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Chiral Symmetry Breaking and Correlations in the Instanton Liquid

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Abstract

We study the instanton liquid model of the QCD-vacuum with the help of Monte-Carlo simulations. At large instanton densities the pseudoparticle system crystallizes. At phenomenologically interesting densities it is in a liquid phase. For three massless flavors we find strong correlations which manifest themselves as a dip in the spectrum around zero. However, when we use phenomenological values for the current quark masses, these correlations are strongly reduced leading to a qualitatively different spectrum. In this case the dip resembles a finite size effect. Also for two massless flavors or less the dip is not present in the thermodynamic limit.

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1. Introduction

Instantons are a very important ingredient of the QCD vacuum [1,2,3,4,5,6], and phenomenological studies [7,8] have revealed the presence of some nontrivial small parameters, allowing for a systematic study of its properties. During the last few years interacting instantons were studied in more detail, both analytically [9,10,11] and numerically [12,13,14,15], and the smallness of all these parameters was confirmed. Recently, it was shown that even very specific properties of the QCD vacuum, such as mesonic correlation functions, are reproduced by this theory [16,17].

The central problem under investigation is the spontaneous breakdown of chiral symmetry in the QCD vacuum, leading to a nonzero quark condensate, light pions *etc.*. It was shown [7,12,13,11,6], that specific quark states, belonging to the so-called "zero mode zone" (ZMZ) are the dominant ones for describing these phenomena. The reason is that these quark states correspond to small eigenvalues of the Dirac operator $i\hat{D} = i\gamma_\mu(\partial_\mu - iA_\mu)$ (where A_μ is the gauge field in the vacuum). For the study of the quark propagator (being essentially the inverse of D) these small eigenvalues are of major importance. In particular, the chiral condensate is proportional to the eigenvalue density at zero.

In this paper we study the instanton liquid model of the QCD-vacuum by a Monte-Carlo simulation of the partition function. This paper constitutes a considerable extension over previous work [18]. Two numerical codes, written independently by both authors, have been compared and matched to give the same results. The increased confidence in our code justified to devote to the study of this model two orders of magnitude more computer time than in previous work [13]. As a result we were able to study the model for larger systems, with greater statistics and for a much wider parameter range. We present the first numerical study of the solid-liquid phase transition in the instanton model of the QCD-vacuum (analytical estimates for the free energy of the instanton-anti-instanton crystal were given

in ref. [10]). It is also for the first time that this model is studied numerically for a large number of flavors. In agreement with analytical estimates of one of the authors [19] our results show a divergence of the density of molecules for more than ≈ 12 massless flavors (for $N_c = 3$, and of course no more than 17.5 massless flavors). Our main goal is the study of chiral symmetry breaking in terms of the spectrum of the Dirac operator (in the ZMZ). Its shape is affected strongly by the correlations in the positions and the orientations of the instantons and the anti-instantons. Because of the fermion determinant (which is given by the product of all eigenvalues), the correlations are such that the eigenvalue density around zero is strongly suppressed. Therefore, they strongly diminish or even lead to a vanishing quark condensate.

The physics of this phenomenon can be expressed in a rather transparent way in terms of the picture suggested in [20,21]. In this work the quark exchange between two pseudoparticles was considered to be a kind of chemical bond. These bonds can give rise to clusters of pseudoparticles. If the cluster is finite (*e.g.* a molecule of an instanton and an anti-instanton), these pseudoparticles cannot really contribute to the spontaneous breaking of a continuous symmetry. Only infinite clusters can lead to the spontaneous breaking of chiral symmetry. However, even the existence of these clusters is not a sufficient condition for chiral symmetry breaking: for example, the crystal phase, to be discussed below, constitutes an infinite cluster. It is an ordered cluster, and it is shown by explicit numerical calculation that it does not break chiral symmetry (but, obviously, it does break many other symmetries like translational invariance and gauge invariance). What is really needed, is the presence of infinite and in some sense disordered clusters. The formation of these clusters depends on the detailed dynamics of the system. The study of the conditions for their formation and the resulting eigenvalue spectra are the essence of this paper.

Apart from the results already mentioned several other surprising results will be presented. We will find that at physically interesting pseudoparticle density the

shape of the ZMZ of the spectrum changes qualitatively between two and three flavors. At zero temperature we do not find a liquid-gas phase transition. The pseudoparticle system appears to exist in a liquid phase.

The instanton liquid model for the QCD-vacuum will be defined in section 2. In this section we also give a brief discussion of the numerical methods used to investigate the partition function. Section 3 contains the bulk of our paper. In this section we investigate the different phases of the system of pseudoparticles. The shape of the eigenvalue density of the zero mode zone is discussed in section 4. Finite size effects and the role of the strange quark mass will be investigated in section 5. In this section we also estimate the chiral condensates. The flavor dependence is evaluated in section 6. Concluding remarks are made in section 7.

2. The instanton liquid model

We consider a liquid of N_+ instantons and N_- anti-instantons in a box of volume V . The partition function of this system of $N = N_+ + N_-$ pseudoparticles can be approximated by [2,3,4,7,12]

$$Z = \int \prod_{I=1}^N d\Omega_I w(\rho_I) \exp\left(-\frac{1}{2} \sum_{I \neq J} \beta(\bar{\rho}_I) u_{int}^{IJ} \det(i\bar{D} + im)\right). \quad (2-1)$$

The collective variables (z_I, U_I, ρ_I) are denoted by Ω_I . The positions z_I range over the inside of the box. The integral over the size ρ_I is cutoff at $\rho\Lambda = 1$. From the numerical results to be presented below, it will become clear that at phenomenologically interesting pseudoparticle densities or lower, our results are insensitive to this cutoff. Although the moduli space of the instantons is $SU(N_c)/SU(2)$, we integrate the orientation U_I over the full gauge group with its normalized invariant measure. The coset space is taken into account by an overall constant [22].

