Pairing, condensation, and superconductivity described by a Hubbard model with an attractive interaction

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We have developed a method for studying superconductivity in the negative-U Hubbard model. It is based on the Hubbard-alloy-analogy approximation applied to the Gor'kov equation for the model. We find that, unlike the case of the BCS solution, the formation of pairs and their condensation into a superconducting ground state take place at two different temperatures. We calculate the condensation temperature T_c for all U and discuss the nature of the normal state which, for large enough U, features a macroscopically large number of pairs. Briefly, we argue that the model has relevance for high-temperature superconductors.

I. INTRODUCTION

Investigating the real-space form of the BCS wave function, Leggett[1] noted that, when the effective attraction between the electrons is strong enough to bind a pair in free space, i.e., without the Fermi sea of the Cooper problem, the ground-state wave function is best described as a Bose-Einstein condensate of bound, "molecular" pairs. Surprisingly, he found no sudden change, as in a phase transition, as the strength of the interaction was increased. However, at finite nonzero temperatures, the physics of the strong-coupling case must be very different from the picture provided by the Bardeen-Cooper-Schrieffer[2] theory. Clearly, for a sufficiently strong interaction, the formation of pairs and their condensation into the superfluid state takes place at two, separate temperatures as in the pre-BCS-theory suggestion of Schafroth *et al.*[3] Indeed, for asymptotically large coupling constants, the problem becomes fairly straightforward to treat. In this regime, Pincus,[4] Robaszkiewicz *et al.*,[5] and Nozières and Schmitt-Rink[6] found that, above the condensation temperature T_c but below the pair-breaking temperature T_p, the electron system becomes equivalent to a hard-core bose gas on a lattice with a charge $2e$ on each particle. In the present paper, our purpose is to propose a tractable approximation scheme which will facilitate the investigation of the most interesting intermediate-coupling regime as well as the weak- and strong-coupling limits, at all temperatures.

As the simplest relevant model we shall study a single-band Hubbard model with an attractive interaction. It is described by the Hamiltonian

$$H=-\sum_{i,j,-\sigma} t_{ij}C^{\dagger}_{i,\sigma}C_{j,\sigma}+U\tfrac{1}{2}\sum_{i,\sigma}C^{\dagger}_{i,\sigma}C_{i,\sigma}C^{\dagger}_{i,-\sigma}C_{i,-\sigma}\ , \qquad (1)$$

where the fermion operators $C^{\dagger}_{i,\sigma}$ and $C_{i,\sigma}$ create and annihilate, respectively, electrons with spin σ in the single tight-binding orbital associated with the site i, t_{ij} is the amplitude for hopping from site j to site i with the diagonal part t_{ii} being the local site energy, $-\varepsilon_0$ and U is, as usual, the interaction energy of two electrons of opposite spin on the same site. In what follows, we shall have in mind the case where the sites labeled by i and j form a three-dimensional lattice. Moreover, we take the interaction energy U to be attractive: $U<0$.

Evidently, the interaction term in the above Hamiltonian favors double occupancy of sites and, hence, charge fluctuations. Indeed, Anderson[7] used a version of this negative-U model to describe strong static binding of electrons at localized centers in amorphous semiconductors.[8,9] Also, very similar models were used to describe a variety of charge-ordering phenomena by Chakravarty *et al.*,[10] Ionova *et al.*,[11] and Lubimov *et al.*[12]

If bound pairs form and they are mobile, superconductivity may also occur. It is this feature of the model we shall focus on. For $|U|$ much less than the bandwidth W ($=2zt$, where t is the nearest-neighbor hoping probability amplitude and z is the number of nearest neighbors), Gorkov decoupling of the equation of motion for the one-particle Green's function leads to the usual BCS-type results. In the opposite limit, $|U|\gg W$, progress can be made by making a canonical transformation which eliminates singly occupied sites and reduces the problem to that of the spin Hamiltonian

$$H_{\rm eff}=-\sum_{i,j}J_{ij}(S_i^{+}S_j^{-}-S_i^{z}S_j^{z})-B\sum_i(2S_i^{z}+1)\ , \qquad (2)$$

where the effective "exchange interaction" $J_{ij}=4t_{ij}^2|U|^{-1}$, the external "magnetic field" $B=\mu-\varepsilon_0$

