ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

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TOWARD THE QUANTITATIVE THEORY OF THE TOPOLOGICAL PHENOMENA IN GAUGE THEORIES III. INSTANTONS AND LIGHT FERMIONS

PREPRINT 87-97

НОВОСИБИРСК

Toward the Quantitative Theory of the Topological Phenomena in Gauge Theories III. Instantons and Light Fermions

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ABSTRACT

The interaction of the pseudoparticles due to the light quark exchange strongly affect the structure of the «instantonic liquid». At large enough N_f these modifications are so strong that the density of the small-size «instantonic molecules» is ultraviolet divergent. Using some simplified models we study how the (chirally asymmetric) «polymer» phase is changed to the (symmetric) «molecular» phase as the pseudoparticle density is lowered. We have made the full-scale simulations for the SU(2) theory with quarks and have found that instantons do generate the quark condensate in its vacuum.

1. INTRODUCTION

The general role of the fermionic degrees of freedom in the gauge theories remains a matter of dispute in literature. The simplest suggestion is the so called «quenched approximation», an assumption that the fermionic determinant can be omitted in the partition function of the gauge fields. The well-known theoretical arguments in its favour are based on the consideration of the large number of colors $N_C \to \infty$ limit. Applications of this idea in lattice numerical experiments are widespread.

In this work we consider the role of light fermions in the theory of the «instantonic liquid», considered in the papers I [1] and II [2] of this series. Probably the main lesson drawn from these studies is a conclusion that the «quenched approximation» is fundamentally wrong in this case. More precizely, we have found that the fermionic determinant is an extremely important ingredient of the theory because it selects quite specific configurations out of the set saturating the statistical sum of the pure gauge theory. This is probably not so surprising because the number of light flavors N_f and the number of colors N_C are comparable, so the above mentioned «$N_C \gg N_f$» arguments do not actually apply.

The central role in what follows is played by the following fundamental fact (being essentially ignored by the «quenched»-based considerations): any topologically nontrivial gauge field configurations is associated with the so called «zero fermionic mode», a normalizable solution of the Dirac equation in this field. For instantons

this fact was discovered by G. t'Hooft [3], but it is a consequence of the general theorem [4]. Therefore, in this case the fermionic determinant is exactly zero which means that such configurations in fact give no contribution to the statistical sum.

The nontrivial effects related to these zero modes have been correlated with some long-standing puzzles of the hadronic spectroscopy. In particular, in the same paper [3] G. t'Hooft has noticed that these effects lead to explicite violation of the U(1) chiral symmetry, driving the Adler—Bell—Jackiw anomaly. In principle it solves the famous Weinberg «U(1) problem», explaining why the mass of the η' meson is so different from all other masses in the pseudoscalar nonet of mesons. Even more interesting are other physical phenomena related to the «zero modes», which are mainly discussed in this work, namely the physics of spontaneous breaking of the $SU(N_f)$ chiral symmetry (below for brevity — SBCS).

Roughly speaking, one may imagine pseudoparticles to be some effective sources (see Fig. 1,*a*) emitting (or absorbing) one quark-antiquark pair of each massless flavor. Any «cluster» of the pseudoparticles may exist in vacuum only due to a kind of «quark-exchange interaction» between them: all quarks and antiquarks emmitted should be absorbed by some another pseudoparticles. This picture suggest the following physical analogue, to be much discussed below. Our *PPs* are similar to some «atoms» (living in 4-dimensional space, of course), while the $N_f \cdot 2$ light fermions exchanged are analogous to a set of «valence electrons».

This analogy immediately suggests a lot of interesting questions. One may ask how the «matter» made of such «atoms» looks like, is it a chaotic «polymer» (examplified in Fig. 1,*c*), or is it made out of separate «molecules» (as in Fig. 1,*d*)? More precizely, is there the «infinite cluster» ranging all over the space, or all such clusters are but finite? As we will see below, the former «conducting» case implies SBCS, while the latter «insulating» phase means that this symmetry remains unbroken.

It is natural to start with the simplest «cluster» possible, the so called «instantonic molecules», (Sections 2, 3). Their investigation provides one more argument in favour of the importance of light fermions. Indeed, if one gradually increases their number N_f he can reach the point where the quark-induced interaction among instantons and anti-instantons is so strong that the density of the «molecules» becomes ultraviolet divergent. (This part of the work was already published in short form in Ref. [5]). As far as we know,

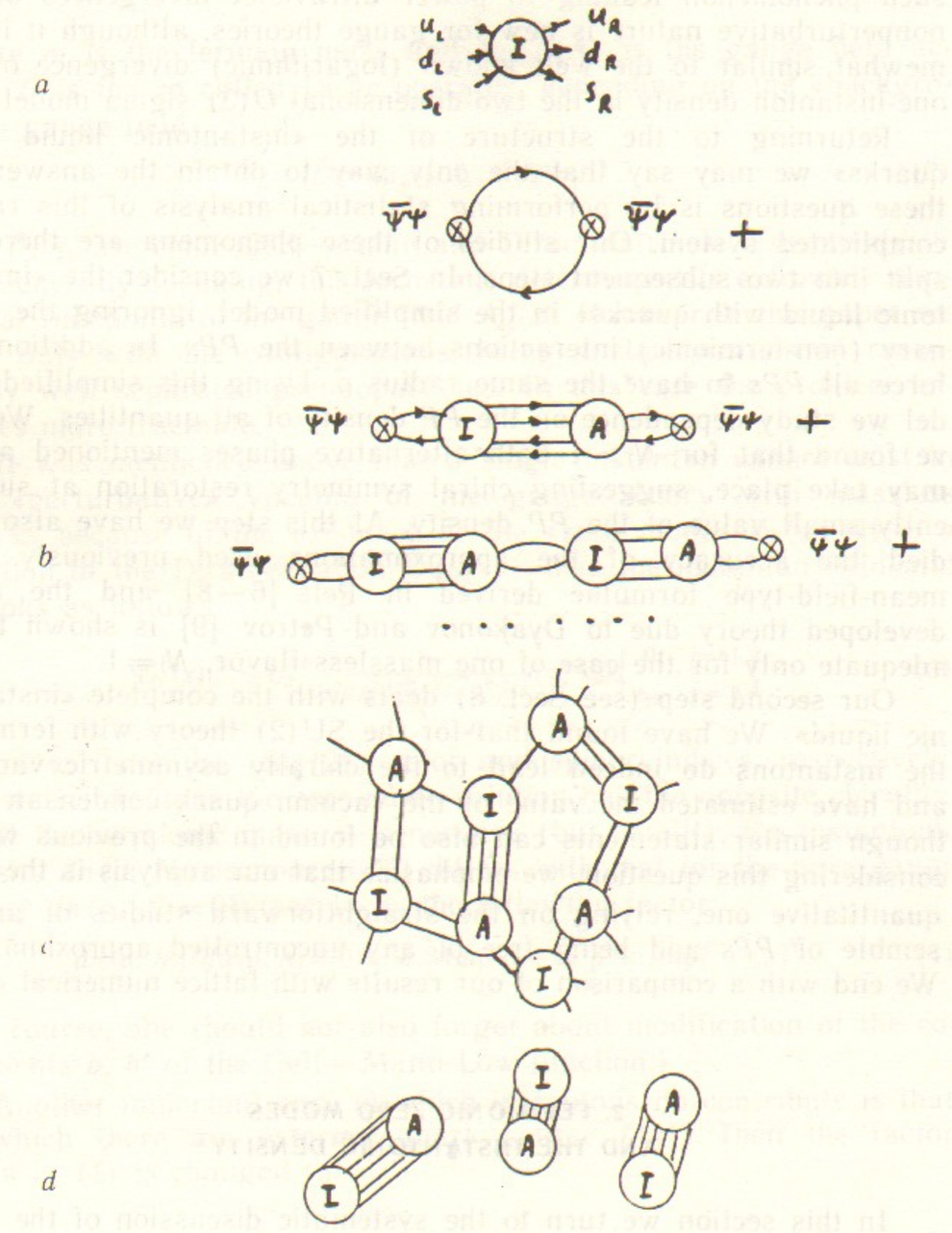


Fig. 1. The instanton-generated effective interaction of the light quarks (*a*). A set of ladder-type diagrams contributing to the correlation function of two $\bar{\Psi}\Psi$ operators at different points (*b*) Schematic picture of a «polymer»-type vacuum (*c*), to be compared to the «molecular» one (*d*).

such phenomenon leading to power ultraviolet divergences of the nonperturbative nature is new for gauge theories, although it is somewhat similar to the well known (logarithmic) divergence of the one-instanton density in the two-dimensional $O(3)$ sigma model .

Returning to the structure of the «instantonic liquid with quarks» we may say that the only way to obtain the answers to these questions is by performing statistical analysis of this rather complicated system. Our studies of these phenomena are therefore split into two subsequent steps. In Sect. 7 we consider the «instantonic liquid with quarks» in the simplified model, ignoring the ordinary (non-fermionic) interactions between the *PPs*. In addition, we force all *PPs* to have the same radius $\bar{\rho}$. Using this simplified model we study dependence on the *PP* density of all quantities. We have found that for $N_f > 1$ both alternative phases mentioned above may take place, suggesting chiral symmetry restoration at sufficiently small value of the *PP* density. At this step we have also studied the accuracy of the approximations used previously. The mean-field-type formulae derived in Refs [6—8] and the more developed theory due to Dyakonov and Petrov [9] is shown to be adequate only for the case of one massless flavor, $N_f = 1$.