The distribution function $w(\rho)$ of the sizes of the pseudoparticles arises from the Jacobian of the transformation of the field variables to the collective variables,

and from the quantum fluctuations around a single instanton [1]. It is given by

$$w(\rho) = C_{N_c} \rho^{-5} \beta_I^{2N_c} \exp(-\beta_{II} - (2N_c - \frac{b'}{2b}) \frac{b'}{2b} \frac{\log \beta_I}{\beta_I}), \quad (2-2)$$

where

$$\begin{aligned} \beta_I &= -b \log \bar{\rho} \Lambda, \\ \beta_{II} &= \beta_I + \frac{b'}{2b} \log \frac{b'}{b} \beta_I, \\ C_{N_c} &= \frac{4.66 \exp(-1.68 N_c)}{\pi^2 (N_c - 1) (N_c - 2)!}. \end{aligned} \quad (2-3)$$

The numerical constants in C_{N_c} were evaluated in the Pauli-Villars renormalization scheme [22]. The cutoff parameter is denoted by Λ . The constants b and b' occurring in the beta-function are given by

$$b = \frac{11}{3} N_c - \frac{2}{3} N_f, \quad b' = \frac{34}{3} N_c^2 - \frac{13}{3} N_c N_f + \frac{N_f}{N_c}, \quad (2-4)$$

where N_c is the number of colors and N_f the number of flavors. The argument of the beta-function depends on the field strength. The contributions of the neighboring pseudoparticles to the field strength are taken into account via an effective radius $\bar{\rho}$ that depends on the surrounding medium,

$$\bar{\rho}_I = \rho_I / (1 + \sum_{I \neq J} \frac{\exp(-0.2 R_{IJ}^2 \rho_J / \rho_I)}{R_{IJ}^2 \rho_J / \rho_I})^{\frac{1}{2}} \quad (2-5)$$

Here, R_{IJ} is a dimensionless distance between pseudoparticles I and J , defined as

$$R_{IJ} = (z_I - z_J) / \sqrt{\rho_I \rho_J}. \quad (2-6)$$

This renormalized radius enters naturally in the so-called ratio Ansatz [23,24] for the gauge field configuration of pseudoparticles. Via the exponential factor it is possible to take into account the modification of the instanton profile at finite pseudoparticle density. The constant in the exponent has been chosen such that the action per pseudoparticle is minimized at the phenomenologically interesting density of one pseudoparticle per fm^3 . In [23] the two body interaction between

pseudoparticles for the ratio *Ansatz* was evaluated numerically. The interaction between an instanton and an anti-instanton can be parametrized by

$$u_{int}^{IJ} = |u|^2 \left[\frac{4d}{(4 + R_{II}^2)^2} + \frac{16}{(3 + R_{II}^2)^3} \right] \frac{4\rho_I^2 \rho_J^2}{(\rho_I^2 + \rho_J^2)^2}. \quad (2-7)$$

The quantity *d* is related to the angle between the relative orientation and the relative position of the two pseudoparticles. It is defined as

$$d = 1 - |Tr \tau_\mu^+ \frac{(z_I - z_I)^\mu}{|z_I - z_I|} U_I U_I^\dagger|^2 / \frac{1}{2} Tr(U_I U_I^\dagger \mathbf{1}_2 U_I U_I^\dagger \mathbf{1}_2), \quad (2-8)$$

and varies between -3 and 1. The $N_c \times N_c$ matrices τ_μ^+ contain the matrices $(\vec{\tau}, -i)_\mu$ in the upper left 2×2 -corner. All other matrix elements are equal to zero. The matrix $\mathbf{1}_2$ projects on the same subspace and is defined by $\mathbf{1}_2 = i\tau_4^+$. The quantity $|u|^2$ which arises as a consequence of the embedding of $SU(2)$ in $SU(N_c)$ is defined by

$$|u|^2 = \frac{1}{2} Tr(U_I U_I^\dagger \mathbf{1}_2 U_I U_I^\dagger \mathbf{1}_2). \quad (2-9)$$

For $SU(3)$ it varies between $\frac{1}{2}$ and 1.

The interaction between two pseudoparticles of the same kind is much weaker. Again we use a parametrization of the numerical results obtained in ref. [23]. They can be summarized by

$$u_{int}^{IJ} = \left(\frac{1}{2} Tr(U_I^\dagger U_I \mathbf{1}_2 U_I^\dagger U_J \mathbf{1}_2) - \left| \frac{1}{2} Tr \mathbf{1}_2 U_I^\dagger U_J \right|^2 \right) \frac{1.6}{(1 + R_{IJ}^2)^3} \frac{4\rho_I^2 \rho_J^2}{(\rho_I^2 + \rho_J^2)^2}. \quad (2-10)$$

In agreement with 't Hooft's multi-instanton solution, for the ratio *Ansatz* we find one orientation for which the interaction between instantons is zero.