$+\frac{1}{2}|U|$ with μ the electronic chemical potential, and the z component of the magnetization M_z is constrained by the relation

$$N^{-1}\sum_{i=1}^{N}\langle S_i^z\rangle=\tfrac{1}{2}(n-1)$$

for n electrons per site. Based on this spin Hamiltonian, a fairly complete discussion of the phase diagram and the low-energy excitation spectrum has been given by Robaszkiewicz *et al.*,[5] Bulaevskii *et al.*,[13] Alexandrov *et al.*,[14] and, most recently, Micnas *et al.*[15] Our work is complementary to these investigations in two respects. Firstly, our scheme extrapolates between the small-(U/W) and the large-(U/W) limits and should, therefore, extend and agree with results based on the Hamiltonian of Eq. (1). Secondly, since we retain the language of the BCS theory and calculate quasiparticle Green's functions and anomalous propagators, we shed light on some of the unconventional phenomena predicted by the effective spin Hamiltonian.

In short, our method is an adaptation of the Hubbard-alloy-analogy approximation[16] for the problem at hand. Recall that Hubbard was dealing with the positive-U Hubbard model. He found that, for $U/W\gg1$, a Hartree-Fock band split into two bands separated in energy by U. For one electron per site, the Hartree-Fock band is half-filled and the system is predicted to be a metal. In the improved alloy-analogy approximation ε_F falls in the gap between the split bands and the system is found to be a Mott-Hubbard insulator. In this state, the electrons occupying the lower Hubbard band are localized. Interestingly, the Bloch vector $\mathbf{k}$ here no longer describes different states of electronic motion but merely different spin arrangements governed by an antiferromagnetic spin Hamiltonian. As shown in Appendix A, this latter is the $U>0$ analogue of Eq. (1) and arises when doubly occupied sites are eliminated by the same canonical transformation. Significantly, the exchange interaction is again given by $J_{ij}^{\mathrm{AF}}=-4t_{ij}^2|U|^{-1}$.

Consequently, we may conclude that the alloy-analogy approximation gives an adequate account of the demanding $U/W\gg1$ limit in the $U>0$ case and, hence, may also suffice in the analogous limit of the $U<0$ sector of the model. Most of this paper can be read as a presentation of evidence that it does.

Having called attention to the connection between the $U>0$ and $U<0$ regimes,[17] we note that the technique we shall develop here is readily applicable for the $U>0$ generalized Hubbard Hamiltonians which are of interest in connection with high-temperature superconductivity.[18]

Our final introductory remark concerns the direct applicability of the above negative-U Hubbard model to the new high-temperature superconductors. Our observation here is that the high-T_c and short coherence length of these superconductors may be taken as hints that such a model is relevant to them as a semiphenomenological description. We may then adopt a strategy which bypasses the real deep issue of what is the pairing mechanism, and limits the investigation to the nature of the condensation. One the basis of some experimental evidence, we shall argue that this may be a fruitful approach to the problem. Alternatively, one may combine an interest in the negative-U Hubbard model with proposals for explicit mechanisms of the attraction. This point of view has been recently explored by Robaszkiewicz *et al.*[19] and Schüttler *et al.*[20] The technique we develop here may prove to be helpful in connection with all these considerations.

The plan of the paper is as follows. In Sec. II we introduce our method of random fields in fairly general terms. In Sec. III we apply it to the problem of superconducting pairing allowing for charge and spin as well as pairing field fluctuations. We do not implement the full theory in this paper. For illustration of its power we study the case where only the local phase of the pairing field is random and introduce the incoherent local pairing (ILP) state. In Sec. IV we study the pairing energies of the BCS and ILP states. In Sec. V we investigate the stability of the ILP state to development of phase coherence and determine the temperature at which full superconducting order sets in. In Sec. VI we attempt to assess the significance of our results.

II. THE METHOD OF RANDOM FIELDS

In the interest of clarity, we now give a brief outline of our method without some of the complications we shall encounter in the next section. We shall also mention some of its previous applications in order to establish its credibility.

The basic idea is due to Hubbard and is sometimes referred to as the alloy-analogy approximation. It has been used and generalized extensively by Cyrot,[21] Hubbard,[22] Hasegawa,[23] Pindor *et al.*,[24] Oguchi *et al.*,[25] Gyorffy *et al.*,[26] Staunton *et al.*,[27] and Economu *et al.*,[28] to mention a few cases. Here we give a slightly modified version of Hubbard's original arguments.