Our second step (see Sect. 8) deals with the complete «instantonic liquid». We have found that for the SU(2) theory with fermions the instantons do indeed lead to the chirally asymmetric vacuum and have estimated the value of the vacuum quark condensate. Although similar statements can also be found in the previous works considering this question, we emphasize that our analysis is the first quantitative one, relying on the straightforward studies of an ensemble of *PPs* and being free of any uncontrolled approximations. We end with a comparison of our results with lattice numerical data.

2. FERMIONIC ZERO MODES AND THE INSTANTONIC DENSITY

In this section we turn to the systematic discussion of the topological effects in the presence of fermions, reminding the reader the main formulae and the terminology used .

The first step made is usually the formal integration over the fermionic fields. Then one proceeds to the partition function of the gauge fields containing the so called fermionic (or Mattew—Salam) determinant

$$Z = \int DA_{a\mu}(x)\ \det\,[i\hat{D}(A_{a\mu}) + im]\ \exp\{-S_{gauge}[A(x)]\} \qquad (1)$$

where m is the fermion mass and $S_{gauge}(A)$ is the gauge field action. $\hat{D}$ is the so called Dirac operator, depending on the «background» gauge field

$$i\hat{D} = (i\partial_\mu + A_{a\mu}\, t^a/2)\,\gamma_\mu \qquad (2)$$

and t^a, γ_μ are color Gell—Mann and Dirac matrixes, respectively.

Generally speaking, this fermionic determinant is extremely nontrivial functional of the gauge field $A_{a\mu}(x)$. However in this paper we deal only with the configurations, being a superposition of reasonably well separated pseudoparticles. In this case the problem becomes more tractable.

It was mentioned above that a single instanton cannot exist in the «perturbative» vacuum of the gauge theory with massless quarks because of the existence of the «zero mode» $\psi_0(x)$. It is a solution of the Dirac equation $\hat{D}\psi_0(x) = 0$ in the instanton field and it looks as follows

$$\Psi_0^{(I)}(x)|_i^\alpha = U_I^{\alpha\beta}\,\frac{\rho}{\pi(2x^2)^{1/2}(x^2+\rho^2)^{3/2}}(\gamma_\mu^{ij}\, x_\mu)\begin{cases} 0 & j=1.2 \\ \varepsilon_{j\beta} & j=3.4 \end{cases} \qquad (3)$$

where α, i are the (SU(2)) color and spinor indices, respectively. For anti-instantons the zero-mode solution has the opposite chirality.

If the fermionic mass m is nonzero (but small!), the instantonic density $dn(\rho, N_f)$ is nonzero. It differs with that for the pure gauge theory $dn(\rho, N_f = 0)$ (see I) by the following factor:

$$dn(\rho, N_f)/dn(\rho, N_f = 0) = [1.34 m\rho\,(1 + m^2\rho^2 \ln(m\rho)^2 + \ldots]^{N_f}. \qquad (4)$$

(Of course, one should not also forget about modification of the coefficients b, b' of the Gell—Mann-Low function.)

Another important case in which instantons do contribute is that in which there are external quark source $J(x)$. Then the factor given in (4) is changed to

$$dn(\rho, N_f)/dn(\rho, N_f = 0) = \{1.34\,[m\rho\,(1 + \ldots) + \int dx\, J^+\psi_0 + c.c]\}^{N_f}. \qquad (5)$$

In particular, in the vacuum possessing a nonzero average of the operator $\bar{\Psi}\Psi$, the so called «quark condensate», the individual small-size instantons can well be present (see discussion and detailed formulae in [10]).

Two comments important for what follows can be made here. First of all, for $N_f=1$ this instanton-generated vertex is bilinear, so it is tempting to assume that instanton generate a kind of an effective quark mass [7]. For $N_f>1$ there appear more complicated multi-fermion operators, and their effect on the quark fields is more difficult to understand. Second observation is as follows: increasing N_f one finds stronger suppression of small-size instantons. In Sect. 4 we show, that it is not the case for the small-size instantonic «molecules».

3. INSTANTONIC MOLECULES

We start their discussion with a remark that similar objects are well known in physics. For example, the well-known planar Heisenberg magnetic (or the so called XY model) is known to have the «vortex molecules» in its low temperature phase. These molecules are melting into some «vortex plasma» at the Beresinsky—Kosterlitz—Thouless transition. Thus, the physics of this transition is somewhat similar to that studied in this work. First discussion of the role of the instanton—anti-instanton molecules for d=4 gauge theories with light fermions was made in Ref. [7], where it was also noted that such «molecules» should dominate if the PP density is small.

The instanton—anti-instanton pair has trivial global topology and, respectively, the nonzero determinant. Its estimate can rather simply be made in the case when the PPs are well separated by sufficiently large distance R exceeding their dimensions ρ. The problem is identical to that of the energy levels of two separated identical atoms, for which the wave functions are just $(\Psi_1\pm\Psi_2)/\sqrt{2}$ and energies are split symmetrically with the gap value equal to twice the nondiagonal matrix element of the Hamiltonian. Quite similarly, in the subspace composed by two «zero modes» $\psi_0^{(I)}$, $\psi_0^{(A)}$ of the instanton and the anti-instanton the Dirac operator can be written in the following matrix form

$$i\hat{D}=\begin{vmatrix}0 & T\\ T^* & 0\end{vmatrix} \tag{6}$$

where T is the so called «zero mode overlap integral», depending on the positions and the orientations of both pseudoparticles. The asymptotics of T at large R is known [11, 9]

$$T(U_I, U_A, R)\underset{R\to\infty}{\to}-\frac{2i\,\rho_I\,\rho_A}{R^4}\,\mathrm{Tr}\,|U_A(R_\mu\,\tau_\mu^+)\,U_I^+| \tag{7}$$

where $\tau_\mu^\mp=(\vec{\tau},\mp i)$. (The asymptotics R^{-3} can be understood as just coming from the propagator of a massless quark.)

Behaviour of T at finite R depends on the particular «ansatz» field configuration used. In II we have considered two of them, the simplest sum ansatz («S») and the «ratio ansatz» («R»). As the former is just a sum over PPs it leads to many specific simplifications in what follows, so in this work we have taken this form for T. Indeed, if

$$A_{a\mu}(x)=U_I^{ab}\,A_{b\mu}^{(I)}(x-z_I)+U_A^{ab}\,A_{b\mu}^{(A)}(x-z_A). \tag{8}$$

one may use the Dirac equations for $\psi_0^{(I)}$, $\psi_0^{(A)}$ very effectively and eliminate either derivatives, or the fields. The latter trick leads to simple dependence on the orientation matrices U describing orientations of pseudoparticles:

$$T(U_I, U_A, R)\approx i\,\mathrm{Tr}\,|U_A(R_\mu\,\tau_\mu^+)\,U_I^+|\,f(R^2). \tag{9}$$

Note that the trace here is nothing else but the cosine of the «relative orientation angle» Φ introduced in II, therefore

$$T(\Phi, R)=\cos\Phi\cdot Rf(R^2). \tag{10}$$

Dependence of T on the distance was evaluated numerically with the following result

$$f(R)\simeq 2/(2.58+R^2)^2. \tag{11}$$

Note that the overlap integral T enters the determinant in rather large power $2N_f$. Therefore, two values of the relative orientation angle $\Phi=0$, π are the most probable ones. It is interesting that it is also the values favoured by the classical dipole interaction (see II).

Note also that in this case T at small distances has some «kinematical» zero, suppressing the contribution of the «compact molecules». Anyway, at small R the very separation of zero modes from all others is meaningless, so we cannot in fact properly describe these objects. Fortunately, our «instanton liquid» turns out to be rather dilute, so we have at least «a posteriori» argument that such «compact molecules» are not very important for the ensemble to be studied.

4. SMALL MOLECULES AT LARGE N_f

The title of this section needs some explanations. By «large N_f» we do not mean $N_f \to \infty$, of course, but rather its values approaching the point where the asymptotic freedom becomes broken. In this connection we remind the two-loop expression for the renormalized charge

$$\frac{8\pi^2}{g^2(k)} = b \ln \frac{k}{\Lambda} + \frac{b'}{2b} \ln \ln \frac{k}{\Lambda} + O\left(\frac{1}{\ln k/\Lambda}\right),$$

$$b = \frac{11}{3} N_C - \frac{2}{3} N_f,$$

$$b' = \frac{34}{3} N_C^2 - \frac{13}{3} N_C N_f + N_f/N_C. \qquad (12)$$

It is seen that if $b \to 0$ than the role of the second term becomes larger. Note also, that b' changes sign in this region. Both facts shows that the theories at which b is small are very specific: the perturbative momentum scale at which (12) holds is shifted to extremely high momenta! All other scales are therefore a subject for some «nonperturbative physics».

As a specific example of the kind we are going to discuss «small molecules». The word « small» means that both the pseudoparticle radii ρ_I, ρ_A, and their separation R are small compared to Λ^{-1}. Therefore, the relevant action is much larger than unity and the semiclassical formulae are applicable. As mentioned in the preceeding section, we also exclude «compact molecules» with $R < \rho_I, \rho_A$ and consider only those with $R > \rho_I, \rho_A$.

Let us start with very «asymmetric» molecules with, say, $\rho_I \gg \rho_A$. It is quite clear that for the anti-instanton one may apply the operator product expansion formalism as in [10] and obtain the small factor $(\rho_A/\rho_I)^{3N_f}$. Thus, suppression of «asymmetric» molecules at large N_f is evident.

Now we turn to the case of very «dilute» molecules, with $R \gg \rho$. In this case the small factor due to zero modes in the quark determinant is as follows

$$\det(i\hat{D}) \sim T^{2N_f}(R) \sim (\rho/R)^{-6N_f} \qquad (13)$$

and very «dilute» molecules are unimportant too.

