Slave-boson mean-field theory for the negative-U Hubbard model

J. O. Sofo and C. A. Balseiro
Centro Atómico Bariloche and Instituto Balseiro, 8400 Bariloche, Argentina
(Received 26 July 1991)

We study the negative-U Hubbard model for arbitrary values of the attractive interaction U and band filling by means of the slave-boson mean-field theory. We analyze both the normal and the superconducting states. We show that for the superconducting state our approach gives results similar to those obtained in the usual BCS mean field; only small renormalization of the bare parameters are obtained for U of the order of the bandwidth W. The energy difference between the normal and the superconducting states is maximum for $U \simeq W$. This energy difference is a measure of the superconducting critical temperature, which increases exponentially for small U and decreases as $1/U$ for large U. We discuss briefly the pair-breaking excitations.

I. INTRODUCTION

The problem of the evolution of the superconducting ground-state and elementary excitations from the weak coupling to the Bose-condensation limit was addressed some years ago by a number of authors.[1–5] The discovery of high-temperature superconductivity has triggered a renewed interest in many aspects of superconductivity, in particular this crossover from Cooper pairing to Bose condensation.

Among the peculiarities of the high-T_c materials, the layered crystalline structures, and the short superconducting coherence length could be responsible for many of the anomalous properties observed in these systems regardless of the particular mechanism leading to superconductivity.

The layered structures could lead to quasi-two-dimensional behavior, while the short coherence length seems to indicate that these systems are in an intermediate regime between the BCS limit, where the size of the Cooper pairs is much larger than the characteristic interparticle distance and the Bose condensation of tightly bound pairs.

At zero temperature the crossover from the weak- to the strong-coupling limits has been analyzed in the context of a BCS theory with a renormalized chemical potential[6] and by using a variational ansatz in two dimensions.[7]

In this work we study the single-band negative-U Hubbard model using the slave-boson formulation in the saddle-point approximation[8] to describe the superconductivity in a system with short-range interactions.

It has been shown recently[9] that this method applied to the positive-U Hubbard model leads to quantitative agreement with quantum Monte Carlo results for the energy and some local observables. Although the repulsive case has been extensively studied with the slave-boson approach,[8–10] for the attractive case the method has not been used. We expect the method to be equally reliable in both cases.

We find that the ground state evolves smoothly from the weak- to the strong-coupling limits. The condensation energy is maximum for the intermediate regime leading to a maximum in the transition temperature. We present results for the pair-breaking energy and the renormalization of the bare parameters.

The rest of the paper is organized as follows: In Sec. II we present the model and the approximation scheme, in Sec. III we present the results, and Sec. IV includes a summary and discussion.

II. SLAVE-BOSON APPROACH

Our starting point is the negative-U Hubbard model, which in the usual notation reads

$$H = -t \sum_{i,j,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} , \quad (1)$$

where $c_{i\sigma}$ are annihilation operators of fermions at site i with spin σ. The hopping matrix element t connects nearest neighbors only, and U ($U > 0$) is the strength of the local attractive interaction.

For the sake of clarity we found it convenient to perform a duality transformation that maps the attractive case into the repulsive one.[11] Although this step is not necessary, for the repulsive case we can take advantage of the experience gained in previous studies. This transformation is equivalent to an electron-hole transformation for the spin-down particles: $c_{i\uparrow} \rightarrow c_{i\uparrow}$ and $c_{i\downarrow} \rightarrow e^{i\mathbf{Q}\cdot\mathbf{R}_i} c_{i\downarrow}^{\dagger}$, where $\mathbf{Q} = (\pi, \ldots)$ and $\mathbf{R}_i$ is the coordinate of site i. The transformed Hamiltonian corresponds to a repulsive Hubbard model with one particle per site and an external magnetic field:

$$\tilde{H} = -t \sum_{i,j,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \frac{U}{2} \sum_{i,\sigma} n_{i\sigma} - \frac{h}{2} \sum_{i} (n_{i\uparrow} - n_{i\downarrow}) , \quad (2)$$

where the effective field $h = U + 2\mu$. The subspace of a fixed number of particles n in the Hamiltonian of Eq. (1)

corresponds to a fixed magnetization $m_z = n - 1$ in the representation of Eq. (2).