We assume that the fermion determinant can be factorized in a factor spanned by the zero modes and in another factor spanned by the continuum modes [9,11]. We further assume that the second factor can be factorized into one-instanton contributions. The resulting quantum corrections are taken into account to one-loop order as originally evaluated by 't Hooft [1]. The first factor involves the

following two overlap matrices [11]

$$\begin{aligned} T_{IJ} &= \int d^4x \phi_I^\dagger(x - z_I) i\gamma_\mu \partial_\mu \phi_J(x - z_J), \\ K_{IJ} &= \int d^4x \phi_I^\dagger(x - z_I) \phi_J(x - z_J) - \delta_{IJ}, \end{aligned} \quad (2-11)$$

where the matrix *K* expresses the nonorthogonality of the zero modes ϕ_I . The zero mode contribution to the fermion determinant is then given by ¹

$$\det(i\hat{D} + im)_{ZMZ} = \frac{\det(T + im(\mathbf{1} + K))}{\det(\mathbf{1} + K)}. \quad (2-12)$$

The matrix *K* which can be obtained analytically in terms of Bessel functions can be parametrized by

$$K_{IJ} = \frac{1}{2} Tr U_I U_I^\dagger \frac{1}{R_{IJ}^2 + 1}. \quad (2-13)$$

We have shown numerically that the matrix *K* in the denominator changes the eigenvalue spectrum and other quantities of interest by only a few percent. Therefore, in our calculations we will not take it into account. The matrix *K* in the enumerator, preceded by a small factor *m*, will also be neglected. The overlap matrix elements T_{IJ} can also be obtained analytically in terms of Bessel functions [9,11]. However, for our numerical simulations we approximate the scalar part of the overlap matrix elements [20,14]

$$T_{IJ} = Tr(\tau_\mu^+(z_I - z_J)_\mu U_I U_I^\dagger) \frac{2}{\rho_I \rho_J (R_{IJ}^2 + 2.0)^2}. \quad (2-14)$$

The total contribution of the fermion determinant is obtained by combining the zero mode part and the continuum part. Apart from a modification of the constants *b* and *b'* (already included in eq. (2-4)) the fermion determinant in the partition function is approximated by

$$\det(i\hat{D} + im) \rightarrow \prod_{f=1}^{N_f} \left(\det(i\hat{D} + im_f)_{ZMZ} \prod_{I=1}^N 1.34 \rho_I \right) \quad (2-15)$$

A more elaborate discussion of the instanton liquid model described above is given in refs. [12,18]. The present model differs from ref. [18] at two points.

¹At this point we differ from Diakonov and Petrov [11].

We have used a different *Ansatz* for the instanton-instanton interaction (see eq. (2-10)), and we have corrected the approximation for the overlap matrix elements T_{IJ} (see eq. (2-14)).

The partition function (2-1) is simulated by means of a Metropolis algorithm. For a given pseudoparticle I , a Metropolis step is taken after the update of ρ_I , after the update of z_I , and after the update of U_I . One iteration consists of $3N$ Metropolis steps. The fermion determinant and the action are evaluated for each of these steps. The fermion determinant is obtained, either from the product of the eigenvalues or directly from a triangular factorization method. With this algorithm we were able to study systems up to 64 pseudoparticles. However, most results described in this work are for 32 pseudoparticles. The new variables in the Metropolis algorithm are obtained by adding an unbiased random number to the old variable. The widths of the distributions of these random numbers are chosen such that an acceptance rate of approximately 50% is achieved for each of the ρ_I , z_I and U_I . The ρ_I are forced to stay in the interval $[0, 1]$. We use periodic boundary conditions. Effectively, the motion of the pseudoparticles is on a torus. The distance between two pseudoparticles is defined as the length of the shortest path on the torus connecting them. In general, one should also take into account contributions from topologically different paths. We checked numerically that contributions involving the next shortest class of paths do not play an important role, and below we will take into account only the shortest path. Unless stated otherwise, our calculations start from a random initial configuration.

A wide variety of tests has been performed to check the algorithm. At this point we only mention that the numerical code was written independently by both authors, and after some work both codes gave identical results. We consider this to be a highly relevant test.

3. Different phases of the system of pseudoparticles

The statistical ensemble of pseudoparticles describing the true vacuum has some optimal pseudoparticle density which is fixed as a compromise between the action and the entropy. In this work we do not attempt to determine this density, but instead study the system in a wide range of densities, even definitely unphysical ones. In this way we hope to obtain a better understanding of the pseudoparticle system at physical densities. In fact there are external parameters that affect the density of pseudoparticles: the temperature and the baryon density of the system. In particular the temperature dependence of the density of instantons has been well studied [25,26]. The main effects are due to the modification of the size distribution of the instantons [25]

$$w(\rho) \rightarrow w(\rho) \exp(-\pi^2 \rho^2 T^2), \quad (3-1)$$

which leads to a temperature dependence of the average size and the average density [27,28,29]. Other effects are that the instanton profile changes as a function of the temperature, leading to a nontrivial temperature dependence of the matrix elements T_{IJ} [28]. We may consider the temperature and the chemical potential (which determines the matter density) as parameters that determine the average size of the instantons.

In this work we do not study the phases of the pseudoparticle system as a function of the temperature, but instead consider the system at zero temperature with the pseudoparticle density as an external parameter. From previous work [20,14,11,30] we know that the pseudoparticle system can exist in three different phases: a solid phase (at high densities), a liquid phase (at medium densities) and a gas phase of instanton-anti-instanton molecules (at low densities). A qualitative picture of these phases is shown in Fig. 1. In this figure instantons are represented by open circles and anti-instantons by full circles. The size of the box is given in units of Λ^{-1} . The fermionic overlap matrix elements T_{IJ} are depicted by full and

dashed lines. For each density we evaluate the maximum value T_{max} of the overlap matrix elements $|T_{II}|$. All pseudoparticle pairs with $T_{max}/2 < |T_{II}| < T_{max}$ are connected by a full line, and all pairs with $T_{max}/4 < |T_{II}| < T_{max}/2$ are connected by a dashed line. Although this recipe is subjective, it gives a good qualitative insight in the different phases of the system. Clearly, in fig. 1a ($N/V_4\Lambda^4 = 256.0$) we see a crystalline phase, and in fig. 1b ($N/V_4\Lambda^4 = 0.0256$) a phase consisting of instanton-anti-instanton molecules is observed. For the physical relevant density of 1 instanton per $f m^4$, Fig. 1c suggests a molecular phase or a phase with small clusters. The situation changes drastically if we decrease the number of massless flavors from 3 to 2. This is shown in Fig. 1d (as in Fig. 1c, $N/V_4\Lambda^4 = 1.0$), where we observe clusters extending over the whole system. For all systems in Fig. 1, the number of colors is equal to 3.