We have shown that the integrals over the ratio ρ_I/ρ_A and R/ρ

are well convergent, and that most important molecules are those with $\rho_I \sim \rho_A \sim R$. If so, their total density in vacuum can be obtained just by the simple dimensional arguments, because the power of the lambda parameter is known from the semiclassical expression

$$\frac{dn_{molecular}}{d\rho d^4 z} \sim \frac{1}{\rho^5} (\rho\Lambda)^{2b(1-\delta)}. \qquad (14)$$

Here δ corrects for the deviations from twice the instanton action (we remind that, at least for the trial functions considered in II, for $R > \rho$ this δ is small, about 0.1).

If $b(1-\delta) < 2$ the density (14) is divergent at small radii: this is the «nonperturbative divergence» mentioned above. The critical value (8 for two and 13 for three colors) is still below the point where the asymptotic freedom is broken. Note also, that because in «compact» molecules the action is reduced stronger, their density may be divergent even earlier. Near this critical point the molecule density (and the nonperturbative vacuum energy density) becomes infinite. Does it really spoil the theory completely, or this infinity may be removed by a sort of «renormalization»?

Note that although being infinitely numerous, the small-size molecules still occupy negligible fraction of space-time: the integral $\int dn(\rho)\rho^4$ is convergent. Similar situation holds with the physical observables. Small molecules affect particle propagation in vacuum, but their contribution to the quark mass is of the order of $\int dn(\rho)\rho^2$, also convergent at the critical point mentioned above. However, at another critical points $b(1-\delta)$ crosses 1, and from this point one has to introduce additive nonperturbative correction to the bare fermionic mass!

Of course, this phenomenon takes place at the unphysical number of light quarks, but they may be used as a test for lattice numerical experiments. (Althogh it is not easy to see small-size molecules on the lattice directly, their influence may be detected indirectly, for example by enhanced deviations from the perturbative scaling.) But the most important consequence of this observation is the statement, that fermions can be the dominant ingredient of the vacuum, leading to extremely complicated field distribution. This probably may help us to understand why in the real world the vacuum is rather inhomogeneous.

5. SPONTANEOUS BREAKDOWN OF THE CHIRAL SYMMETRY

First of all, it is necessary to say what is the SBCS phenomenon under consideration. Let us discuss some gauge theory with the fermions, and let us study the limit in which their mass tends to zero. As the interaction of these fermions is transfered by the vector fields which do not change chirality, the left and the right-handed components of these fields become quite independent in this limit. In particular, one may independently rotate them in the flavor space, which is the chiral symmetry under consideration.

However, the limit $m \to 0$ may in fact be not so simple: the ground state of the theory may turns to be asymmetric. More precizely, if fermions move in some external gauge field $A(x)$ which is not weak, the Dirac operator $iD(A)$ may have eigenvalues λ very close to zero. If so, the (Euclidean) propagator (being an inverse to $(i\hat{D}+im)$ and therefore looking simple in terms of its eigenvalues λ and eigenfunctions $\Psi_i(x)$)

$$S(x,y)=\sum_i \frac{\Psi_i(x)\Psi_i^+(y)}{\lambda_i+im} \qquad (15)$$

is singular in the limit $m \to 0$. Taking $y=x$ and performing the trace, one may proceed to the so called quark condensate:

$$\langle \bar{\Psi}\Psi \rangle = \frac{1}{V}\,\mathrm{Tr}\int dx\, S(x,x) = -\frac{1}{V}\sum_{\lambda_i \geqslant 0} \frac{m}{\lambda_i^2+m^2}. \qquad (16)$$

(We have used the fact that in average the condensate is the same at all points and have integrated over x, using the normalization condition of the modes. We also have used the fact that, due to the chiral symmetry, all eigenvalues goes in pairs, $\pm|\lambda|$).

In the limit $m \to 0$ one may rewrite (16) in terms of the eigenvalue spectrum density $dn/d\lambda$ and specify the order of both limits considered

$$|\langle \bar{\Psi}\Psi \rangle| = \lim_{(m\to 0)} \cdot \lim_{(V\to\infty)} \cdot \left(\frac{\pi}{V}\frac{dn}{d\lambda}\bigg|_{\lambda=0} \right) \qquad (17)$$

where V is the 4-dimesional volume considered. Expression (17) is currently used in lattice numerical experiments as a practical signal for SBCS. For any gauge field configuration the spectrum of the

Dirac operator is found numerically and the level density $dn/d\lambda|_{\lambda=0}$ is determined from some extrapolation to be discussed below.

Using these formulae it is easy to explain why instantons may be more important for SBCS than any other gauge field fluctuations. Consider some field configuration made of $N_I = N_A$ *PPs*. As the total topological charge is zero, there is no reason to have exactly zero modes, but if the *PPs* overlap weakly then there should be eigenvalues λ very close to zero. Thus, being interested in $dn/d\lambda|_{\lambda=0}$ at zero we naturally study the fermionic states related to them. It is analogous to evaluation of a conductivity of a condensed matter considering only electrons in energy zones near the Fermi level.

The first attempt to point out whether *PPs* really lead to spontaneous breaking of the chiral symmetry or not was made by Caldi [12], who has considered the ladder-type diagrams (see Fig. 1,*b*) summed by the Bethe — Solpeter equation. On this way one may at least formulate some sufficient instability condition for the chirally symmetric vacuum.

Later this problem was studied in the mean-field approximation (for the quark condensate) by Carlitz and Creamer [6], Callan, Dashen and Gross [7] and myself [8]. This approach lead to some estimate of the quark condensate etc. Generally speaking equations of Ref. [6] are a complicated set of integral equations for the distribution over the *PP* parameters, but if one forces all instantons to have the same radius $\bar{\rho}$ they become just simple algebraic equations, leading to the following results [8]:

$$M_{det} = \pi\bar{\rho}/\bar{R}^2,$$
$$|\langle \bar{\Psi}\Psi \rangle| = 1/(\pi\bar{\rho}\bar{R}^2). \qquad (18)$$

(Here we have used $N_C=2$ and, for clarity of the presentation, have used the mean interparticle spacing $\bar{R}=n_{PP}^{-1/4}$ instead of the *PP* density.)

The former quantity in (18) is the so called «determinantal mass», to be much discussed below. It characterizes the mean value of the fermionic determinant, which is specially put in such a form that in the expression (4) for the instanton density one should substitute the «bare» mass m by $(m+M_{det})$. In other terms, M_{det} is the «geometric mean» of the eigenvalues because $M_{det} = \det(i\hat{D})^{1/N}$ where N is the number of *PPs*. One should not mix this quantity with the so called «quark effective mass» introduced in many works

Two parameters $\bar{\rho}$, $\bar{R}$ were phenomenologically estimated in [8] for the QCD vacuum (we have briefly considered it in I), and the mean field estimates (of course, for $N_C=3$) were shown to produce the values of the quark condensate and the «determinantal mass» of quite reasonable magnitude. Also the condition derived by Caldi was satisfied, thus it was concluded in [8] that the chiral symmetry seems to be broken by instantons.

Recently discussion of the subject was revived by Dyakonov and Petrov [9]. First, they have qualitatively discussed what happens if the positions and orientations of the *PPs* are random (we will refer to such an ensemble of *PPs* as the «random model»). In this case one may expect the nonzero quark condensate at any finite *PP* density. Indeed, it is easy to show that for such «random model» the eigenvalue spectrum has the semi-circular shape with the peak at zero and with the width of the order of mean overlap integral of the zero modes. As this integral at large *PP* separation R behaves as $1/R^3$, this model predicts at small *PP* densities that

$$M_{det}\sim\bar{\rho}^2/\bar{R}^3,$$
$$|\langle\bar{\Psi}\Psi\rangle|\sim 1/\bar{\rho}^2\bar{R}. \qquad (19)$$

Second, in Refs [9] a more quantitative theory is developed, considering fermions in the «$N_C\gg N_f$» approximation (as mentioned by its authors). However, we prefer to look at their theory at another angle, as the theory of the case $N_f=1$. This is most clearly seen from the second paper [9] in which Dyakonov and Petrov have not started with formal integration over the quark fields Ψ, leading to the fermionic determinant, but instead have introduced the following statistical sum

$$Z_\Lambda=\int D\Psi^+ D\Psi\, e^{\int dx\,\Psi^+(i\hat{\partial})\Psi}\int\prod_{I,A=1}^{N} d\Omega_I\, d\Omega_A\left\{|im-\int dx\,\Psi^+(i\hat{\partial})\,\psi_0^{(I)}|\times\right.$$
$$\left.\times|im-\int dx\,\psi_0^{+(I)}(i\hat{\partial})\,\Psi|\;|im-\int dx\,\Psi^+(i\hat{\partial})\,\psi_0^{(A)}|\,|im-\int dx\,\psi_0^{(A)}i\hat{\partial}\,\Psi|\right\}^{N_f} \qquad (20)$$

where $d\Omega_I(d\Omega_A)$ is the element of the collective coordinates for the instanton (anti-instanton) and N is the number of instantons, equal to that for the anti-instantons. Introduction of such statistical sum means that the quark propagator is approximated by two terms

$$S(x,y)=S^{free}(x,y)+\sum_{I,A}\frac{\psi_0^{I,A}(x)\,\psi_0^{+I,A}(y)}{(-im)} \qquad (21)$$

where S^{free} is the free quark propagator, which is a kind of interpolation, valid both at small and large distances.