The superconducting order parameter of the Hamiltonian (1) $\Delta = \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$ corresponds to a staggered magnetization in the x-y plane of Hamiltonian (2) $\tilde{\Delta} = \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle e^{i\mathbf{Q}\cdot\mathbf{R}_i}$. The superconducting state is then obtained as a state with staggered magnetization in the x-y plane and total magnetization $m_z = n - 1$ along the z direction. To obtain this state we add to the Hamiltonian of Eq. (2) a constrain by means of a Lagrange multiplier $\lambda^{(0)}$. The total Hamiltonian is given by

$$H_S = \tilde{H} - \frac{\lambda^{(0)}}{2} \sum_i [\eta_i (c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}) - m_x] , \tag{3}$$

where $\eta_i = e^{i\mathbf{Q}\cdot\mathbf{R}_i}$. Once the energy of the system with this constraint is evaluated, it is minimized with respect to m_x. The normal phase is then characterized by $m_x = 0$, the superconducting phase by $m_x \neq 0$. The magnetization m_x in the positive-U representation corresponds to an off-diagonal long-range order (ODLRO) of the negative-U model.

In the slave-boson approach the partition function of the system is written in a functional-integral form in terms of four auxiliary boson fields: e_i, $p_{i\sigma}$, and d_i. Following Kotliar and Ruckenstein[8] each boson is associate with a given electronic configuration: empty (e_i), single-occupied ($p_{i\sigma}$) and double-occupied (d_i) states of Hamiltonian (3). Completeness relation and charge conservation give the following identities:

$$e_i^\dagger e_i + p_{i\uparrow}^\dagger p_{i\uparrow} + p_{i\downarrow}^\dagger p_{i\downarrow} + d_i^\dagger d_i = 1 \tag{4}$$

and

$$c_{i\sigma}^\dagger c_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i . \tag{5}$$

These constraints are introduced through Lagrange multipliers $\lambda^{(1)}$ and $\lambda^{(2)}$.

In terms of the auxiliary boson fields the Hamiltonian are given by

$$\begin{aligned} \bar{H} = & -t \sum_{i,j,\sigma} z_{i\sigma}^\dagger c_{i\sigma}^\dagger c_{j\sigma} z_{j\sigma} + U \sum_i d_i^\dagger d_i - \frac{h}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow}) \\ & - \frac{\lambda^{(0)}}{2} \sum_i \eta_i (y_{i\uparrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow} y_{i\downarrow} + y_{i\downarrow}^\dagger c_{i\downarrow}^\dagger c_{i\uparrow} y_{i\uparrow} - m_x) \\ & - \sum_i \lambda_i^{(1)} (e_i^\dagger e_i + p_{i\uparrow}^\dagger p_{i\uparrow} + p_{i\downarrow}^\dagger p_{i\downarrow} + d_i^\dagger d_i - 1) \\ & - \sum_{i,\sigma} \lambda^{(2)} (c_{i\sigma}^\dagger c_{i\sigma} - p_{i\sigma}^\dagger p_{i\sigma} - d_i^\dagger d_i) , \end{aligned} \tag{6}$$

where $z_{i\sigma}$ changes the number of bosons at site i and is given by

$$\begin{aligned} z_{i\sigma} = & \frac{1}{\sqrt{1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma}}} \\ & \times (e_i^\dagger p_{i\sigma} + p_{i\bar{\sigma}}^\dagger d_i) \frac{1}{\sqrt{1 - e_i^\dagger e_i - p_{i\bar{\sigma}}^\dagger p_{i\bar{\sigma}}}} . \end{aligned} \tag{7}$$

The choice of the operator $z_{i\sigma}$ is not unique. The form given in Eq. (7) guarantees that, at a saddle-point level, the $U = 0$ limit is well described. The operator $y_{i\sigma}$ in Eq. (6) is given by

$$y_{i\sigma} = \frac{1}{\sqrt{1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma}}} p_{i\sigma} \frac{1}{\sqrt{1 - e_i^\dagger e_i - p_{i\bar{\sigma}}^\dagger p_{i\bar{\sigma}}}} . \tag{8}$$

Here again, as in the case of the operator $z_{i\sigma}$, we take the representation of $y_{i\sigma}$, which gives the exact result for the uncorrelated state.

