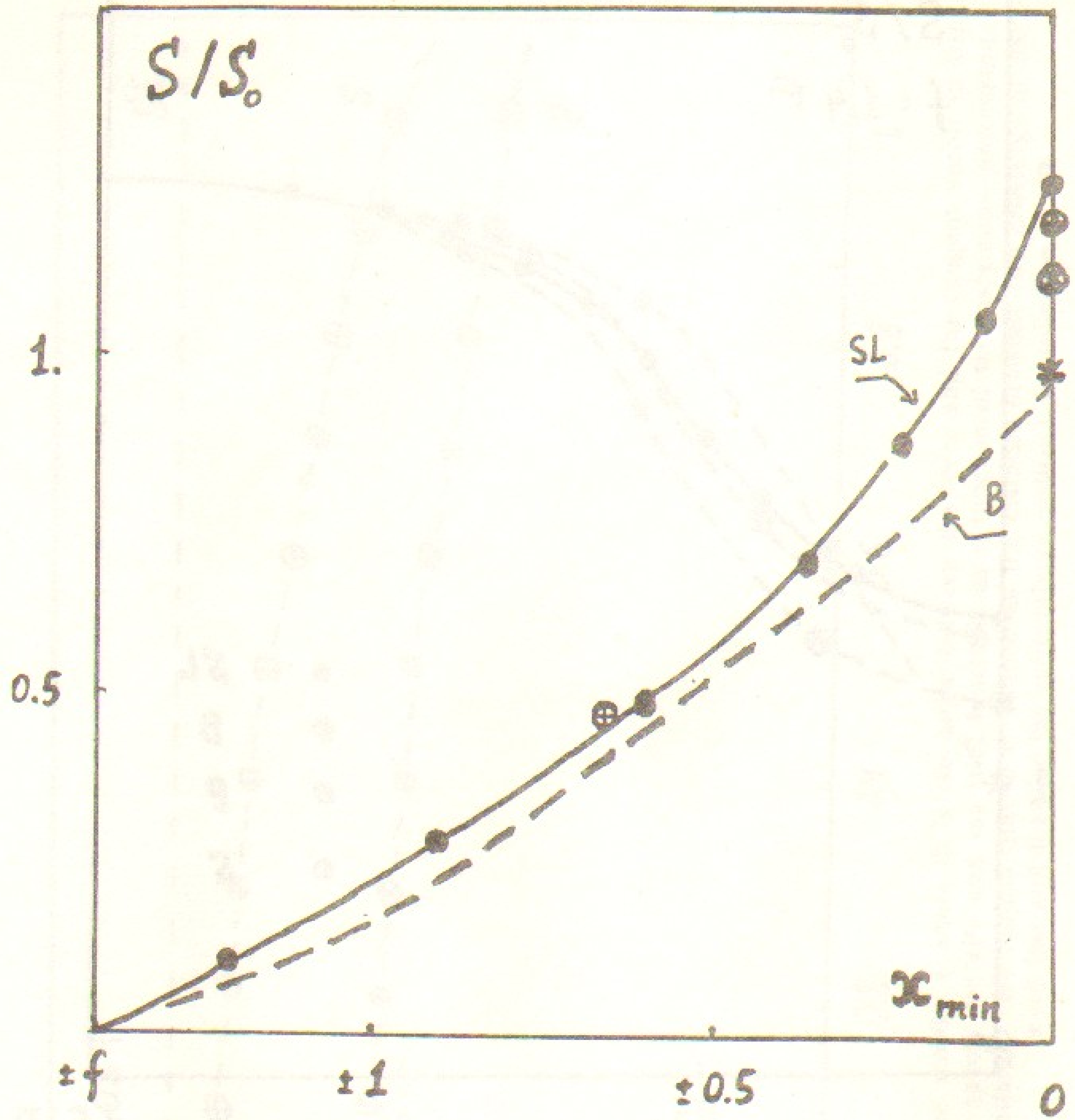


*Fig. 6.* The action $S$ (in unites of the instanton action $S_0$) for the flutons versus the maximal distance of the curve from the well bottom $x_{max}$ All notations are as in Fig. 5. The ansatz $B$ results shown by the dashed line also correspond to the semiclassical fluctons discussed in Section 3.