In the limit of very high densities the average distance $\bar{R}$ between the pseudoparticles is very small. The matrix elements of T_{II} are proportional to $\bar{R}/\bar{\rho}^2$. One factor $\bar{\rho}$ will be cancelled by the contribution from the continuum part of the fermion determinant. Therefore, in the limit $\bar{R} \rightarrow 0$ only configurations for which $\bar{R}/\bar{\rho} \rightarrow const.$ are relevant. This result is confirmed by our Monte-Carlo simulations. For a system of 32 pseudoparticles we show in Fig. 2 $N/V_4\bar{\rho}^4$ as a function of $\bar{R} = (V\Lambda^4/N)^{1/4}$. We conclude that in the limit $\bar{R} \rightarrow 0$ also $\bar{\rho} \rightarrow 0$. Consequently, $\beta(\bar{\rho})$ approaches infinity in this limit. In the absence of quantum fluctuations we expect the system to crystallize. This should happen even for a small number of flavors (e.g. $N_f = 1$).

At lower densities, the quantum fluctuations will become more substantial. Eventually, these fluctuations will lead to the melting of the crystal. As is clear from the way ρ enters in the partition function, for a given phase the dimensionless density $N/V_4\bar{\rho}^4$ will depend only logarithmically on N/V_4 . In Fig. 2 we observe that this parameter is almost constant for a wide range of densities. The depletion at very low densities is due to the cutoff of the size distribution at $\rho\Lambda = 1$. Its value (around 1/3) agrees with the value suggested on a phenomenological basis by one

of the authors [7]. We want to stress that the value of this parameter is also very stable with respect to variations of other parameters of the system (see e.g. Fig. 12 for the flavor dependence of this parameter). From Fig. 11 we also conclude that the pseudoparticles shrink inversely proportional to their average distance. This clearly illustrates the presence of a mutual repulsion at short distances. Two effects will affect the correlations in this fluid. The interactions between the pseudoparticles may lead to the formation of polymers (at high densities) or molecules (at low densities). On the other hand, quantum fluctuations, which increase with increasing $\bar{\rho}$, will lead to a break-up of these pseudoparticle chains. *A priori*, it is not clear whether, and in what sense, the quantum fluctuations will destroy the correlations in the liquid. Naively, we expect stronger correlations at higher densities. This should be contrasted to the case where the size of the instantons is determined by the value of the temperature. In previous work this case was studied in a simplified model with a fixed radius for the pseudoparticles [20,14]. In this case the quantum fluctuations (which are determined by the average size of the pseudoparticles) do not depend on N/V_4 . Therefore, at low densities the liquid of pseudoparticles will organize itself in a gas of instanton-anti-instanton molecules. At this point the chiral symmetry will be restored. In this work the size of the instantons will always be determined dynamically by the partition function. In the dilute limit we will observe mainly effects due to the cutoff of the size distribution $\rho\Lambda = 1$. Therefore, this limit extends well into the strong coupling domain, and conclusions cannot be considered reliable.

The integrand in eq. (2.1) shows a discontinuity at the transition between the crystalline phase and the liquid phase. This is illustrated in Fig. 3 where we plot the average internal energy per particle $\langle S \rangle$ (defined as the average of the logarithm of the integrand in eq. (2.1)) as a function of the average distance $\bar{R}$. We observe a phase transition at a density of $N/V_4\Lambda^4 \approx 65.0$. The increase of $\langle S \rangle$ in the liquid phase is mainly due to the increase of the average size of the pseudoparticles. Of course, the free energy must be continuous at the transition

between the two phases. In order to investigate this point, we define a quasi-entropy in terms of the acceptance rate of the Metropolis algorithm. Let P_{ρ_I} be the probability that a new value of ρ_I is accepted. Analogously, we can define P_{z_I} and P_{U_I} . To settle the normalization we choose the new variables independent of the old ones. Then we can define a quasi-entropy per particle by

$$S_M = \log P_\rho + \log P_z + \log P_U. \quad (3-2)$$

The dependence of S_M on the pseudoparticle density is shown in Fig. 4. The discontinuity between the crystalline phase and the liquid phase exactly matches the discontinuity in S . In the liquid phase, P_ρ and P_U increase monotonically as a function of the density, whereas P_z has a maximum around $a = 3$.

Next we analyze the crystal phase in more detail. At very high densities the total action will be dominated by the $I\bar{I}$ interaction (2-7). Consequently, $|u|^2$ will be maximized and d will be minimized. From the first condition we learn that the relative orientation matrix $U_I U_I^\dagger$ factorizes in a 2×2 block, and in a $(N_c - 2) \times (N_c - 2)$ block. The matrices in each of the blocks are unitary. Up to a phase factor $\alpha \in \mathbb{Z}_2$, the $SU(2)$ factor of the matrix in the upper 2×2 block is determined by the second condition,

$$\mathbf{1}_2 U_I U_I^\dagger \mathbf{1}_2 = \alpha^{II} \frac{i\tau_\mu^-(z_I - z_I)}{|z_I - z_I|}. \quad (3-3)$$

Consequently, an $SU((N_c - 2) \times U(1) \times Z_{N_c})$ subgroup of $SU(N_c)$ is not broken by the crystal [10] (for $N_c = 2$, only a Z_2 subgroup remains unbroken). When we move around a plaquette P the product of the relative orientation matrices must be equal to one. This results in the following consistency conditions,

$$\prod_{II'P} \frac{i\tau_\mu^-(z_I - z_I)}{|z_I - z_I|} \alpha^{II'} = 1. \quad (3-4)$$

It can be verified that the phase factors $\alpha^{II'}$ cannot be gauged away². For the overlap matrix T we find,

$$T_{II'} \sim \alpha_{II'}. \quad (3-5)$$

²The product of $R^{II'} i\tau_\mu^-$ around a plaquette P is equal to -1 . Therefore, also $\prod_{II'P} \alpha^{II'} = -1$.