In the Hamiltonian of Eq. (6) the fermion variables appear in a bilinear form and can be integrated out exactly. The boson variables are treated in the saddle-point approximation. This approximation is equivalent to replacing the boson operators by numbers in Eq. (6). Clearly in this type of approach the terms of the Hamiltonian that contain products of fermion and boson operators are treated in an approximated way. In particular, in the present case, the kinetic energy and the pairing energy—proportional to $\lambda^{(0)}$—are evaluated at a mean-field level. This way of treating the slave-boson fields presents a poor approximation. In the large-U limit, the pairing energy dominates, and it would be convenient to evaluate it in a more rigorous way. To do so, we proceed in the following way.

The Hamiltonian of Eq. (3) describes electrons in the presence of an external magnetic field. This effective field has a component along the z direction given by the chemical potential μ of the original Hamiltonian of Eq. (1) and a staggered field in the x-y plane given by the pairing-order parameter. We perform a rotation at each site of the lattice such that the effective magnetic field induces a magnetization along the z direction of the new coordinates system. This corresponds to a rotation of an angle θ ($-\theta$) along the x-z plane in sublattice A (B). After performing the rotation we introduce the boson fields. The angle θ is calculated self-consistently. In this way in the large-U limit the pairing energy is evaluated exactly.

In the mixed boson-fermion representation the Hamiltonian reads

$$\begin{aligned} \bar{H}_R = & -t \cos\theta \sum_{i,j,\sigma} z_{i\sigma}^\dagger c_{i\sigma}^\dagger c_{j\sigma} z_{j\sigma} - t \sin\theta \sum_{i,j} \eta_i (z_{i\uparrow}^\dagger c_{i\uparrow}^\dagger c_{j\downarrow} z_{j\downarrow} - z_{i\downarrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow} z_{j\uparrow}) \\ & + U \sum_i d_i^\dagger d_i - \frac{h\cos\theta + \lambda^{(0)} \sin\theta}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow}) - \frac{\lambda^{(0)} \cos\theta - h \sin\theta}{2} \sum_i \eta_i (y_{i\uparrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow} y_{i\downarrow} + y_{i\downarrow}^\dagger c_{i\downarrow}^\dagger c_{i\uparrow} y_{i\uparrow}) \\ & - \sum_i \lambda_i^{(1)} (e_i^\dagger e_i + p_{i\uparrow}^\dagger p_{i\uparrow} + p_{i\downarrow}^\dagger p_{i\downarrow} + d_i^\dagger d_i - 1) - \sum_{i,\sigma} \lambda^{(2)} (c_{i\sigma}^\dagger c_{i\sigma} - p_{i\sigma}^\dagger p_{i\sigma} - d_i^\dagger d_i) + \frac{\lambda^{(0)} m_x}{2} . \end{aligned} \tag{9}$$

As we have mentioned above, the angle θ is evaluated self-consistently to achieve the condition that the magnetization at each site points along the z direction. The angle θ depends on the pairing field $\lambda^{(0)}$, for the normal state $\lambda^{(0)} = \theta = 0$, and Hamiltonian (9) reduces considerably. In what follows we study two phases: (i) the normal phase ($\lambda^{(0)}, m_x = 0$) and (ii) the superconducting phase ($\lambda^{(0)}, m_x \neq 0$).

III. RESULTS

In this section we present the results corresponding to the normal and superconducting phases.