Consider the equation of motion for the one-particle finite-temperature Green's function.[2]

$$G_{\sigma\sigma}(i,j;\tau)=-\langle\,\mathcal{T}_\tau\{C_{i,\sigma}(\tau)C_{j,\sigma}^\dagger(0)\}\,\rangle\ , \tag{3}$$

where the imaginary time $\tau=it/\hbar$, $\langle\ \rangle$ denotes the average with respect to the equilibrium density matrix corresponding to the Hubbard Hamiltonian in Eq. (1), $\mathcal{T}_\tau$ is the usual "time"-ordering operator, and $C_{i,\sigma}(\tau)$ evolves in imaginary time τ according to the Heisenberg picture. The standard arguments yield the following equation of motion:

$$\sum_l\left[\left(-\frac{\partial}{\partial\tau}+\mu\right)\delta_{i,l}+t_{il}\right]G_{\sigma\sigma}(l,j;\tau)+U\langle\,\mathcal{T}_\tau[C_{i,-\sigma}^\dagger(\tau)C_{i,-\sigma}(\tau)C_{i,\sigma}(\tau)C_{j,\sigma}^\dagger(0)]\,\rangle=\hbar\delta_{i,j}\delta(\tau)\ . \tag{4}$$

Evidently, in this formulation of the problem, the principle task of the many-body theory is to provide a tractable scheme for finding the four-point expectation value on the left-hand side of Eq. (4) in terms of the Green's function $G_{\sigma\sigma}(i,j;\tau)$. The Hartree-Fock approximation is given by the decoupling

$$\langle \mathcal{T}_\tau[C^\dagger_{i,-\sigma}(\tau)C_{i,-\sigma}(\tau)C_{i,\sigma}(\tau)C^\dagger_{j,\sigma}(0)]\rangle = -\bar{n}_{i,-\sigma}(\tau)G_{\sigma\sigma}(ij;\tau) , \quad (5)$$

where $\bar{n}_{i,-\sigma}(\tau)$ is the average occupation number defined as

$$\bar{n}_{i,\sigma}(\tau)=\langle C^\dagger_{i,\sigma}(\tau)C_{i,\sigma}(\tau)\rangle \quad (6)$$

and is usually independent of τ. Substituting Eq. (5) into Eq. (4) leads to the Hartree-Fock, self-consistent, one-electron problem where the electron described by $G_{\sigma\sigma}(l,j;\tau)$ moves in the average electrostatic field due to the other electrons with opposite spin.

The method of random fields is a way of going beyond the Hartree-Fock approximation by taking into account some of the fluctuations in the average field seen by an electron. Explicitly, one decouples the four-point average in Eq. (4) but makes up for some of the error by allowing the occupation number $n^\nu_{i,\sigma}$ to fluctuate about its mean $\bar{n}_{i,\sigma}$. This leads to

$$\sum_l \left[\left[-\frac{\partial}{\partial\tau}+\mu-Un_{i,-\sigma}\right]\delta_{i,l}+t_{il}\right]\tilde{G}_{\sigma\sigma}(l,j;\tau) = \hbar\delta(\tau)\delta_{i,j} , \quad (7)$$

where the Green's function $\tilde{G}_{\sigma\sigma}(l,j;\tau)$ describes an electron moving in the random field which takes the value $Un_{i,\sigma}$ at the lattice point labeled by i. The prediction of the theory for the one-particle Green's function $G_{\sigma\sigma}(i,j;\tau)$ is the average of $\tilde{G}(i,j;\tau)$ over a suitably defined ensemble of configurations labeled by the sets $\{n_{i,\sigma}\}$. Namely,

$$G_{\sigma\sigma}(i,j;\tau)=\langle \tilde{G}_{\sigma,\sigma'}(i,j;\tau;\{n_{i,\sigma}\})\rangle . \quad (8)$$

At this point recipes differ.[16,22,26,28] We advocate the following simple procedure. We allow the charge densities $n_{i,\sigma}$ at each site i to take on a finite number of characteristic values $n^\nu_{i,\sigma}$ labeled by $\nu=1,2,3,\ldots$, etc. We treat the occupation numbers $n_{i,\sigma}$ as independent random variables and assign to each occurrence $n^\nu_{i,\sigma}$ the probability $P_i(\nu)$. Thus, the average in Eq. (8) is with respect to the distribution

$$P(\{\nu_i\})=\prod_i P_i(\nu_i) . \quad (9)$$

To complete the prescription we must now select the characteristic values $n^\nu_{i,\sigma}$ and determine the corresponding probabilities $P_i(\nu_i)$.