The phase factors are such that the fermion determinant is maximized. Of course, apart from the already mentioned invariances, the orientations are only determined up to a global special unitary transformation.

Numerically, a crystal structure is found by starting from a random initial configuration at the very high density of $N/V\Lambda^4 = 1.6 \cdot 10^6$. The equilibrated configuration was used as a starting point for densities allowing a crystalline phase. Only for a total number of pseudoparticles equal to 16 a crystal structure was found. No crystal formation was observed for 32 pseudoparticles (calculations for other particle numbers were not performed). In the latter case the pseudoparticles cannot be distributed evenly over the four dimensions. Also the boundary conditions might play a role in the formation of a crystal. The crystal is a simple cubic lattice with instantons and anti-instantons on alternate sites [10] (a $4d$ generalization of the $NaCl$ lattice). However, in 4 dimensions, we have two distinct possibilities for the positions of the anti-instantons, given the lattice of the instantons. This can be understood as follows: suppose that an orthogonal set of unit vectors is given by $\{e_k\}$. Then the positions of the pseudoparticles are given by $\sum m_k e_k$. The instantons are at the positions with $\sum m_k$ odd, and the anti-instantons at the positions with $\sum m_k$ even. When we translate either the instantons or the anti-instantons by $\frac{1}{2}(e_1 + e_2 + e_3 + e_4)$, a different simple cubic lattice is obtained. The reason is that the distance from the center to a corner of a $4d$ cube is the same as the length of a rib of this cube.

In Fig. 5, we show the crystal as found from the numerical simulations. We show four different layers of the unit cell, which are labeled by the x_4 coordinate. Anti-instantons are denoted by full circles and instantons by open circles. The two different possibilities for the choice of the simple cubic crystal correspond to the interchange of layer one and layer three. The configuration in Fig. 5 was found for $N_f = 3$. For $N_f = 1$ layer one and layer three are interchanged. Pseudoparticles of the same kind do not interact when their relative orientations point in the unit direction. Therefore, two pseudoparticles of the same kind can be located at the

same position. Indeed, this possibility is realized, as can be seen from Fig. 5. For $N_f = 1$ we find even four pairs of pseudoparticles located at the same position.

The relative orientation between the pseudoparticles can be expressed in terms of the distribution of d defined in eq. (2-8). In absence of fluctuations we expect a single peak at $d = -3$ for the crystalline phase. In the liquid phase we only expect correlations between nearby pseudoparticles. After averaging over all pairs the total distribution will be close to random. The actual situation for the instanton-anti-instanton case is shown in Fig. 6a. For the crystalline phase the peak at $d = -3$ is smeared but the distribution is completely different from the case of random orientations (dashed line). For the phenomenologically interesting density of $N/V_4\Lambda^4 = 1$ the relative orientation is close to random. From the difference in area one can estimate that for each instanton there are approximately three anti-instantons for which the value of d is smaller than in the random case.

In Fig. 6b we show the relative orientation for pseudoparticles of the same kind. At a density of $N/V_4\Lambda^4 = 1$ their distribution is identical to the random distribution. In the crystal phase we expect two peaks. One peak at $d = 1$ for pseudoparticle pairs with the same x_4 coordinate, and another peak at $d = -1$ for pairs with different x_4 coordinates. This is confirmed by Fig. 6b.

As discussed above, in the crystalline phase the distribution of norm $|u|^2$ is peaked at $|u|^2 = 1$ for pseudoparticles of different chirality (see Fig. (7a)). For $N/V_4\Lambda^4 = 1$, its distribution is identical to the random case. The distribution of $|u|^2$ for pseudoparticles of the same chirality is not very different (see Fig. 7b). Now, the distribution for $N/V_4\Lambda^4 = 1.0$ (full line) differs slightly from the random distribution (dashed line).

Finally, we show in Fig. (8) the size distribution for an instanton density of $N/V_4\Lambda^4 = 1$. Its distribution is very close to gaussian. From this figure it is clear that our results do not depend on the cutoff at $\rho\Lambda = 1$. Deviations from a gaussian behavior are only found for large values of the average size where the cutoff at $\rho\Lambda = 1$ plays an important role. From mean field arguments one concludes that

the width of the size distribution is proportional to $1/\sqrt{N_c}$ [31].

4. Shape of the spectrum in the zero mode zone

When the collective coordinates of the pseudoparticles are distributed randomly, we expect that the eigenvalue density of the matrix T is reminiscent to the eigenvalue density of an uncorrelated gaussian random matrix. Indeed, in the large N_c limit one can prove [9,31] that the shape of the eigenvalue spectrum is semicircular. The result for finite N_c is more complicated and can only be obtained numerically. The result for a random distribution of the collective coordinates and $N_c = 3, N_f = 3$ is given by the dashed-dotted line in Fig. 9a. When we take into account the fermion determinant and the interaction between the pseudoparticles the results are completely different. The most remarkable feature is dip in the spectrum around zero. Since the eigenvalues are expressed in units of $\bar{\rho}^{-1}$ the spectrum does not change over a wide range of pseudoparticle densities. Only when the size distribution is affected by the cutoff at $\rho\Lambda = 1$ does the width of the eigenvalue distribution decrease, indicating the formation of a molecular phase.