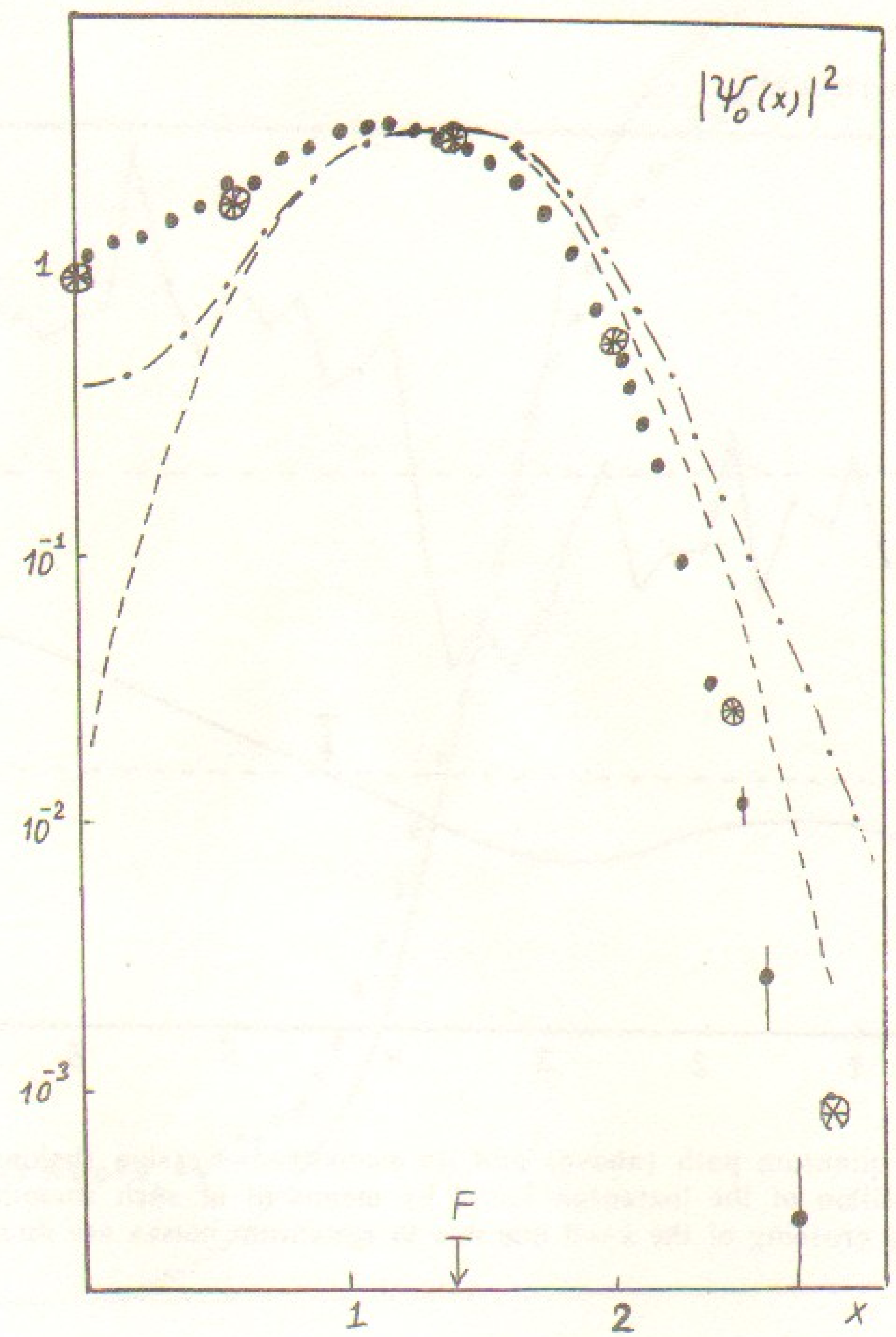


*Fig. 7.* The time-averaged coordinate probability (or the ground state wave function squared) at $f=1.4$. The points are straightforward «large lattice» simulations. The dashed and the dash-dotted lines correspond to the semiclassical flucton theory described in Section 3, the former for the linear oscillator and the latter for the double-well potential. Note that for the latter case one should add contributions of all types of the paths shown in Fig. 1. The points shown by stars correspond to «adiabatic switching» method and «small lattice» calculations (see text).