A. The normal phase

In order to study the phase without ODLRO we set, in Hamiltonian (9), $\lambda^{(0)} = \theta = 0$. After integration of the fermion variables and performing the saddle-point approximation for the boson fields, we obtain the following free energy for the system:

$$f_N = -\frac{k_B T}{M}\sum_k \ln\left\{1+\cosh\left[\beta\left(q\varepsilon_k - \frac{h}{2}\right)\right]\right\} + Ud^2 + \left(\frac{h-U}{2}\right)m_z - \frac{U}{2} - k_B T \ln 2 , \quad (10)$$

where

$$q = \langle z_{i\sigma}\rangle^2 = \frac{4d^2}{1-m_z^2}[1-2d^2+\sqrt{(1-2d^2)^2-m_z^2}] . \quad (11)$$

Here ε_k is the dispersion relation of the uncorrelated band, and $d^2 = \langle d_i^\dagger d_i\rangle$. Note that d^2 is the probability of a single occupation for the original Hamiltonian (1) with a local attraction.

This free energy has been minimized with respect to the Lagrangian multipliers $\lambda^{(1)}$ and $\lambda^{(2)}$. After minimization with respect to d^2 and h, we obtain—as expected—two phases that correspond to $q = 0$ for large U and $q \neq 0$ for small U.

If $q = 0$, electrons cannot propagate as independent particles; this phase corresponds to a situation in which there is a real two-particle bound state below the bottom of the one-particle band. The electrons are bound in pairs, and the system behaves as a collection of hard-core bosons. In the present approximation, however, the boson mass is infinite; only by including fluctuations around the saddle-point have the bosons acquired a finite mass. An alternative way to study the large-U limit is by means of a canonical transformation of the original Hamiltonian (1);[12–14] with this procedure it is easy to show that the effective hopping matrix element for the bosons is of the order of t^2/U.

The phase with $q \neq 0$ corresponds to a state with unbound electrons, which can propagate as independent particles, although the effective mass is strongly renormalized by a factor q. In this regime our approximation suggests[15] that the system will behave as a Fermi-liquid system. However, some authors speculate that in two dimensions the system may behave as a marginal Fermi liquid.

The critical value of U at which a bound state occurs is given by

$$U_c = 2W[1+\sqrt{n(2-n)}] , \quad (12)$$

assuming a rectangular band of width $2W$.

In Fig. 1 the mass-renormalization factor q, the probability of single-occupied sites and the energy per site are shown as a function of U for $n = 0.6$. For $U > U_c$ the mass renormalization q and the probability of single-occupied sites are zero, and the energy is given by $-Un/2$. The same quantities (q, d, and E) are shown in Fig. 2 as a function of the particle density n. As Eq. (12) indicates, for $U < 2W$ ($U > 4W$) the mass-renormalization factor q is different from zero (equal to zero) for the whole range of concentrations. For $2W < U < 4W$ there is a critical density n_c such that for $n < n_c$ there is a real bound state, while for $n > n_c$ the electrons can propagate as independent particles.

The pairing energy in the normal phase is given by the minimum energy $\tilde{\Delta}$ needed to flip a spin. This quantity is zero for $U < U_c$ and increases for $U > U_c$ to reach, in the large-U limit, the value $\tilde{\Delta} = U$. To flip a spin in the negative-U Hubbard model corresponds to changing the number of particles in the transformed Hamiltonian of Eq. (3). The pairing gap is given by the Mott gap of a polarized system in the positive-U representation.