The same qualitative behavior is found for $N_f = 3$ and $N_c = 2$ (see Fig. 9b). In this case the dip near zero is even more pronounced. However, for $N_c = 3, N_f = 2$ (see Fig. 9c) the picture is qualitatively different. In this case the dip at $\lambda = 0$ resembles a finite size effect. This will be confirmed in section 5 where we discuss the dependence of the shape of the dip on the size of the system. Only at much lower densities a spectrum characteristic for a molecular phase is observed. These results indicate that the fermion determinant plays a major role in establishing correlations in the instanton liquid.

The spectrum for the crystalline phase resembles a band spectrum found in ordinary solids. This result is shown in Fig. 9d. The fact that the eigenvalue

density at zero approaches zero is a nontrivial result. As an analogue consider the density of states on the Fermi sphere for an ordinary solid. Whether the eigenvalue density is zero (for an insulator) or nonzero (for a conductor) cannot be argued on general grounds.

The eigenvalue spectra can be summarized by the geometric average of the eigenvalues m_{det} . This so-called 'determinantal mass' should not be confused with the effective quark mass. In a molecular phase m_{det} is nonzero whereas the vacuum state is chirally symmetric with a zero effective quark mass. In Fig. 10 we show the dependence of m_{det} on the average distance $\bar{R}$ of the pseudoparticles. The results for the crystal phase are for 16 pseudoparticles, and all other results for 32 pseudoparticles. In the liquid phase m_{det} shows an extremely weak dependence of the pseudoparticle density. The m_{det} for random collective coordinates (denoted by a star) is much smaller. The result for $N_f = 2$ and $N_c = 3$ is in between the random result and the three flavor-three color result. In agreement with the displayed spectra, for $N_c = 2$ a large determinantal mass is found.

5. Finite size effects and the role of the strange quark mass

Only for isolated pseudoparticles do we find rigorously zero eigenvalues of the Dirac operator. For a finite system two pseudoparticles cannot be further apart than the size of the system, and strictly speaking there are no zero eigenvalues. The smallest eigenvalue is determined by the size of the system. A typical scale is given by the absolute value of the overlap matrix elements T at a separation of the order of the size of the system. We find

$$|T|/\Lambda \sim \frac{2}{\bar{\rho}\Lambda} \left(\frac{\bar{\rho}}{a} \right)^3, \quad (5.1)$$

where a is the linear size of the system. For a typical system of 32 pseudoparticles in a box with $a\Lambda = 2.2$ we find that $|T|/\Lambda \approx 0.05$.

We already observed a significant difference between the zero mode spectrum for two flavors and for three flavors. At a phenomenologically interesting pseudoparticle density of $N/V_4\Lambda^4 = 1$ the dip near zero for two flavors differs qualitatively from the dip for three flavors. In the latter case the dip is much more pronounced. If this dip is a finite size effect its area should decrease for an increasing number of pseudoparticles. In Fig. 11a we show the eigenvalue distributions for $N_f = 2$ and $N_c = 3$ for different pseudoparticle numbers. Results for 16 pseudoparticles are given by a dotted line, for 32 pseudoparticles by a dashed line and for 64 pseudoparticles by a full line. The pseudoparticle density is $N/V_4\Lambda^4 = 1.0$, and the quark masses are equal to zero. This figure strongly suggests that the dip at $\lambda\Lambda = 0$ is a finite size effect which should vanish in the thermodynamic limit.

Exactly the same series of calculations was performed for three flavors. The results are shown in Fig. 11b. Now, the spectra for 32 and 64 pseudoparticles are quantitatively similar. Moreover, for all pseudoparticle numbers essentially no eigenvalues are found for $\lambda\Lambda < 0.05$.

The number of flavors can be varied continuously. We find a gradual transition from the two flavor case to the three flavor case. A best estimate for the critical number of flavors would be 2.5. As will be shown in next section, for a large number of flavors we expect a phase of instanton-anti-instanton molecules. Consequently, the existence of this transition is not surprising. However, the occurrence of this transition at only 2.5 flavors was unexpected. Since a nonzero value of the strange mass effectively interpolates between two and three flavors, we expect to find a critical mass. For a mass below this mass the eigenvalue density at zero is zero, and above this mass it converges to some nonzero value in the thermodynamic limit. We performed calculations for only a limited number of mass values. The results for realistic quark masses (0.05 Λ , 0.05 Λ , 1.0 Λ) are given in Fig. 11c. The dip at zero appears to disappear in the thermodynamic limit, and we conclude that it is a finite size effect. For the instanton liquid the strange mass is rather 'heavy' than 'light'. It is not possible to discriminate these finite size effects from

other sources for a dip as *e.g.* due to the two-pion intermediate state contribution [20]. We also performed calculations for 3 colors and 3 flavors of equal mass at a density of $N/V_4\Lambda^4 = 1.0$. For masses of $m_f/\Lambda = 0.03$ the dip at zero is still present whereas for masses of m_f/Λ the dip vanishes in the thermodynamic limit.