For one quark flavor it is possible to integrate over the instanton parameters and then proceed to the effective quark theory of the type

$$Z=\int D\Psi^+ D\Psi\exp|-\int\Psi^+(i\hat{\partial}+M_{eff})\,\Psi\,dx|. \qquad (22)$$

It is possible because in the $N_f=1$ case the t'Hooft vertices have the structure $\Psi^+\Psi$, but we do not think this trick is useful for $N_f>1$, when this effective interaction leads to multi-fermion operators and cannot be taken into account just by the «effective mass». Dyakonov and Petrov have obtained the following results:

$$M_{det}\simeq 0.9\bar{\rho}/\bar{R}^2,$$
$$|\langle\bar{\Psi}\Psi\rangle|\simeq 0.55/\bar{\rho}\bar{R}^2. \qquad (23)$$

(Again we have put $N_C=2$ and consider all ρ equal to $\bar{\rho}$. Note that (23) differs with the mean field estimates (18) just in some numerical factors.) In Sect. 7 we are going to confront these results with our numerical data.

6. GENERAL DISCUSSION OF THE INSTANTON LIQUID WITH QUARKS

We have mentioned in the introduction that in order to formulate some questions about the structure of this complicated statistical system it is helpful to use a physical analogue, looking at the pseudoparticles as at some «atoms» and at the light quarks as some «valence electrons». Further, the eigenvalue spectrum of the Dirac operator is somewhat analogous to that of the atomic Hamiltonian. The nonzero eigenvalue density at $\lambda=0$ is analogous to the nonzero state density at the Fermi level. If so, the presence or absence of SBCS is reduced to the question whether our «instantonic liquid with quarks» is a conductor or an insulator.

Generally speaking, there are a number of possibilities. The simplest one, being the «random model» mentioned above, implies that the matter is «amorphous», with the «atoms» making some chaotic

«polymer» all over the space. If so, the spectrum is continuous and SBCS takes place. This is similar to the conductivity of semiconductors with impurities: whatever small is the impurity density, the so called «jump conductivity» is always nonzero.

However, in contrast to the impurity atoms in semiconductors the *PPs* in vacuum are strongly correlated. Moreover, one of the most important source of such correlations is the light fermion exchanges, the interaction we study in this work.

For example, if these correlations lead to some ordered phase (a «crystal»), the eigenvalue spectrum has zones, leading either to well conducting or to perfectly insulating phases. Another possibility is that the *PPs* are united in small clusters, say the «molecules» considered above. As it was argued by Callan, Dashen and Gross [7], such phase may be the case if the *PP* density is sufficiently small.

It is easy to show that in the dilute «molecular» vacuum there is no SBCS. Indeed, in this case the eigenvalues are just the overlap integrals, and therefore their distribution at small λ is directly related to the distribution over the sizes R of the molecules

$$\left.\frac{dn}{d\lambda}\right|_{\lambda\to 0} \sim \lambda^{2N_f-4/3} \tag{24}$$

where we have used $T\sim 1/R^3$. Therefore, in this case the eigenvalue density at $\lambda\to 0$ is vanishing, together with the quark condensate.

Note, that one should still prove that the «dilute molecular» phase is stable. Consider for example the chain-type cluster containing 4 *PPs*. If one integration over the space-time is taken apart, the remaining integration looks as follows:

$$Z_{(\square)}\sim V\int d^4z_2\, d^4z_3\, d^4z_4 [T(z_1-z_2)\, T(z_2-z_3)\, T(z_3-z_4)\, T(z_4-z_1)]^{N_f} \tag{25}$$

and one can see that indeed there is one special case $N_f=1$, for which this integral diverges at large z. The same is true for other «chains», which means that in the case $N_f=1$ the «dilute molecular» vacuum cannot take place even at arbitrarily small *PP* density. (This conclusion nicely matches with the absence of any symmetry to be broken in this case, but of course it is not a convincing argument: one may well have some first-order transitions without any symmetries to be broken!)

For $N_f>1$ all finite clusters lead to convergent expressions, which means that at arbitrarily small densities it is statistically favourable to split them into the smallest unites, the molecules, which lead to larger statistical sum. Thus, in this case the «molecular vacuum» should indeed take place.

Considering the problem at finite densities we face very nontrivial combinatorical problem. As for any statistical problem, one should compromise the opposite trends governed by the «energy» and the «entropy». The «lowest energy» (namely the maximal fermionic determinant) configuration is some rather complicated crystall (first discovered in Ref. [13] in another context). It has 16 *PPs* with nontrivial orientations as the elementary unite, and the overlap integrals for all neighbours are maximal. The entropy is of course maximal for the «random model» (RM) mentioned above.

7. SBCS IN A SIMPLIFIED MODELS

Because of the complexity of the problem we start our analysis with the discussion of some simplified models for the ensemble of pseudoparticles. The first one is «random model» (RM) mentioned above, an ensemble of *PPs* with random positions and orientations. We confront this model to the «correlated model» (CM), in which the distribution over positions and orientations of *PPs* is governed by the quark-exchange interaction. For simplicity in this section we (i) take all radii ρ of the *PPs* equal and (ii) ignore the non-fermionic interactions (considered in II). The only free parameter of the model is the dimensionless parameter $n_{PP}\bar{\rho}^4=(\bar{\rho}/\bar{R})^4$.

More precizely, the properties of the «correlated model» are defined by the following partition function Z, modelling the zero-mode part of the fermionic determinant

$$Z=\int\left(\prod_{I,A=1}^{N} dU_I\, dU_A\, d\rho_I\, dz_A\right)(-1)^N\left[\det\begin{vmatrix} 0 & T_{AI} \\ T^*_{IA} & 0\end{vmatrix}\right]^{N_f}. \tag{26}$$

For N instantons and N anti-instantons the NN matrix T_{IA} consists of the «overlap integrals» of all instantonic and all anti-instantonic zero modes. Expressions for T_{IA} are considered in Sect. 3. The $2N\cdot 2N$ matrix in (26) is Hermitean and its eigenvalues are real, also due to the block-structure of this matrix they are doubled, $\pm|\lambda|$, and the sign factor stands to make the weight positive.

We have made numerical simulation for the ensemble of *PPs* governed by this weight function. Straightforward averaging of the

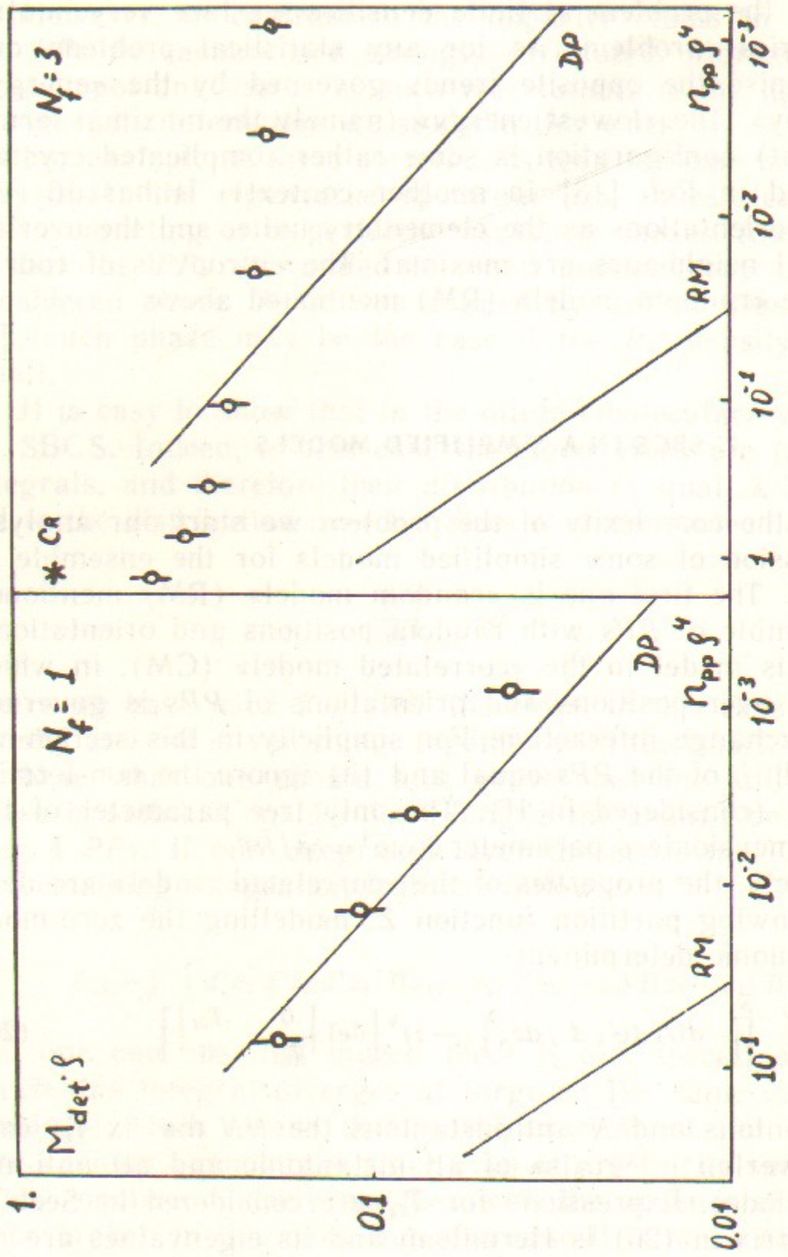


Fig. 2. The so called «determinantal mass» M_{det} (the geometric mean of the eigenvalues of the overlap matrix) versus the pseudoparticle density n_{pp} for $N_f=1$ (*a*) and $N_f=3$ (*b*). The curves marked «RM» mean the random model (see text), while the curve marked «DP» shows the results of Dyakonov and Petrov [9]. The «star» marked CR near the star in the upper left corner stands for the instanton—anti-instanton «crystal». The points correspond to our data for the «correlated model» defined in the text.

determinant over random configurations was found completely impossible, because it fluctuates by orders of magnitude. Therefore we have simulated configurations by the Metropolis algorithm, explicitely evaluating the determinant at each updating. (Here the formula $Z\sim|\det T|^2$ is useful.) For small Langevin-type updating there exist simple approximate expressions for the variations of the determinant, but we have found this method to be more slow. We have considered up to 34 pseudoparticles in a box with periodic boundary conditions. For each pair of pseudoparticles our program have selected the shortest way out of all topologically distinct ones on this 4-torus.