One of the principle features of our method is a self-consistency condition which determines the characteristic fluctuations: $\{n^\nu_{i,\sigma}\}$. In the interest of clarity we shall describe this condition in two steps. Firstly, we give the recipe as a sequence of "gedanken" calculations. Secondly, we propose a practical scheme for implementing them.

To begin with, consider an ensemble of sets $\{n^{\nu,\text{old}}_{i,\sigma}\}$. By solving Eq. (7) and using the weights in Eq. (9), we can calculate the partially averaged charge densities $\bar{n}^{\ \nu}_{i,\sigma}$ in terms of the Fourier coefficients $G_{\sigma\sigma}(i,j;\varepsilon_n)$ defined by

$$G_{\sigma\sigma'}(i,j;\tau)=\frac{1}{\beta}\sum_n e^{-i\varepsilon_n\tau}G_{\sigma\sigma}(i,j;\varepsilon_n) \quad (10)$$

by evaluating the formula

$$\bar{n}^{\ \nu}_{i,\sigma}=+\frac{1}{\beta}\sum_n e^{i\varepsilon_n\delta}\langle G_{\sigma\sigma}(i,i;\varepsilon_n)\rangle_{i,\nu} , \quad (11)$$

where ε_n is the usual Matsubara "frequency" $(\pi/\beta)(2n+1)$, δ is a positive infinitesimal energy, and $\langle\ \rangle_{i,\nu}$ denotes an average over the ensemble of all configurations with the charge densities $n^{\nu\ \text{old}}_{i,\sigma}$ on the ith site. In principle, $\bar{n}^{\ \nu}_{i,\sigma}$ in Eq. (11) can be calculated for all sites and for each allowed local configuration $n^{\nu,\text{old}}_{i,\sigma}$ for $\nu=1,2,\ldots$. When this is done, a new ensemble of configurations is created. Let us denote it by $\{n^{\nu,\text{new}}_{i,\sigma}\}$. Our procedure is to repeat the whole calculation using $\{n^{\nu,\text{new}}_{i,\sigma}\}$ in place of $\{\bar{n}^{\ \nu,\text{old}}_{i,\sigma}\}$ and continue to iterate until $\{\bar{n}^{\ \nu,\text{new}}_{i,\sigma}\}$ agrees with $\{n^{\nu,\text{old}}_{i,\sigma}\}$ within some prescribed limit; in other words, until we have reached a fixed point of the algorithm.

The problem of an electron moving in a random potential field has a vast literature.[29] For the particularly simple example above, where the potential function depends on a set of independent random variables, there is a well-tried method, called the coherent-potential approximation (CPA), for dealing with it.[30,31] In what follows we adopt this technique. The CPA can be shown to be a mean-field theory of disorder[32] and, hence, our theory will treat the fluctuations about the Hartree-Fock potential in the spirit of a mean-field theory.

Of course, the above procedure is to be carried out for a fixed set of probabilities $P_i(\nu)$. Specifying instructions for choosing these is the final step in defining the method. There are two different approaches which have been used successfully. The first is that adopted by Hubbard in his classic paper[16] where he introduced the method of random fields. It consists of choosing a set of intrinsic probabilities on the basis of physical intuition. The second approach views the probabilities $P_i(\nu)$ as parameters to be determined by requiring that some quantity, like the ensemble-averaged free energy, is a minimum.[22,23,26] In this paper we shall make use of both schemes. In the interest of efficient presentation we shall not describe them here any further but give such details as will be necessary later on when our particular applications have been more fully explained.