The value of the chiral condensate is related to the eigenvalue density $\nu(\lambda)$ by

$$\langle \bar{u}u \rangle = -\frac{N}{V_4} \int d\lambda \frac{m_f \nu(\lambda)}{m_f^2 + \lambda^2} / \int d\lambda \nu(\lambda). \quad (5-2)$$

For the eigenvalue density given in Fig. 11c for $N = 64$ we find a value of $(1.21 \pm 0.03)\Lambda^3$ for $\langle \bar{u}u \rangle$, a value of $(0.73 \pm 0.01)\Lambda^3$ for $\langle \bar{s}s \rangle$. When also evaluated the eigenvalue spectrum for $N = 64$ and quark masses equal to $(0.05\Lambda, 0.05\Lambda, 0.7\Lambda)$. Now, we find $(1.19 \pm 0.03)\Lambda^3$ for $\langle \bar{u}u \rangle$ and $(0.87 \pm 0.01)\Lambda^3$ for $\langle \bar{s}s \rangle$. The ratio $\langle \bar{s}s \rangle / \langle \bar{u}u \rangle$ is equal to 0.60 and 0.73, respectively. Although the value is bigger than in ref. [18] (in this reference there is an error in the approximate expression for the overlap matrix elements T_{IJ}), it is still smaller than the accepted value of 0.8. In agreement with ref. [15,14] we find that $\langle \bar{u}u \rangle$ is insensitive to small variations of the value of the strange quark mass near the physical point. Of course, by decreasing the value of the strange quark mass to zero we obtain the qualitatively different result for three massless flavors.

6. The instanton liquid for many flavors

When we increase the number of massless flavors, the fermion determinant is raised to an equally high power. Consequently, in order to avoid small eigenvalues stronger correlations will be induced in the instanton liquid. More specifically, for a larger number of flavors an increasing number of molecules and small clusters will be present. For more than $\frac{11}{2}N_c$ flavors asymptotic freedom is violated. Obviously, this will result in a liquid with very different properties. We will not discuss this case any further.

As was noted by one of us [19], already for a smaller number of flavors we will find a genuine nonperturbative divergence in the sense that the density of the instanton-anti-instanton molecules diverges. Since the size distribution is proportional to $\rho^{\frac{11}{2}N_c - \frac{3}{2}N_f - 5}$, the average size shifts to smaller values for a larger number of flavors. It is only possible to maintain a large fermion determinant when the pseudoparticles organize themselves into clusters of a small volume. Due to phase space factors only the molecular clusters are relevant. In this case the system can be analyzed in more detail. The size distribution for a single molecule is proportional to

$$w(\rho_I, \rho_T) \sim (\rho_I \rho_T)^{b-\delta+2-b\delta}. \quad (6-1)$$

The 2 in the exponent arise from the integral over the relative position of the instanton-anti-instanton pair. The term $b\delta$ is due to the $I\bar{I}$ -interaction. For the most attractive orientation the value for δ is only 0.23. For $\frac{11}{2}N_c \geq N_f \geq \frac{11}{2}N_c - 2/(1-\delta)$ there is an ultra-violet divergence. When this condition is obeyed the Monte-Carlo simulations will not equilibrate. Instead, molecular configurations with smaller and smaller value of the average size will be generated.

The analytical estimates discussed above have been confirmed by our Monte-Carlo simulations. In Fig. 12 we show the flavor dependence of the average size of the pseudoparticles. For 12 flavors the Metropolis algorithm no longer equilibrates. For 10 flavors the average size is extremely small but nonzero. The flavor dependence of m_{det} is displayed in Fig. 13. After a gradual increase, it saturates at the molecular value. The projection of the 4d box of pseudoparticles on the xy -plane ($N_f = 9, N_c = 3$) is shown in Fig. 14. There are no bonds between different molecules. Bonds inside a molecule are no longer visible.

7. Discussion and Conclusions

This work essentially confirms all qualitative features of the instanton liquid found in previous works. Apart from this several new results have been found. The correlations induced by the fermion determinant were investigated in greater detail and with much better statistics. We found that they are responsible for a dip in the spectrum, which already for three massless flavors seems to prevail in the thermodynamic limit. In the case of two massless flavors the dip is qualitatively different and resembles a finite size effect. Therefore, it is not surprising that a quark mass for one of the quarks of the order of the strange quark mass also reduces these correlations considerably: also in this model the chiral symmetry is broken. For a pseudoparticle density of $N/V_4\Lambda^4 = 1.0$ we find phenomenologically acceptable values for the chiral condensates. We have thus found that the physical point is in a region where a strong rearrangement takes place. Both molecules and polymers seem to be present in considerable quantities. This makes the problem both nontrivial and interesting.

At very high instanton densities, the pseudoparticle system is in a solid phase. The liquid-solid phase transition takes place at a pseudoparticle density $N/V_4\Lambda^4 = 65.0$, a definitely unphysical density, which agrees qualitatively with previous analytical estimates [10]. In this crystalline phase we do not find eigenvalues near zero. The chiral symmetry is unbroken.

At very low densities the pseudoparticle system is in a gas phase of instanton-anti-instanton molecules. However, no clear transition to this phase is observed, and conclusions concerning this phase (at zero temperature) are unreliable because it is in the strong coupling domain. Moreover, the liquid phase is contaminated by molecules especially at a larger number of massless flavors.

When we increase the number of colors the average size of the instantons increases whereas the deviations from the average size decrease: the vacuum becomes more homogeneous. On the other hand, when we increase the number of massless

flavors the average size of the instantons decreases whereas the deviations from the average size increase. Moreover, correlations induced by the fermion determinant lead to the formation of small cluster and molecules: the vacuum becomes more inhomogeneous.

In lattice QCD calculations, one works with a typical quark mass of $50 - 100 \text{ MeV}$. When all three quarks are in this mass range no dip occurs. This suggests the possibility that QCD simulations with dynamical fermions might give qualitative different results for quark masses in the range $5 - 10 \text{ MeV}$. However, it should be noted that the present lattice size allows for only a few pseudoparticles which is insufficient to observe most of the phenomena mentioned above.

Our present calculations can be improved in several ways. We will mention two of them. In the first place, in order to determine the average pseudoparticle density we should have studied the grand canonical partition function. In the second place, we might improve on the *Ansatz* for the multi-instanton configuration. This would lead to a modified interaction between the instantons. Another important question which we have not really solved is the qualitative difference in the spectrum between two and three massless flavors. In particular, we do not understand which properties of the system are responsible for these correlations at precisely this number of massless flavors.