In Fig. 2 we have plotted some results for the «geometric mean» value of eigenvalues $M_{det}=(\det i\bar{D})^{1/NN_f}$, the «determinantal mass» mentioned above. First of all, one should look at the curve marked «RM», corresponding to the random model. It gives much smaller determinants than it was actually observed for the «correlated model», even at densities $O(1)$. It means that the correlations induced by the fermion exchange are quite significant at any density.

Our second observation follows from the comparison of $N_f=1$ and $N_f=3$ cases, shown on this picture. One can see that the line «DP», corresponding to the Dyakonov—Petrov theory, is indeed reproduced in the former case while at the $N_f=3$ case the dependence is quite different: the determinant tends to some constant at small densities, which means dominance of some finite-size clusters.

In Fig. 3 we show behaviour of the quark condensate with density in both cases. (This quantity is determined from the eigenvalues found. Note by the way, that in contrast to determinant, one cannot just calculate the spectrum of the smaller matrix T: this is clear already from the fact that it is not generally symmetric and therefore have complex eigenvalues.) For $N_f=1$ again there is reasonable agreement with the *DP* theory, the condensate decreases with density, but remains nonzero. In the $N_f=3$ case the behaviour found is much more complicated. We definitely observe that at small *PP* densities the condensate drops, which is correlated with the transition into a «molecular» phase. In the density region roughly indicated in this figure we have strong evidences for the «mixed phase» behaviour. If one drow a picture of spatial *PP* distribution he finds that in this density region it is sometimes very inhomogeneous, containing both relatively dense «drops» with few molecules occupying all the remaining space.

In Fig. 4 we display the eigenvalue distributions at few densi-

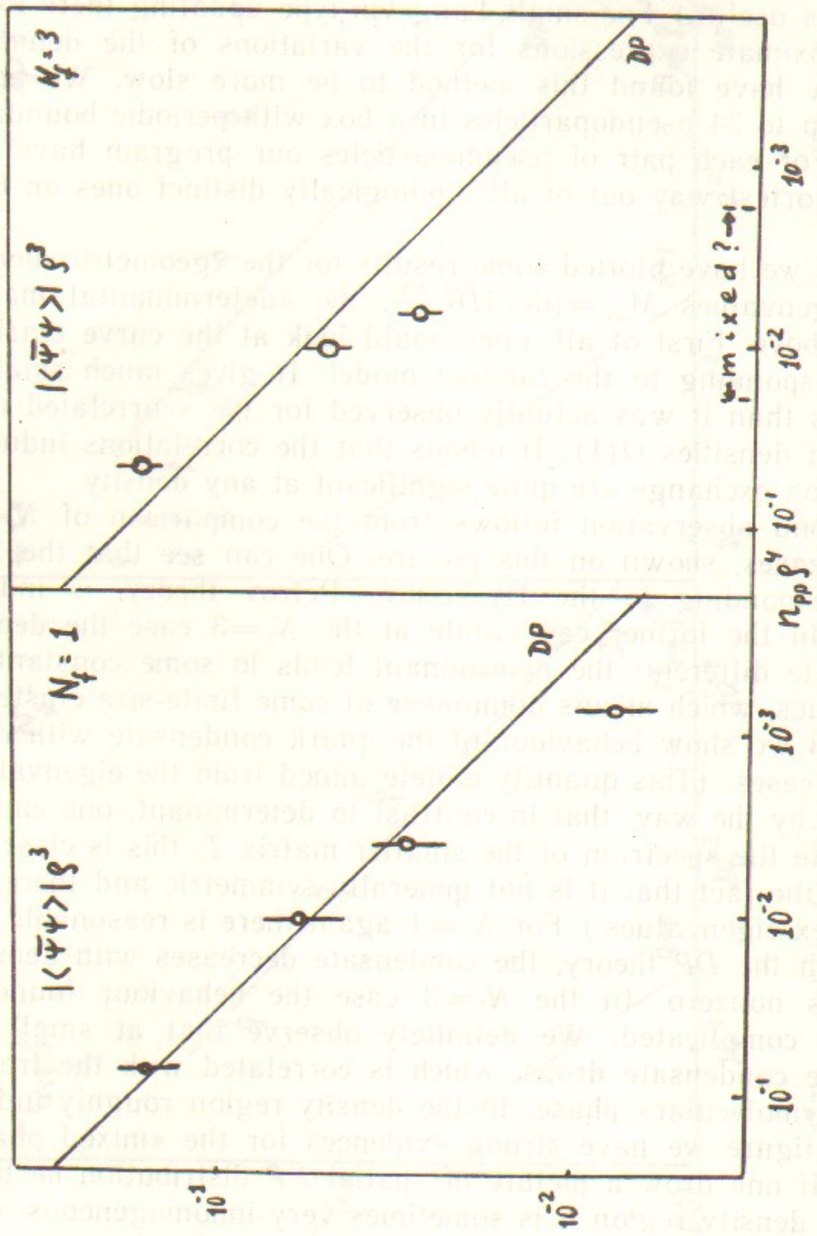


Fig. 3. The quark condensate versus the *PP* density. Notations are the same as in Fig. 2.

ties. One can see that for $N_f=1$ one has a Gaussian-type spectrum for all densities, with more narrow peak at smaller densities. However, for $N_f=3$ the behaviour is completely different. The two-peak structure of the spectrum was found in the transition region, with one peak at zero (being due to a «polimer») and another at larger λ, corresponding to the «molecules». The magnitudes of both peaks are changed with density, till the former one disappears at some n_{pp}.

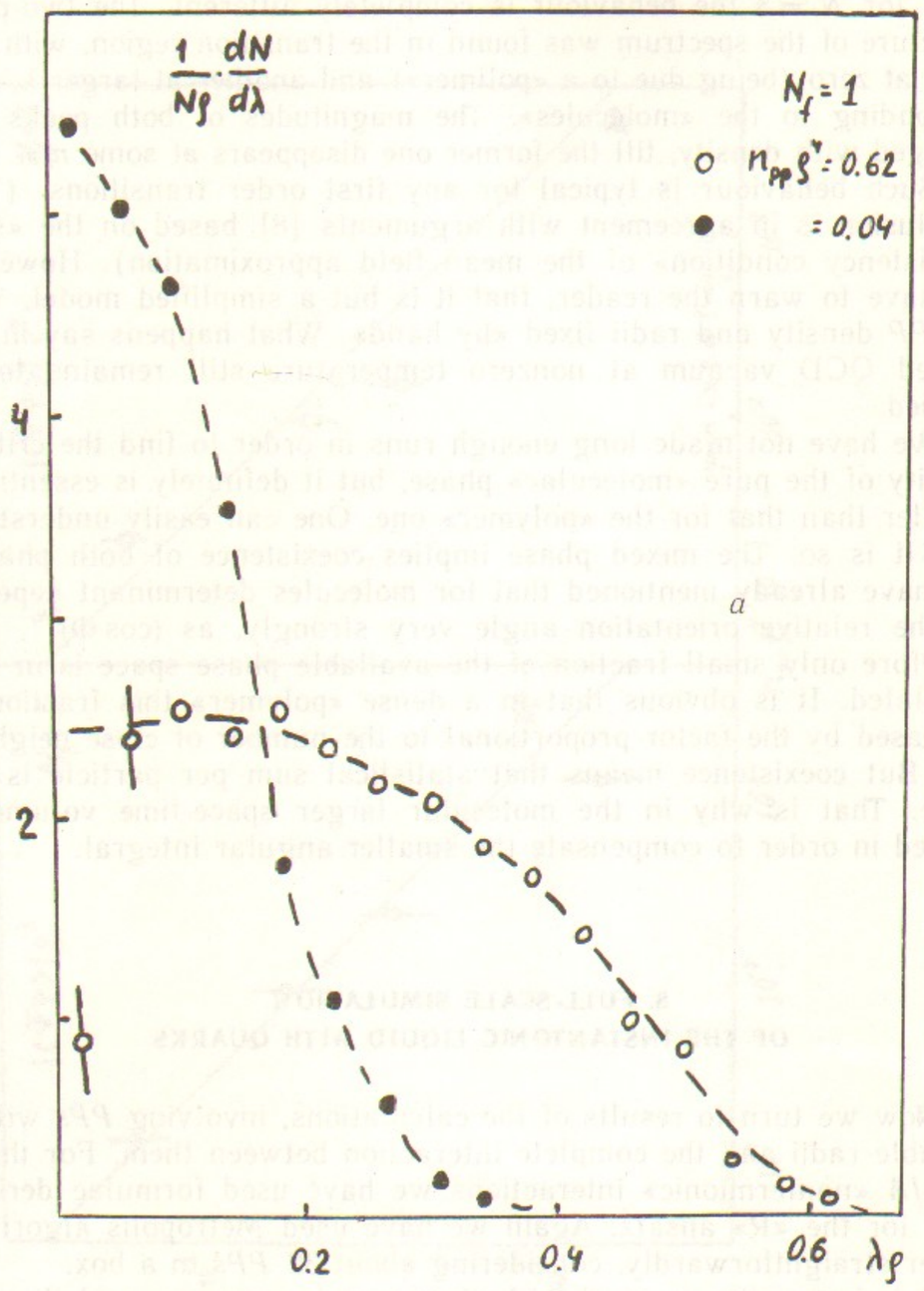
Such behaviour is typical for any first order transitions. (This conclusion is in agreement with arguments [8] based on the «self-consistency condition» of the mean field approximation). However, we have to warn the reader, that it is but a simplified model, with the *PP* density and radii fixed «by hand». What happens say in the heated QCD vacuum at nonzero temperature still remains to be studied.