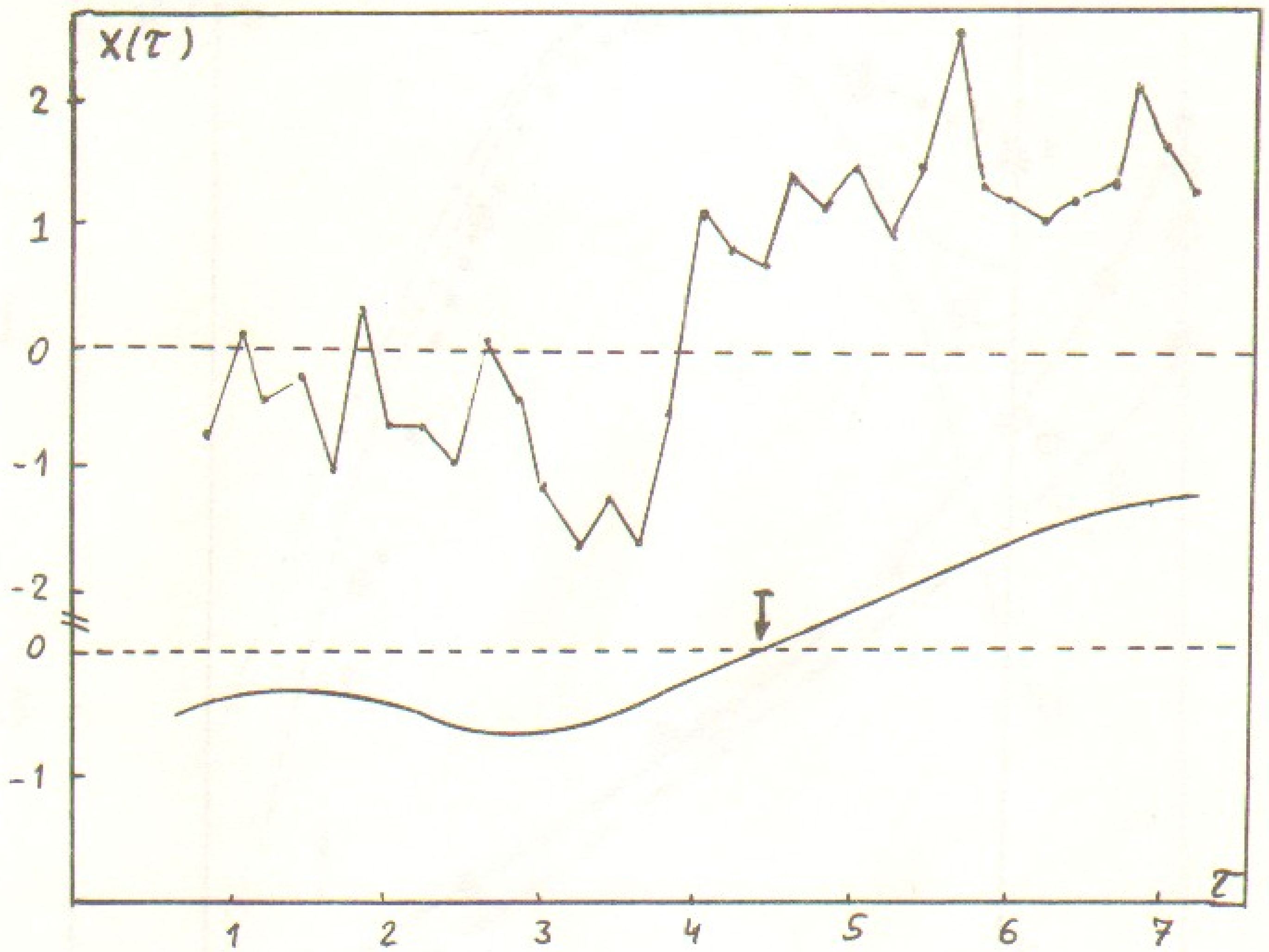


*Fig. 8.* Some quantum path (above) and its «smoothed» version (below). An arrow shows the position of the instanton found by means of of such smoothening, while auxilliary crossing of the $x=0$ line due to «quantum noise» are diregarded.