We calculate the chemical potential of the system ($\mu =$

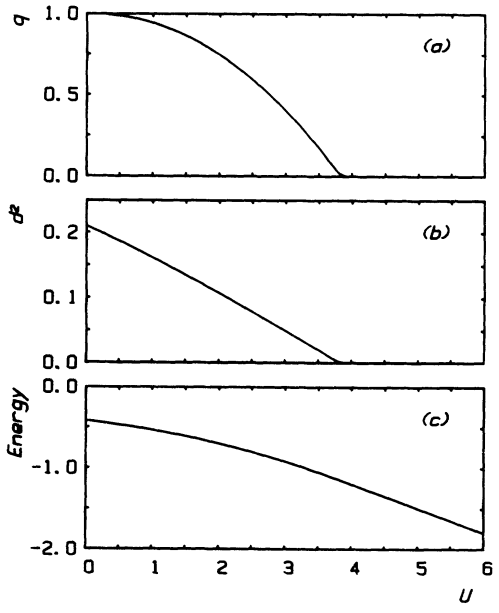

FIG. 1. Mass-renormalization factor q (a), probability of single-occupied sites d^2 (b), and energy per site (c) as a function of U in the normal phase. Calculations are for a particle density $n = 0.6$, and bandwidth $W = 1$.

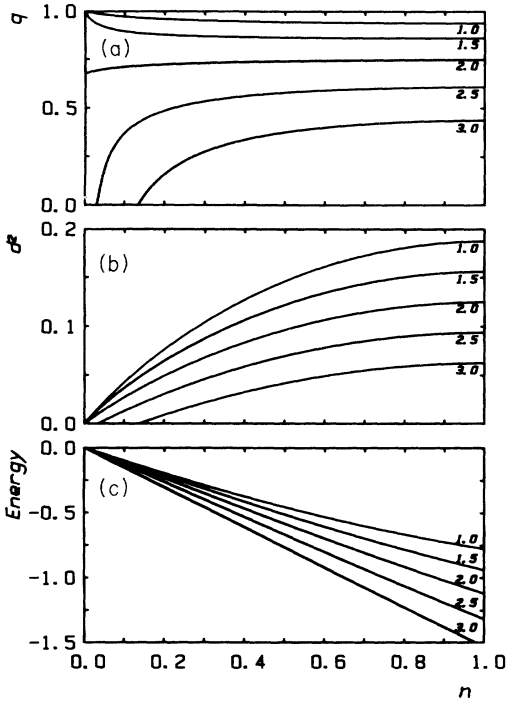

FIG. 2. Mass-renormalization factor q (a), probability of single-occupied sites d^2 (b), and energy per site (c) as a function of the particle density n in the normal phase and calculated for different values of U as indicated in the figure, and $W = 1$.

$\partial f_N/\partial n$) as a function of n for different values of U. The results are shown in Fig. 3. As can be seen, there is a change in behavior when $U = 2W$. For $U > 2W$ there is a region at low density where μ is independent of n,

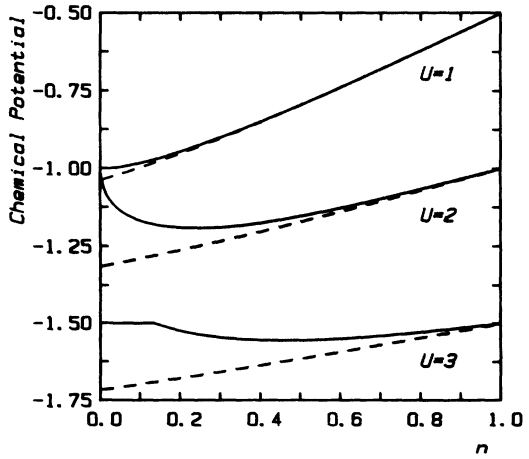

FIG. 3. Chemical potential μ as a function of the particle density n in the normal phase (full line) and in the superconducting phase (dashed line). The curves correspond to different values of the interaction parameter U as indicated in the figure, and bandwidth $W = 1$.

indicating the existence of the bound state, which can accommodate a finite number of pairs. The bound state lies at $-U/2$. For $U < 2W$, $\mu \to -W$ as $n \to 0$, and in all cases $\mu \to -U/2$ as $n \to 1$. For the parameters studied, there is always a range of densities where the chemical potential decreases with n, indicating an instability of the system. For this density the system is characterized by a negative compressibility. This is not surprising, since the normal phase does not correspond to the ground state of the system. As we show below, the state with ODLRO always has lower energy than the normal state and is well behaved.