We have not made long enough runs in order to find the critical density of the pure «molecular» phase, but it definitely is essentially smaller than that for the «polymer» one. One can easily understand why it is so. The mixed phase implies coexistence of both phases. We have already mentioned that for molecules determinant depends on the relative orientation angle very strongly, as $(\cos\Phi)^{2N_f}$, and therefore only small fraction of the available phase space is in fact populated. It is obvious that in a dense «polymer» this fraction is increased by the factor proportional to the number of close neighbours. But coexistence means that statistical sum per particle is the same. That is why in the molecular larger space-time volume is needed in order to compensate the smaller angular integral.

8. FULL-SCALE SIMULATION OF THE INSTANTONIC LIQUID WITH QUARKS

Now we turn to results of the calculations, involving *PPs* with a variable radii and the complete interaction between them. For the *II* and *IA* «nonfermionic» interactions we have used formulae derived in II for the «R» ansatz. Again we have used Metropolis algorithm rather straightforwardly, considering about 32 *PPs* in a box.

It is instructive to start with some simple estimates and then report numerical results. For pure gauge theory we have found in II that the typical radius $\bar\rho$ is small in the Λ_{PV} unites: $\bar\rho\simeq\frac{1}{3}\Lambda_{PV}^{-1}$.



a

Fig. 4.

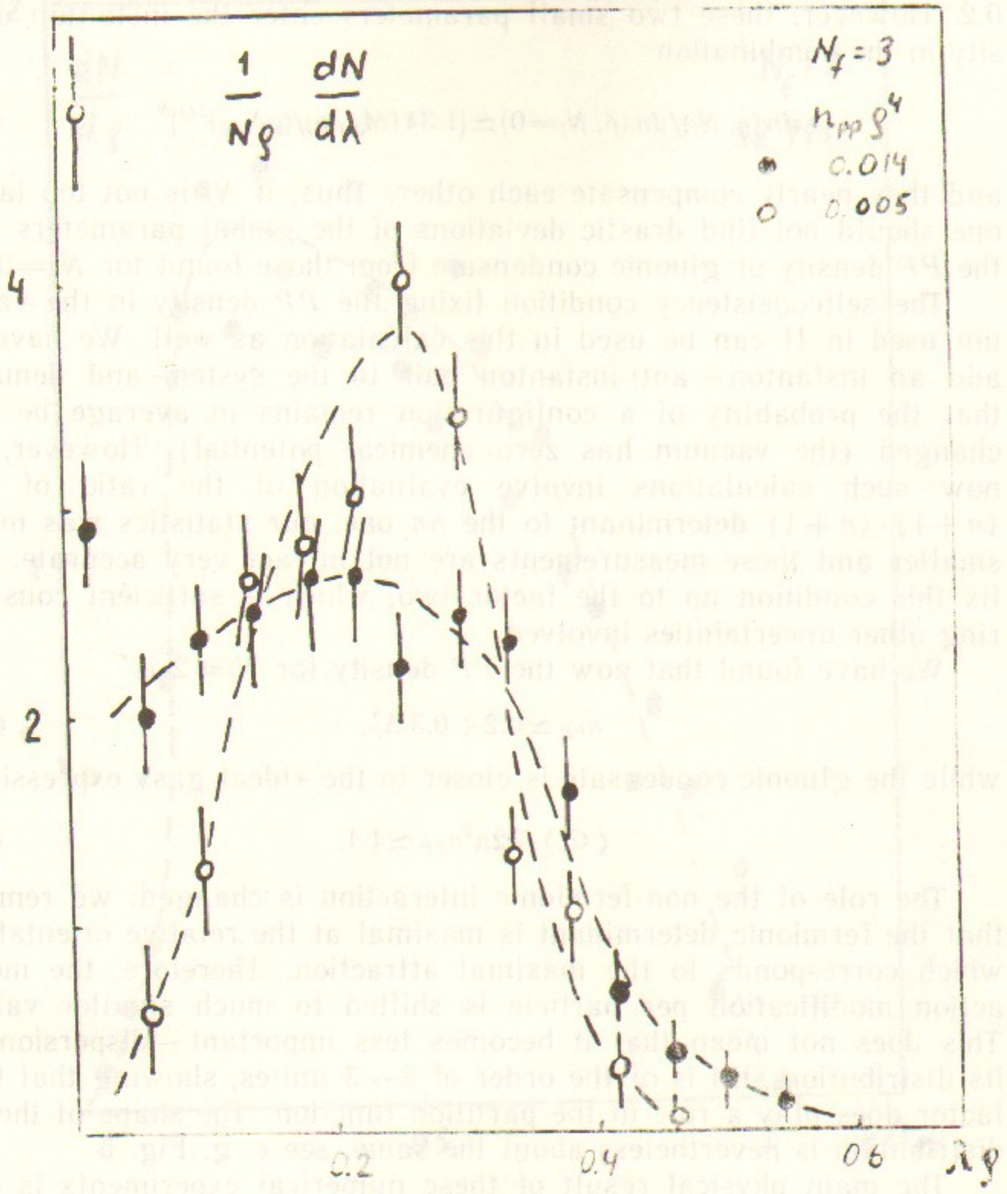


Fig. 4. The eigenvalue distribution for few values of the *PP* density.

Another nontrivial small numerical parameter is the «determinantal» mass: from the results given above we see that $M_{det}\bar{\rho}$ is about 0.2. However, these two small parameters enter the instanton density in the combination

$$dn(\rho, N_f)/dn(\rho, N_f=0) \simeq [1.34 (M_{det}\rho)/(\rho\Lambda_{PV})^{2/3}]^{N_f} \quad (27)$$

and they nearly compensate each other. Thus, if N_f is not too large one should not find drastic deviations of the global parameters like the PP density or gluonic condensate from those found for $N_f=0$.

The selfconsistency condition fixing the PP density in the vacuum used in II can be used in this calculation as well. We have to add an instanton—anti-instanton pair to the system and demand that the probablity of a configuration remains in average be unchanged (the vacuum has zero chemical potential). However, as now such calculations involve evaluation of the ratio of the $(n+1)\cdot(n+1)$ determinant to the nn one, our statistics was much smaller and these measurements are not in fact very accurate. We fix this condition up to the factor two, which is sufficient considering other uncertainties involved.

We have found that now the PP density for $N_f=2$ is

$$n_{PP} \simeq 0.2 \div 0.3\, \Lambda_{PV}^4 \quad (28)$$

while the gluonic condensate is closer to the «ideal gas» expression

$$\langle G^2 \rangle / 32\pi^2 n_{PP} \simeq 1.1. \quad (29)$$

The role of the non-fermionic interaction is changed: we remind that the fermionic determinant is maximal at the relative orientation which corresponds to the maximal attraction. Therefore, the mean action modification per particle is shifted to much smaller value. This does not mean that it becomes less important—dispersion of its distribution still is of the order of 2—3 unites, showing that this factor does play a role in the partition function. The shape of the ro distribution is nevertheless about the same, see e. g. Fig. 5.

The main physical result of these numerical experiments is our conclusion that the resulting vacuum does possess the nonzero quark condensate. In order to make it one should consider the eigenvalue distribution shown in Fig. 5. Another (and the more standard) plot is the dependence of the condensate on the small quark mass, see Fig. 6. Both our system and that studied on the lattice have finite volume, therefore this spectrum at small eigenvalues is distorted and some extrapolation to the zero mass is necessary.