We have a few suggestions for the effects that might affect the strong correlations in the case of three massless flavors. We remind the reader that not all types of gluonic fluctuations have been taken into account properly. Actually, the semiclassical calculation is correct for gluon wavelengths up to a scale of $\bar{\rho}$. In this range of wavelengths fluctuations of order Λ^{-1} are not included correctly. First of all, they are in the strong coupling domain, where the gaussian approximation is inadequate. Second, even if this problem is ignored, and one proceeds semiclassically, one should evaluate the gaussian fluctuations around the many-instanton configuration. The breakup of the problem into fluctuations around one-instanton solutions is certainly not sufficient.

At the moment we do not know how to incorporate these long-range gluonic fluctuations. Neither do we understand in which way they can produce confinement. We are convinced that they will not affect the gross features of the instanton system (such as the total density *etc.*). However, these long range fluctuations may affect long range correlations between the instantons, presumably randomizing the system and lead to the absence of a dip in the thermodynamic limit.

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Figure Captions

- Fig. 1. Projection on the xy -plane of the $4d$ hypercube containing pseudoparticles. Instantons are depicted by open circles and anti-instantons by full circles. The full lines and the dashed lines show the strength of the overlap matrix element T_{II} (the precise definition is given in the text). The pseudoparticle density $N/V_4\Lambda^4$ is equal to 256.0, 0.0256, 1.0 and 1.0 in Figs. 1abcd, respectively. The results are for 2 (Fig. 1d) and 3 (Figs. 1abc) massless flavors.
- Fig. 2. The gas factor $(N/V_4)^{1/4} \bar{\rho}$ for a system of 32 pseudoparticles as a function of the average distance $\bar{R}\Lambda$. The quark masses are equal to zero. The full line is drawn to guide the eye. Further comments are in the legend of the figure.
- Fig. 3. The average action $\langle S \rangle$ for a system of 32 pseudoparticles as a function of the average distance. For further details we refer to the caption of Fig. 2.
- Fig. 4. The quasi-entropy S_M (see eq. (3-2)) for a system of 32 pseudoparticles as a function of the average distance $\bar{R}$. For further comments we refer to the caption of Fig. 2.
- Fig. 5. Three-dimensional sections of the unit cell of the four dimensional instanton crystal. Instantons are denoted by open circles and anti-instantons by full circles.
- Fig. 6. Distribution of the relative orientation of the pseudoparticle pairs as given by d (see eq. (2-8)) for a system containing 16 (for $N/V_4\Lambda^4 = 256.0$) or 32 (for $N/V_4\Lambda^4 = 1.0$) pseudoparticles. The case where the orientations and the positions are distributed randomly is shown by a dashed line. All flavors are massless. In Fig. 6a we show results for pseudoparticles of a different kind, and in Fig. 6b we show results for pseudoparticles of the same kind. In Fig. 6b the curve for the random case coincides with the full curve for $N/V_4\Lambda^4 = 1.0$.

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Fig. 7. The distribution of $|u|^2$ for a system of 16 (for $N/V_4\Lambda^4 = 256.0$ or 32 (for $N/V_4\Lambda^4 = 1.0$) pseudoparticles. The instanton-anti-instanton case is shown in Fig. 7a and the instanton-instanton case in Fig. 7b. In Fig. 7a the random case (dashed curve in Fig. 7b) coincides with the full curve. All quarks are massless.

Fig. 8. The size distribution for a system of 32 pseudoparticles at a density of $N/V_4\Lambda^4 = 1.0$. All quarks are massless.

Fig. 9. The eigenvalue distribution of the overlap matrix T . The curves for $N/V_4\Lambda^4 = 16.0$ in Fig. 9a and the curve in Fig. 9d are for a system of 16 pseudoparticles. All other curves are for 32 pseudoparticles. The results shown in Fig. 9b and Fig. 9c are for systems that only differ in the number of colors and the number of flavors from systems presented in Fig. 9a. In all cases the quarks are massless.

Fig. 10. The determinantal mass m_{det} for a system of 16 (for $\bar{R} \leq 0.35$) or 32 (for $\bar{R} \geq 0.35$) pseudoparticles as a function of $\bar{R}$. The curves have been drawn to guide the eye.

Fig. 11. The N -dependence of a pseudoparticle system with a density $N/V_4\Lambda^4 = 1.0$. Fig. 11a is for 2 massless flavors, Fig. 11b for three massless flavors and Fig. 11c for three flavors with realistic quark masses.

Fig. 12. The average size $\bar{\rho}\Lambda$ as a function of the number of flavors for a system of 32 pseudoparticles with a density of $N/V_4\Lambda^4 = 1.0$. All flavors are massless. The curve has been drawn to guide the eye.

Fig. 13. The determinantal mass m_{det} as a function of the number of flavors for a system of 32 pseudoparticles with a density of $N/V_4\Lambda^4 = 1.0$. All flavors are massless. The line has been drawn to guide the eye.

Fig. 14. Projection on the xy -plane of the four dimensional hypercube containing 32 pseudoparticles. The results are for 9 massless flavors and 3 colors. The size of the box $a\Lambda$ is equal to 2.378. For more details we refer to the caption of Fig. 1.

Fig. 1a

Fig. 1b

Fig. 1d

Fig. 1c

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6a

Fig. 6b

Fig. 7a

Fig. 7b

Fig. 8

Fig. 9a

Fig. 9b

Fig. 9c

Fig. 9d

Fig. 10

Fig. 11a

Fig. 11b.

Fig. 11c.

Fig. 12

Fig. 13

Fig. 14