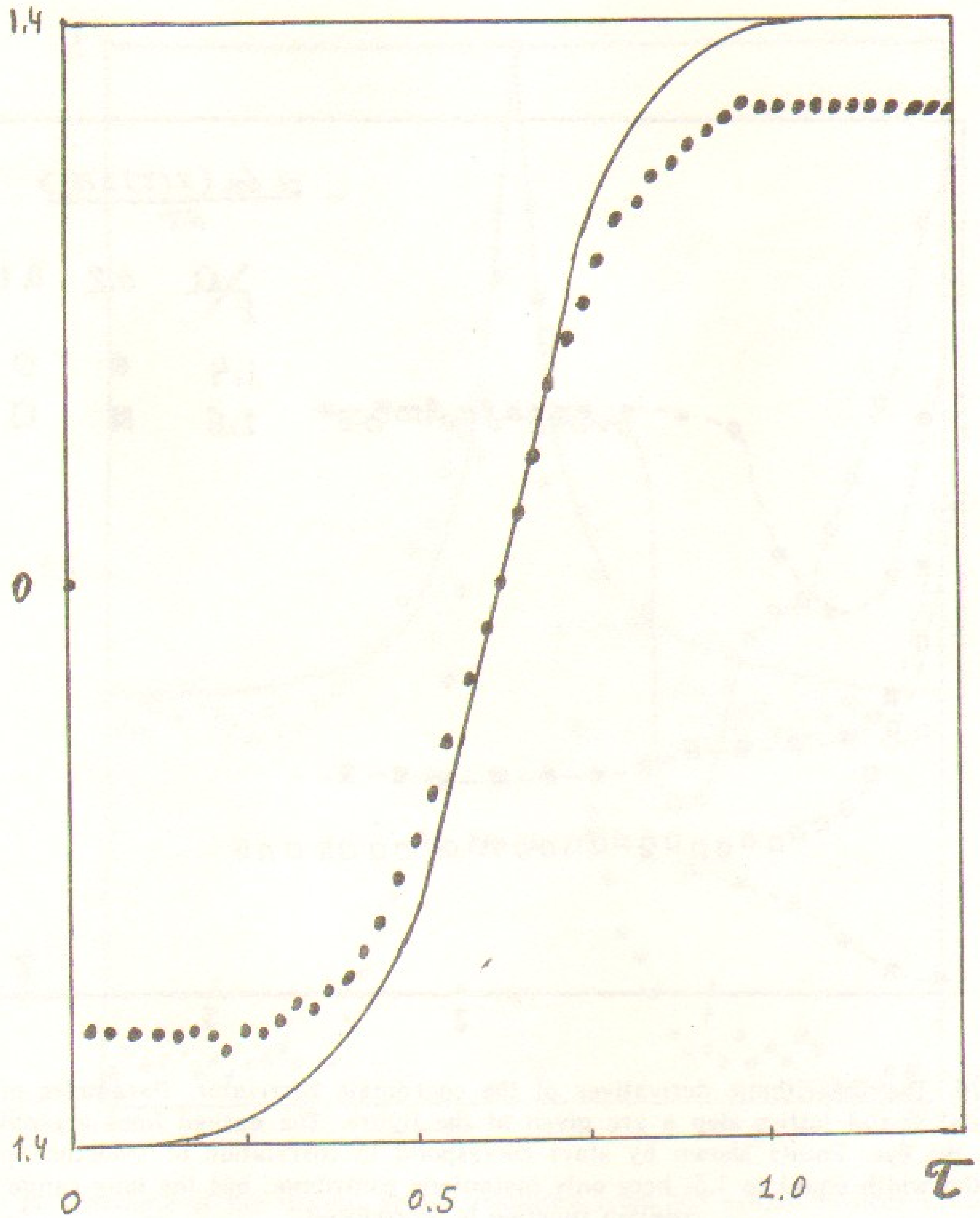


*Fig. 9.* The instanton shape as given by the semiclassical theory (the solid line) and that found from the «large lattice» numerical experiment (dots). The mean coordinate value for «ordinary oscillations» is not $+f$ because the wells are asymmetric (there are cubic and other odd terms in deviations).