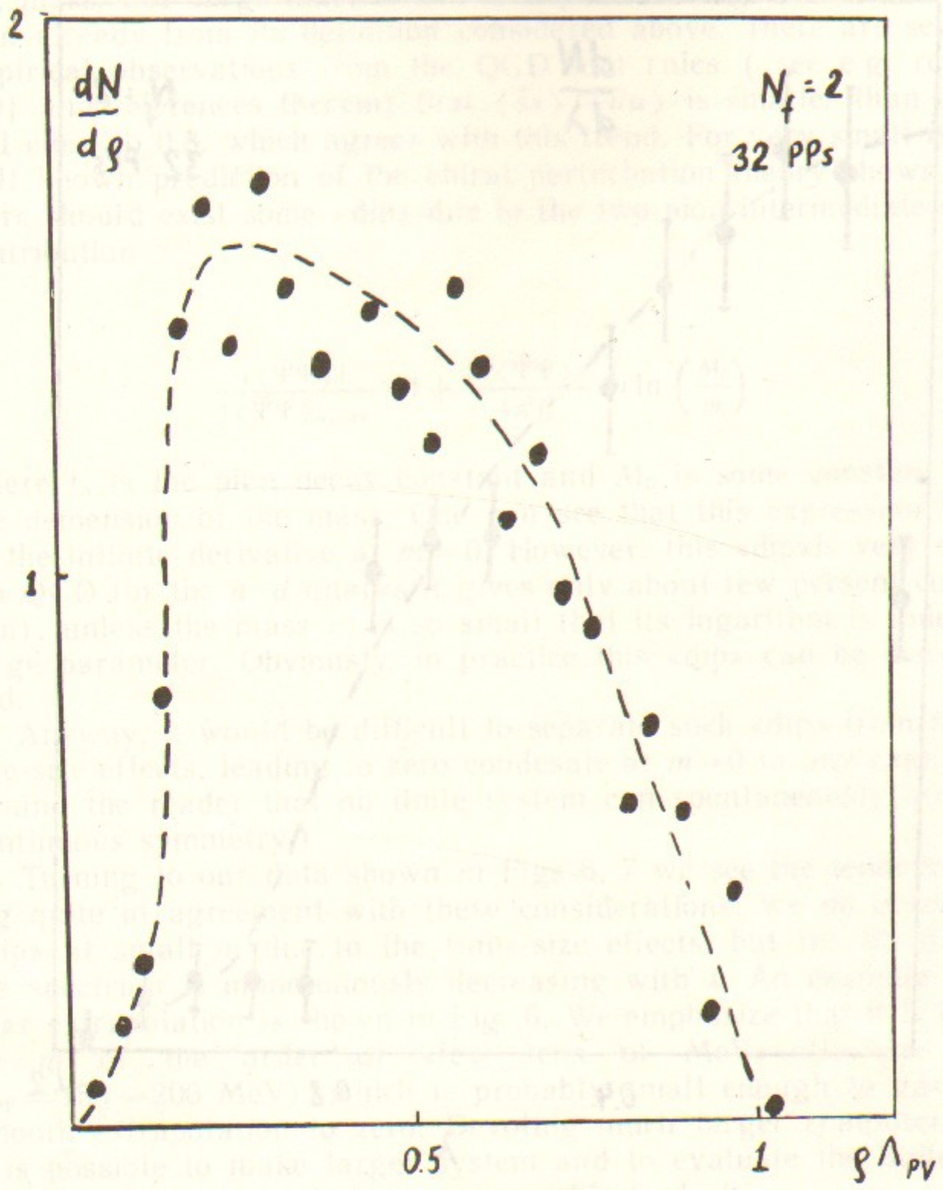


Fig. 5. Distribution of the pseudoparticles over ρ in the «instantonic liquid with quarks» at $N_f=2$.

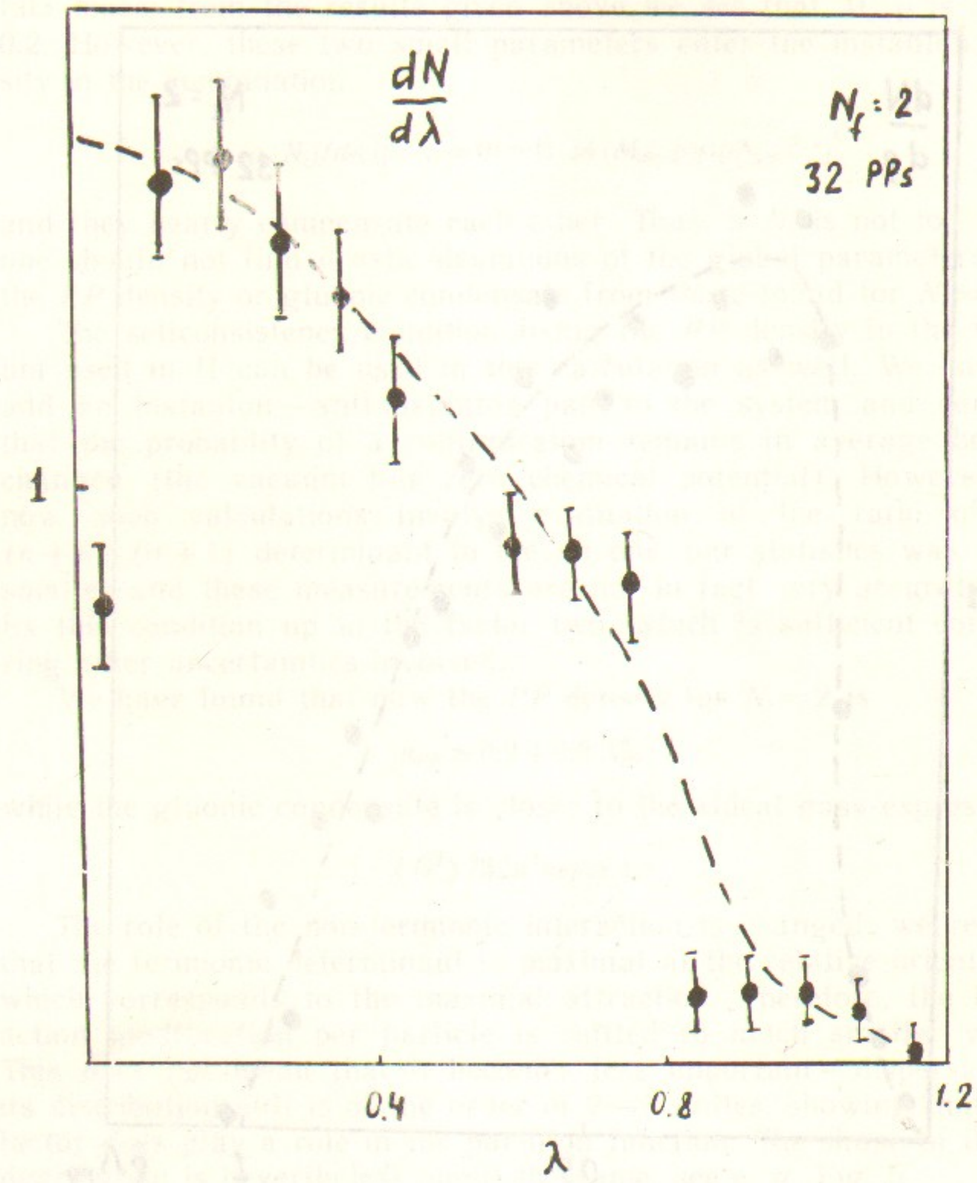


Fig. 6. The eigenvalue distribution for the «instantonic liquid with quarks» at $N_f=2$.

Before making this extrapolation it is instructive to discuss the general information concerning dependence of the $\langle\bar\Psi\Psi\rangle$ on the quark mass. For large mass it is trivially decreasing as 1/m, as it is seen already from its definition considered above. There are several empirical observations from the QCD sum rules (see e.g. review [19] and references therein) that $\langle\bar ss\rangle/\langle\bar uu\rangle$ is smaller than unity and close to 0.8, which agrees with this trend. For very small m the well known prediction of the chiral perturbation theory shows that there should exist some «dip» due to the two-pion intermediate state contribution

$$\frac{|\langle\bar\Psi\Psi\rangle|}{|\langle\bar\Psi\Psi\rangle_{m=0}|}=1+\frac{3|\langle\bar\Psi\Psi\rangle|}{4\pi^2 f_\pi^4}\,m\ln\left(\frac{M_0}{m}\right)$$

where f_π is the pion decay constant and M_0 is some constant with the demension of the mass. One can see that this expression leads to the infinite derivative at $m=0$. However, this «dip»is very small (in QCD for the u, d quarks it gives only about few persent correction), unless the mass m is so small that its logarithm is indeed a large parameter. Obviously, in practice this «dip» can be disregarded.

Anyway, it would be difficult to separate such «dip» from the finite-size effects, leading to zero condesate at $m\to0$ in any case. (We remind the reader that no finite system can spontaneously break a continuous symmetry.)

Turning to our data shown in Figs 6, 7 we see the tendency being quite in agreement with these considerations: we do observe a «dip» at small m due to the finite-size effects, but for $\lambda > 0.1\,\Lambda_{PV}$ the spectrum is monotonously decreasing with λ. An example of linear extrapolation is shown in Fig. 6. We emphasize that it is based on m of the order of «few tens of MeV» (if one take $\Lambda_{PV}=150-200$ MeV), which is probably small enough to garantee smooth extrapolation to zero. Devoting much larger computer time it is possible to make larger system and to evaluate the finite size effects from the data, but we were unable to do it.