B. The superconducting phase

In this phase we minimize the free energy with respect to the ODLRO parameter m_x. The free energy in the saddle-point approximation is given by

$$f_S = -\frac{k_B T}{M}\sum_k \ln\left[1+\cosh\left(\beta E_k\right)\right] + Ud^2 - \frac{Un}{2} + \frac{hm_z}{2} + \frac{\lambda^{(0)}m_x}{2} - k_B T \ln 2 , \tag{13}$$

where

$$\begin{aligned} E_k &= \sqrt{(q_0\varepsilon_k - h_1)^2 + (q_1\varepsilon_k + \lambda_1)^2} , \\ h_1 &= \frac{1}{2}\frac{hm_z + \lambda^{(0)}m_x}{\sqrt{m_x^2+m_z^2}} , \\ \lambda_1 &= \frac{g}{2}\frac{\lambda^{(0)}m_z - hm_x}{\sqrt{m_x^2+m_z^2}} , \\ q_0 &= \frac{qm_z}{\sqrt{m_x^2+m_z^2}} , \\ q_1 &= \frac{qm_x}{\sqrt{m_x^2+m_z^2}} , \\ q &= \frac{4d^2[1-2d^2+\sqrt{(1-2d^2)^2-m_x^2-m_z^2}]}{1-m_x^2-m_z^2} \\ g &= \langle y_{i\uparrow}^\dagger y_{i\downarrow}\rangle = \frac{2\sqrt{(1-2d^2)^2-m_x^2-m_z^2}}{1-m_x^2-m_z^2} . \end{aligned} \tag{14}$$

This free energy is to be minimized with respect to the parameters m_x, h, $\lambda^{(0)}$, and d^2.

In this phase the behavior of the system is qualitatively the same for all values of U. In Fig. 4 we show the factor q and the probability of a single-occupied site for different values of the band filling. For the sake of completeness the self-consistent value of the angle θ is also shown. Note that $q \simeq 1$ for all values of U. The maximum correction to this value is about 5% for $U/W \simeq 1$. In contrast to the result obtained for the normal phase the renormalization of the quasiparticle excitations in the superconducting state is very small. This means that the quasiparticles and, as we will see below, the energy of the system are well described by the BCS mean field, which corresponds to $q = 1$. The pair-breaking gap is, as in the normal phase, of the order of U for large U. It should be noted, however, that the pair-breaking excitations are not the ones that will destroy the off-diagonal long-range order

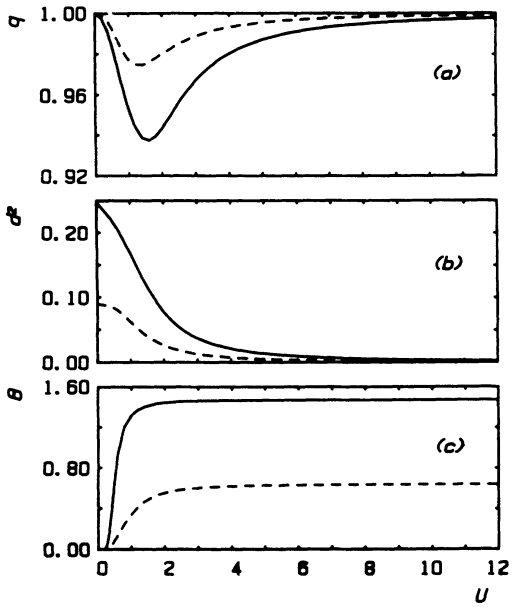

FIG. 4. Mass-renormalization factor q (a), probability of single-occupied sites d^2 (b), and angle of rotation of the quantization axis for the spin θ (c) as a function of U in the superconducting phase with a bandwidth $W = 1$. The corresponding particle densities are $n = 0.2$ (dashed line) and $n = 0.9$ (full line).