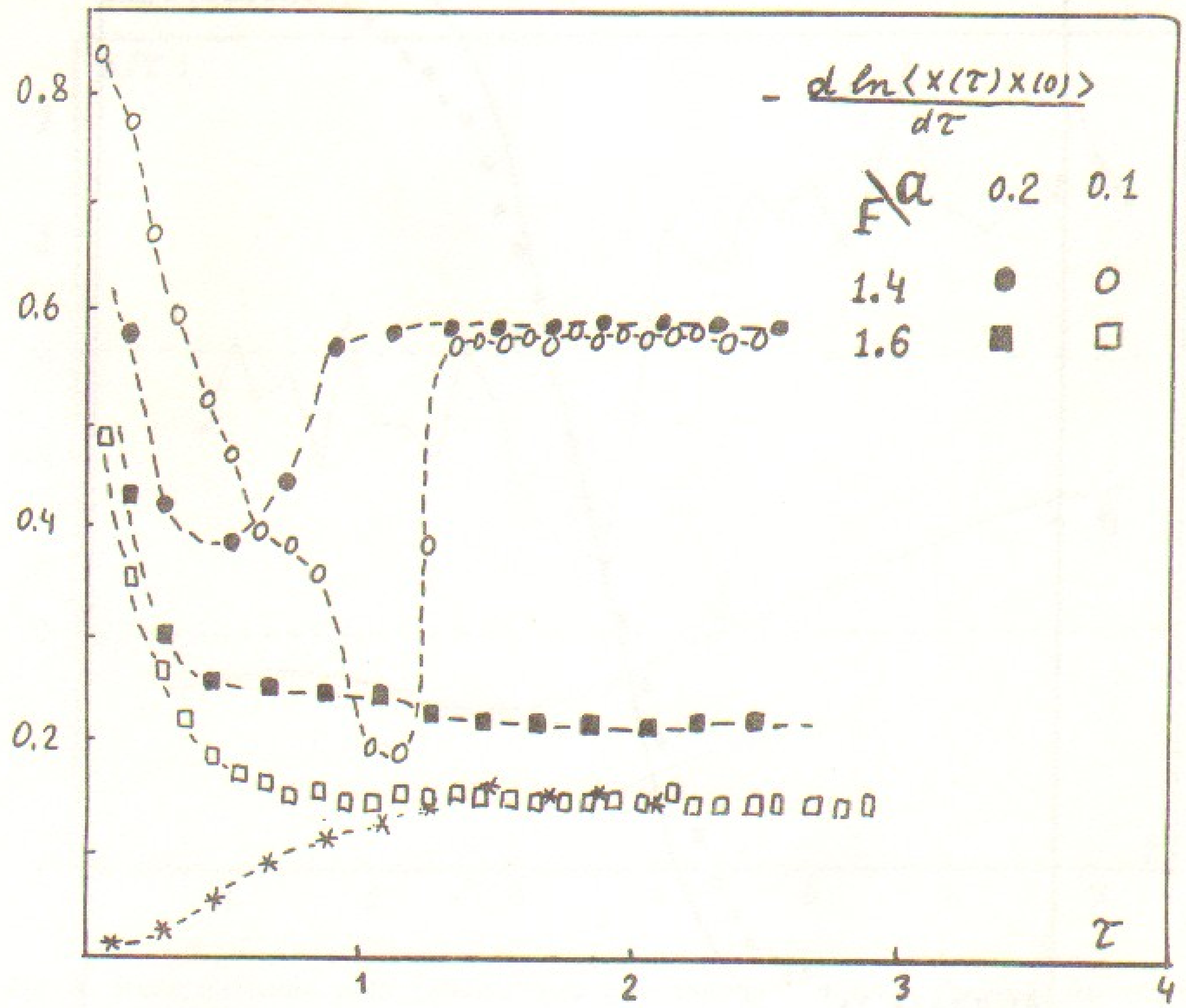


*Fig. 10.* The logarithmic derivatives of the coordinate correlator. Parameter of the potential $F$ and lattice step a are given at the figure. The dashed lines are only to guide the eye. Points shown by stars correspond to correlation of smoothed paths with the width equal to 1.5: here only instantons contribute, but the long-range correlation function is reproduced.