It is instructive to compare all this with the lattice data. First, they make an extrapolation from somewhat larger masses. Second, their extrapolation to $m\to0$ has the positive slope, that is, their condensate is increasing with (small) quark mass (see e.g.[14]). Thus, their eigenvalue spectrum is qualitatively different from ours. There is no direct contradiction here: they have all modes of (huge) fermi-

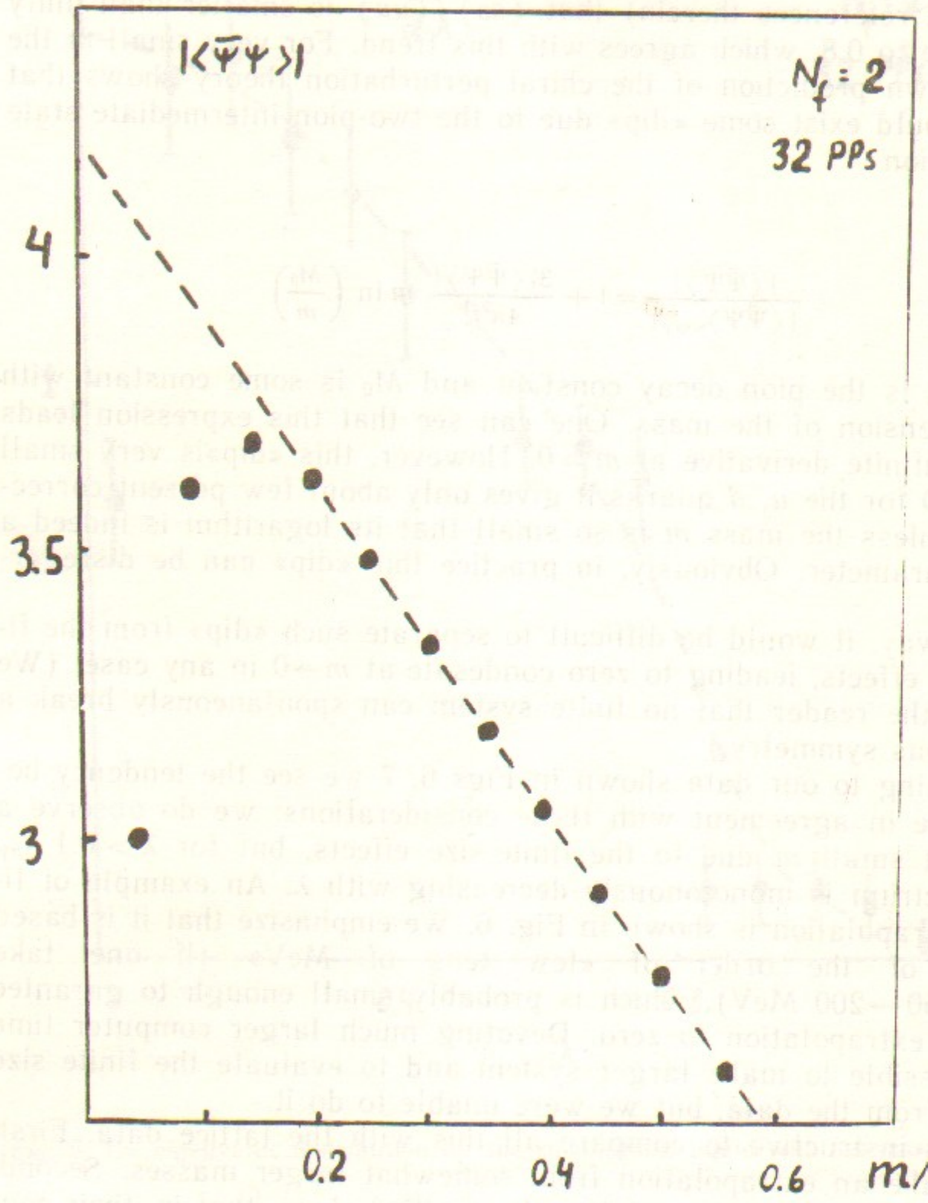


Fig. 7. Dependence of the quark condensate on the small quark mass.

onic matrix while we have considered only the «quasizero» ones, belonging to instantons. It may well be that our effect is just not the dominant one. However, it remains to be explained how to reconcile these lattice data with the phenomenology, suggesting the opposite trend at all mass scales.

One may look at these lattice data at some different angle too. Their box size is such that they actually work at «temperature» (the inverse of the box length in the Euclidean time) which varies between about 0.5 and 1.5 of the critical temperature for chiral symmetry restoration. Near the phase transition our eigenvalue spectra discussed in the preceeding section also have a minimum at zero. (It was due to the smaller role of the «infinite cluster» in this region.) Can this nonzero temperature be the explanation of the difference between our and lattice data?

Our final number for the quark condensate can be expressed in terms of the gluonic condensate scale

$$\frac{|\langle\bar{\Psi}\Psi\rangle|^{1/3}}{\langle G^2\rangle^{1/4}} \simeq 0.26-0.28\,, \quad (N_f=2)\,. \tag{30}$$

Such number is very stable, independing on the details such as our poor accurasy of the selfconsistency condition ($F_{N+1}=1$) measurements etc. The absolute value is as follows

$$|\langle\bar{\Psi}\Psi\rangle|^{1/3} \simeq (0.8-1.2)\Lambda_{PV}\,. \tag{31}$$

The best available lattice data [14] (for the SU(2) group and the explicite account for the dynamical fermions) lead to

$$|\langle\bar{\Psi}\Psi\rangle|^{1/3} = \begin{cases} 3.3\langle\langle\Lambda_{\overline{MS}}\rangle\rangle & (N_f=0) \\ 5.1\langle\langle\Lambda_{\overline{MS}}\rangle\rangle & (N_f=4) \end{cases} \tag{32}$$

where $N_f=0$ means «quenched approximation». (Note that «$\Lambda_{\overline{MS}}$» calculated from Λ_L is practically equal to our Λ_{PV}, see their relation with the lattice unites in [18].)

These results suggest $\langle\bar{\Psi}\Psi\rangle$ much larger than was found in our calculations. However, if one try to fix the «physical scale» somehow (e. g. from the critical temperature of the chiral symmetry restoration, putting it between 200 and 300 MeV) he also finds that the scale (32) is about twice larger than the phenomenological QCD value for the quark condensate.

The same can be said in another way. Including measurements

of the gluonic condensate (by Iwasaki et al., see II for reference) one finds the dimensionless ratios of scales are as follows

$$\frac{|\langle\bar{\Psi}\Psi\rangle|^{1/3}}{\langle G^2\rangle^{1/4}}=\begin{cases}0.40 & (N_f=0,\ \text{lattice})\\ 0.27 & (\text{QCD})\end{cases} \tag{33}$$

Note, that the phenomenological value is smaller (and very close to our one (30)).

Completing this section we may say that we have found that «instantonic liquid» does provide a nonzero contribution to the quark condensate. Its remains to be clarified whether it is the main effect or not. We have made some critical remarks concerning the lattice data for $\langle\bar{\Psi}\Psi\rangle$. As a positive suggestion for lattice studies we suggest to check whether small eigenvalues are correlated with the presence of well separated instantons (seen by the «cooling»method) in their ensemble of gauge field configurations or not.

9. CONCLUSIONS AND DISCUSSION

The main conclusion which can be drawn from this work was already mentioned in the introduction: it is the statement that the presence of light fermions makes the structure of the «instantonic liqiud» much more complicated compared to pure gauge theory. Roughly speaking, if the latter system is analogous to a nonideal gas made of «atoms», in the former one these «atoms» are also connected by some «chemical bonds» into a complicated «polymer». Apart from the case $N_f=1$, all simple approximations suggested previously turns to be quite inadequate for its description.

Our numerical experiments are also but first exploratory studies of the problem. Their main result is the model itself, which is shown to be practical for even modest computers. This statement is rather nontrivial, because the system studied in this work is much more complicated than those usually studied in statistical mechanics applications. Indeed, it looks as a solution of the Dirac equation for quarks moving in many complicated and randomly placed potential wells at each updating!

And nevertheless it is demonstrated that a fermionic determinant in the «zero mode approximation» is quite tractable. We typically worked with about 30 *PPs* in a box, which is not so large number in 4 dimensions. However, it is already essentially larger than the

number of instantons seen in current lattice experiments, which have observed few *PPs* (if any). Straightforward lattice approach has to face a problem of computing determinant of a huge matrices. In most cases these determinants are too small, and it often is so because apart of thousends of «normal» modes, there are several «quasi-zero modes» due to wrongly placed pseudoparticles!

Using once more an analogy with atomic physics, we may say that it seems hopeless to understand a condenced matter by solving the Schreodinger equation for all electrons. It is reasonable to select a small subset of the «valence» ones, which determine the states near the «Fermi level». If the picture of the «instantonic liquid» is reasonable, we have such a possibility, and it would be a mistake not to benefit from such tremendous simplification of a complicated problem.

There are no many specific applications in this work, but using our data for the «instantonic liquid with quarks» it is possible to study all instanton-induced effects, in particular, their contribution to various correlation functions. Previous experience shows that most of the properties of the pseudoscalar mesons [8, 9] and baryons [15] may be explained on this way. We hope to report these calculations in latter works of this series.

Another potential applications deal with a superdense matter. In Sect. 7 we have considered the phase transition with the chiral symmetry restoration as the *PP* density is lowered. It was considered above as a purely methodical example. However it is known [16, 17] that in the excited matter (heated to some nonzero temperature, compressed to high baryonic charge density etc.) the instantons are suppressed. Therefore, these studies may have quite real applications, for example for high energy heavy ion experimental program aiming to observe the so called «quark-gluon plasma». Sharp transition from the «polymer»-type phase to dilute «molecular» phase found in this work may lead to observable consequences in this case. We are going to turn to this in separate publications.

ACKNOWLEDGMENTS

It is a pleasure to thank my colleges and friends V.L. Chernyak, D.I. Dyakonov, V.Yu. Petrov, M.A. Shifman and A.I. Vainshtein who have contributed to this work by multiple critical comments and helpful suggestions.

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E.V. Shuryak

Toward the Quantitative Theory of the Topological Phenomena in Gauge Theories III. Instanton and Light Fermions

Э.В. Шуряк

К количественной теории топологических явлений в калибровочных теориях поля III. Инстантоны и легкие фермионы

Ответственный за выпуск С.Г.Попов

Работа поступила 28 мая 1987 г.
Подписано в печать 23.07 1987 г. МН 08283
Формат бумаги 60×90 1/16 Объем 2,6 печ.л., 2,1 уч.-изд.л.
Тираж 250 экз. Бесплатно. Заказ № 97

Набрано в автоматизированной системе на базе фотонаборного автомата ФА1000 и ЭВМ «Электроника» и отпечатано на ротапринте Института ядерной физики СО АН СССР,
Новосибирск, 630090, пр. академика Лаврентьева, 11.