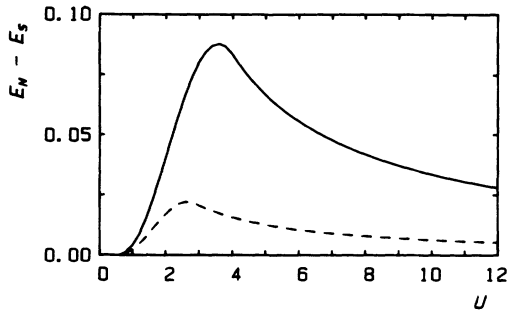

FIG. 5. Difference between the energy of the normal phase E_N and the energy of the superconducting phase E_S as a function of the interaction parameter U for two-particle densities: $n = 0.1$ (dashed line) and $n = 1.0$ (full line), with a bandwidth $W = 1$.

for large U. In both, the superconducting and the normal states all the particles are bound in pairs for large U.

The chemical potential of the superconducting phase as a function of n is shown in Fig. 3. In this phase the compressibility is always positive.

The difference between the energy of the normal phase E_N and the energy of the superconducting phase E_S is shown in Fig. 5. As U increases from zero, this energy difference increases exponentially. It goes through a maximum, and it decreases as $1/U$ for large U. Clearly the critical temperature T_c will behave roughly as this energy difference. However, to calculate T_c one should evaluate the entropy. Unfortunately the saddle point presented in this work gives the wrong entropy for the system, and in order to do the thermodynamic one should correct the mean field by including corrections around the saddle point.

IV. SUMMARY AND DISCUSSION

In this work we have studied the negative-U Hubbard model using slave bosons in the saddle-point approximation. We have obtained solutions for both the normal and the superconducting states.

The normal state obtained within this approximation is qualitatively different from the normal state described in the usual BCS mean field. The existence of real bound pairs in the former is a feature that is not present in the latter. This causes the energy difference between the normal and the superconducting state (see Fig. 5) to go as t^2/U for large U, while in the BCS mean field it is of the order of U. It is clear that in this limit the superconductivity will be destroyed because of the loss of coherence and not by pair-breaking excitations.

For the superconducting state, we have shown that in order to obtain a qualitatively correct description at the saddle-point level, a particular representation of the original Hamiltonian is to be used. The BCS mean-field theory is a very good description of the superconducting phase for all values of U and densities.

The method can be generalized to study the interplay between superconductivity and charge-density waves for $n \simeq 1$—a nearly half-filled band. The charge-density-wave state in the positive U representation of Hamiltonian (1) is described by a staggered magnetization along the z axis and can be included in a straightforward way by including a different order parameter.

ACKNOWLEDGMENT

We are partially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.

[1] A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter*, edited by A. Pekalski and J. Przystawa (Springer-Verlag, Berlin, 1980), p.13.
[2] D. M. Eagles, Phys. Rev. **188**, 456 (1969).
[3] M. Randeria, J. Duan, and L. Shieh, Phys. Rev. Lett. **62**, 981 (1989).
[4] R. T. Scalettar, E. Loh, J. Gubernatis, A. Moreo, S. White, D. Scalapino, R. Sugar, and E. Dagotto, Phys. Rev. Lett. **62**, 1407 (1989).
[5] K. Miyake, Prog. Theor. Phys. **69**, 1794 (1983).
[6] P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).

[7] M. Randeria, J. Duan, and L. Shieh, Phys. Rev. B **41**, 327 (1990).
[8] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).
[9] L. Lilly, A. Muramatsu, and W. Hanke, Phys. Rev. Lett. **65**, 1379 (1990).
[10] M. Lavagna, Phys. Rev. B **41**, 142 (1990).
[11] H. Shiba, Prog. Theor. Phys. **48**, 2171 (1972).
[12] S. Robaskiewicz, R. Micnas, and K. A. Chao, Phys. Rev. B **23**, 1447 (1981)
[13] A. Alexandrov and J. Ranninger, Phys. Rev. B **23**, 1796 (1981)
[14] A. G. Rojo, J. O. Sofo, and C. A. Balseiro, Phys. Rev. B **42**, 10 241 (1990)
[15] P. Nozières (unpublished).