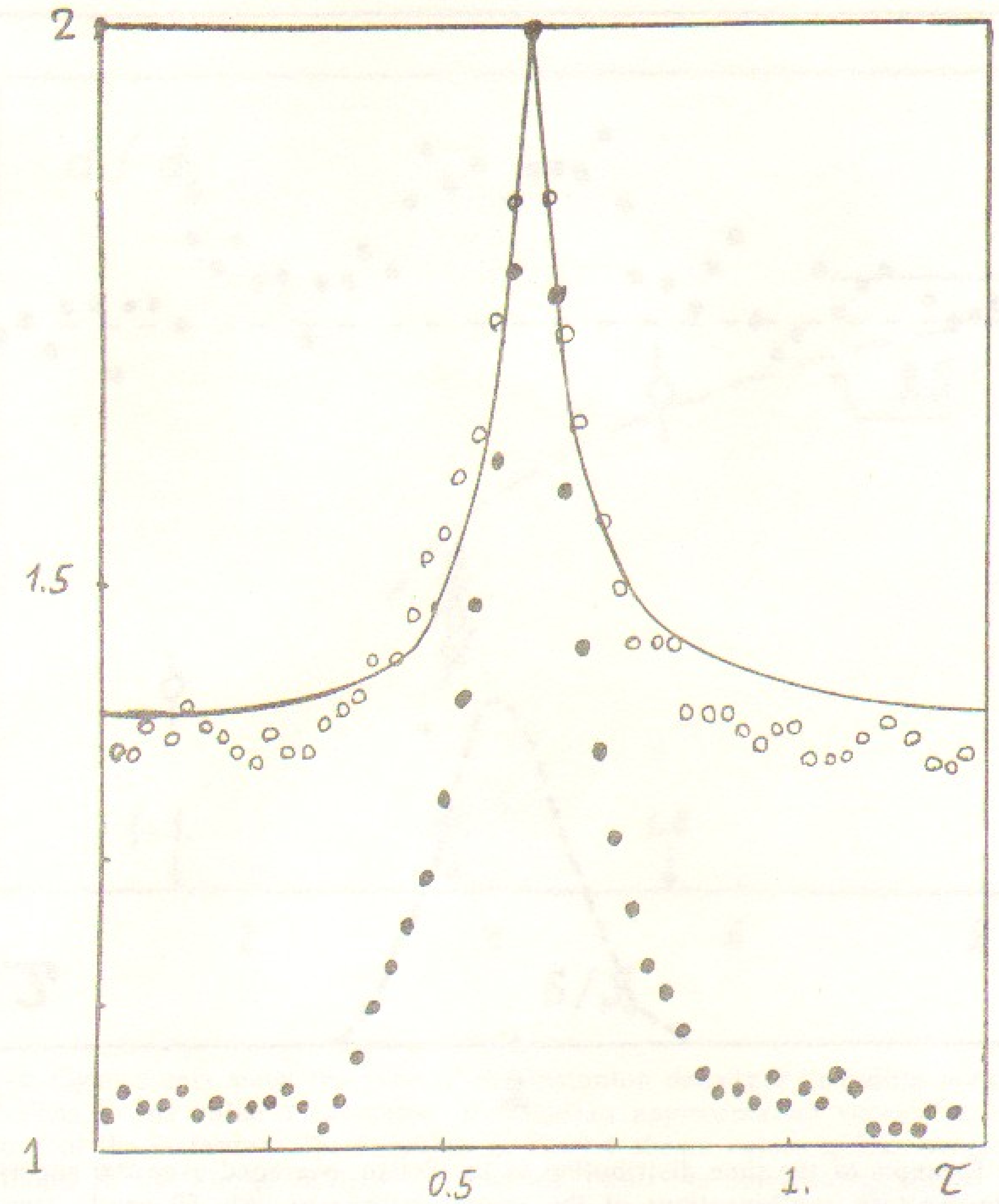


*Fig. 11.* Example of the flucton profile resulting from the «small lattice» calculation with contstraint at some point $x=2$. The curve corresponds to the classical path described in Section 3 the open and the closed points are for the linear oscillator and for the double-well system, respectively. (The calculations reported are made with the very small lattice step $a=0.025$ and, unlike the data given at Fig. 10, are insensitive to it.)

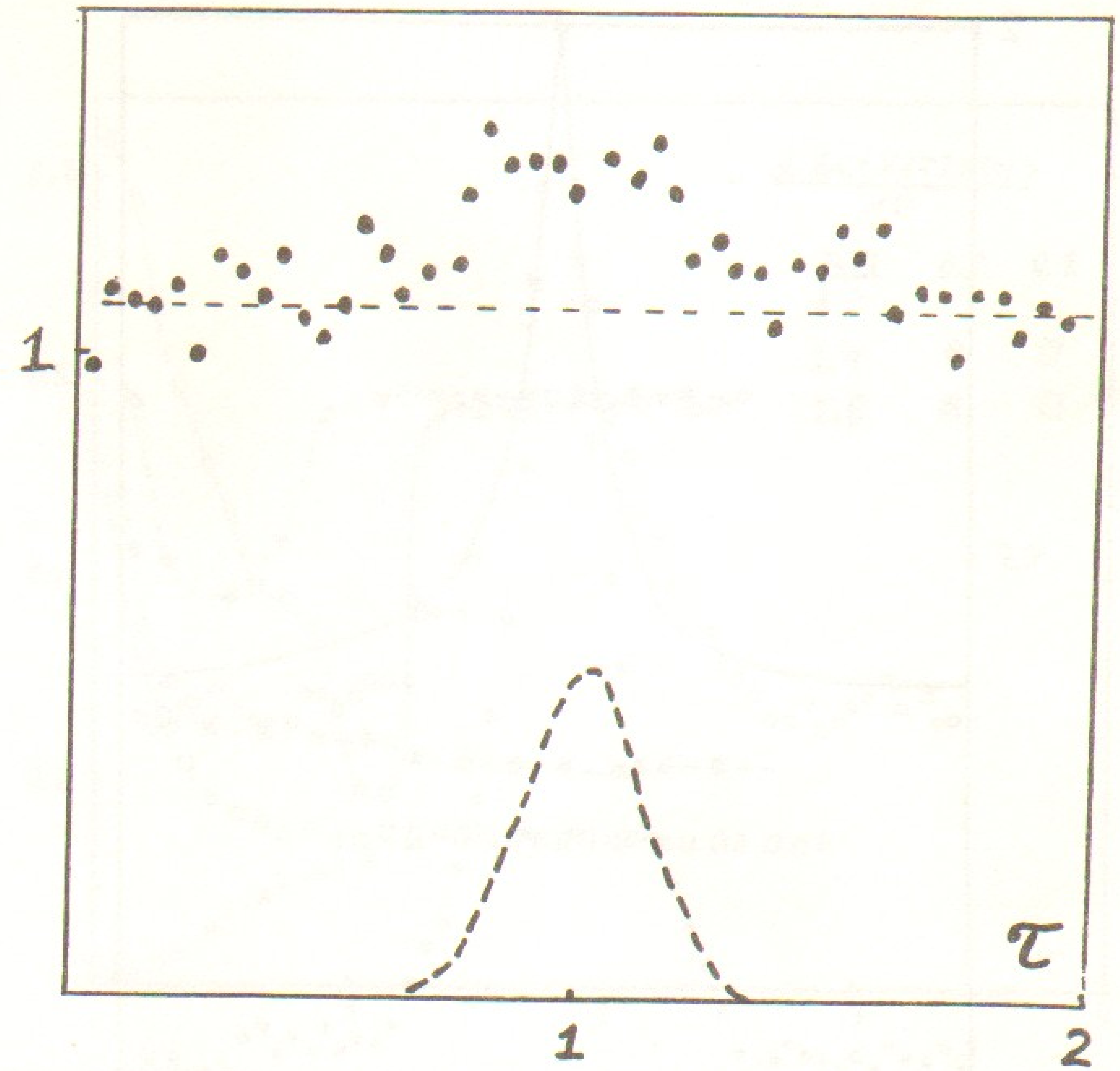


*Fig. 12.* Example of the time distribution of the action, avereged over 200 superimposed instanton-type configurations of the «small lattice» of only 50 points (the time step is $a=0.04$) with the antiperiodic boundary conditions. The dashed line below corresponds to the classical instanton solution, the dashed straight line above shows the mean «quantum noise» level measured in control cofigurations without instantons. Although a trace of the instanton is definitely seen, quantitative measurements are impossible.



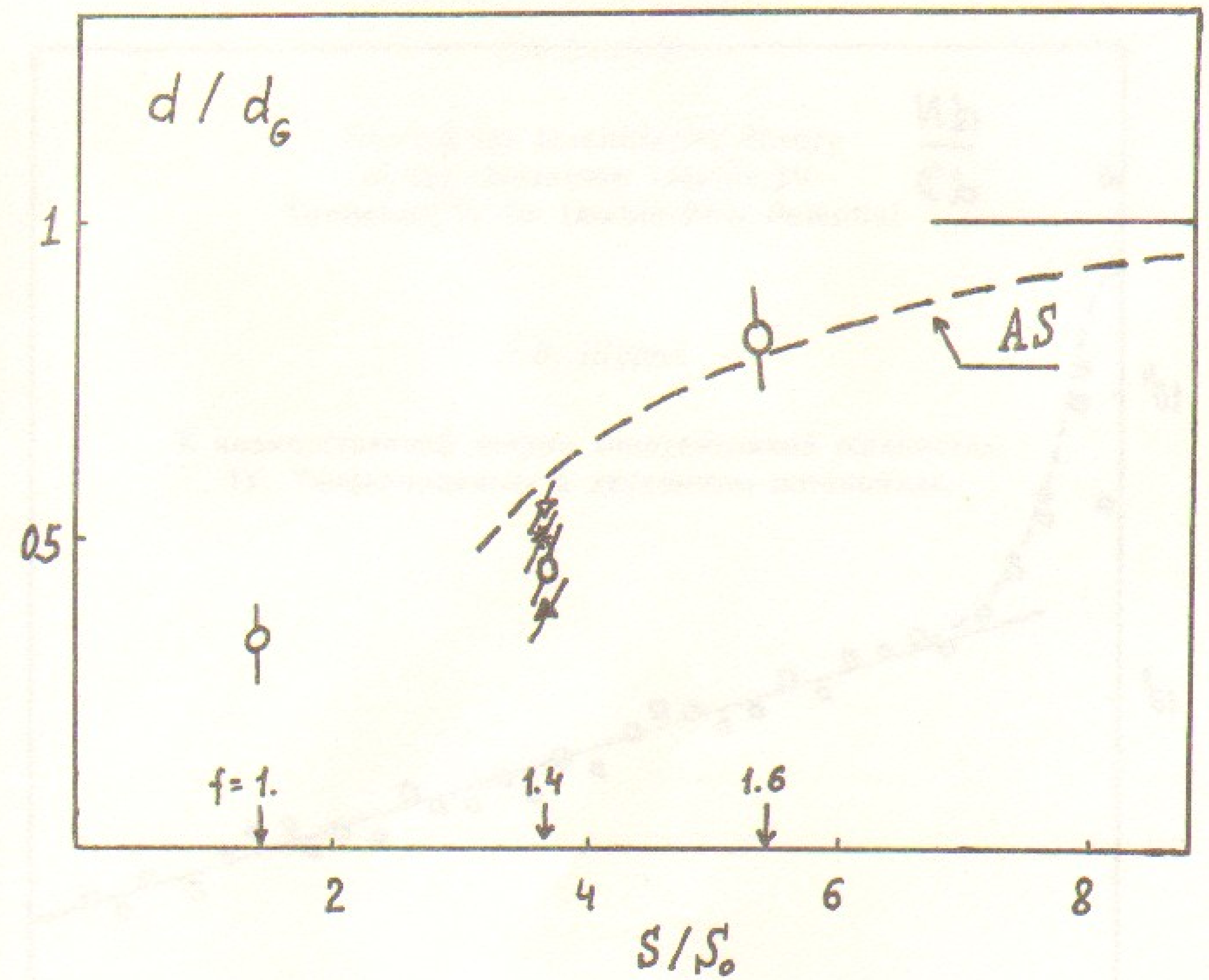


*Fig. 13.* Open points show the ratio of the instanton density $d$ including nongaussian corrections to the value $d$ calcuated in Gaussian approximation versus the classical action $S$ of the instanton. The triangles at $F=1.4$ shows values of the instanton density found in the «large lattice» calculations (with the smothening widths 0.1 and 1.5, upper and lower points). The star corresponds to $1/\langle D \rangle$ found from instanton separation distribution, see Fig. 11. The dashed line corresponds to the correction [5]. It is seen that the semiclassical theory becomes valid at $S$ value about 6.

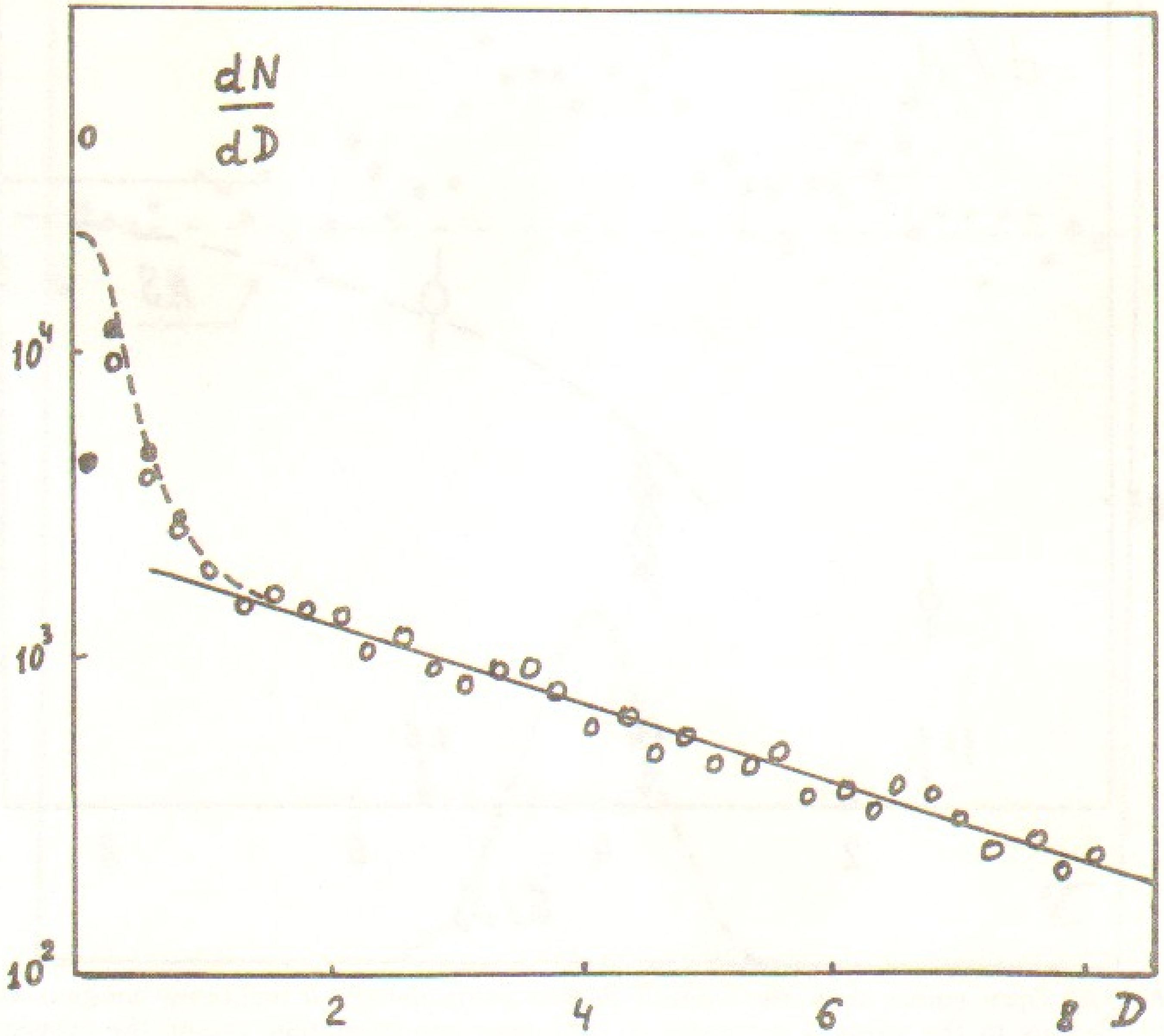


*Fig. 14.* Distribution over the instanton time separation $D$. The open points corresponds to the «large lattice» data with $T=40$, $a=0.2$ and the «naive» definition of the instanton (as the crossing of the $x=0$ line). The closed points are for the paths smoothed with the widths 0.1 (eliminating some «quantum noise» but affecting the most close pairs). The solid line for large $D$ is the exponential fit $\exp(-0.29 \cdot D)$, while the dashed one correspond to the correcion for the instanton—anti-instanton attraction, taken from the Fig. 5 for the «streamline».



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**Toward the Quantitative Theory of the «Instanton Liquid» IV. Tunneling in the Double-Well Potential**

*Э.В. Шуряк*

**К количественной теории «инстантонной жидкости». IV. Туннелирование в двухямном потенциале.**

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