Let us now be more specific and consider, explicitly, the example of four possible fluctuations: $n^{\nu=+}_{i,\sigma}, n^{\nu=-}_{i,\sigma}, n^{\nu=\uparrow}_{i,\sigma}, n^{\nu=\downarrow}_{i,\sigma}$ on each site. For simplicity, we take the + and − sites as pure charge fluctuations about the mean occupation number $\bar{n}_i$. Namely,

$$n^+_{i\uparrow}=n^+_{i\downarrow}=\tfrac{1}{2}(\bar{n}_i+\delta n) , \quad n^-_{i\uparrow}=n^-_{i\downarrow}=\tfrac{1}{2}(\bar{n}_i-\delta n) . \quad (12)$$

Moreover, the $\uparrow$ and $\downarrow$ states are taken to be pure spin fluctuations. This implies that

$$n_{i\uparrow}^{\uparrow}+n_{i\downarrow}^{\uparrow}=\bar{n}_i\ ,\quad n_{i\uparrow}^{\downarrow}+n_{i\downarrow}^{\downarrow}=\bar{n}_i\ , \tag{13a}$$

$$n_{i\uparrow}^{\uparrow}-n_{i\downarrow}^{\uparrow}=\bar{\mu}_i\ ,\quad n_{i\uparrow}^{\downarrow}-n_{i\downarrow}^{\downarrow}=\bar{\mu}_i\ , \tag{13b}$$

where $\bar{\mu}_i$ is the magnetic moment on the site i and, to preserve conceptual simplicity, up ($\uparrow$) and down ($\downarrow$) refers to the same axis of spin quantization on each site. However, we note that it is frequently useful to allow the orientation of the local axis of spin quantization to vary from site to site.[22,23,26]

We shall now briefly summarize the theory for these simple fluctuations. The central feature of the CPA is the Green's function $G_{\sigma\sigma}^{c}(i,j;\varepsilon_n)$ which describes the motion of an electron at the Matsubara frequency ε_n, on a nonrandom, effective lattice. This Green's function satisfies the following equation of motion:

$$\sum_l\{[i\varepsilon_n+\mu-\Sigma_{i,\sigma}(\varepsilon_n)]\delta_{i,l}+t_{il}\}G_{\sigma\sigma}^{c}(l,j;\varepsilon_n)=\delta_{i,j}\ , \tag{14}$$

where $\Sigma_{i,\sigma}(\varepsilon_n)$ is the energy-dependent complex coherent potential at site i. Consider now an impurity in this lattice at point i, described by the potential

$$V_{i,\sigma}^{\nu}=Un_{i,-\sigma}^{\nu}\ . \tag{15}$$

It is easy to show that the impurity Green's function is given by

$$G_{\sigma\sigma}^{\nu}(i,i;\varepsilon_n)=[1-\tilde{V}_{i,\sigma}^{\nu}(\varepsilon_n)G_{\sigma\sigma}^{c}(i,i;\varepsilon_n)]^{-1}G_{\sigma\sigma}^{c}(i,i;\varepsilon_n)\ , \tag{16}$$

where

$$\tilde{V}_{i,\sigma}^{\nu}=V_{i,\sigma}^{\nu}-\Sigma_{i,\sigma}(\varepsilon_n)\ .$$

The well-known CPA condition which determines the coherent potential $\Sigma_{i,\sigma}(\varepsilon)$ may now be written as

$$\sum_{\nu}P_i(\nu)G_{\sigma\sigma}^{\nu}(i,i;\varepsilon_n)=G_{\sigma\sigma}^{c}(i,i;\varepsilon_n)\ . \tag{17}$$

Note that the above relation describes an infinite set of coupled equations: one for each site. As will be seen later, this inhomogeneous CPA is a useful formal device.[26–28] However, it can be solved explicitly only in the homogeneous limit where all sites are the same, e.g., $\Sigma_{i,\sigma}(\varepsilon_n)=\Sigma_{\sigma}(\varepsilon_n)$ for all i. In this case Eq. (17) can be readily solved, for $\Sigma_{\sigma}(\varepsilon)$, by numerical iteration.

Recently, the spin-only sector of the above theory played an important role in the theory of metallic magnetism.[22,23,26] Deployed in the context of a positive-U Hubbard model, it facilitated the description of the paramagnetic state. In contrast to the Stoner theory, where, after the demise of long-range magnetic order at the Curie temperature T_c, there is only Pauli paramagnetism, the inclusion of spin fluctuations led to a disordered local moment (DLM) state[22,23,26] with the Curie-Weiss susceptibility. The high-temperature incoherent local pairing state, which we shall discover in the context of the negative-U Hubbard model, will be shown to be the superconducting analogue of this DLM state.

From the formal point of view it may be helpful to note that, in the above applications, many authors[21–23] arrived at the method advocated here via a functional integral representation of the partition function. In these approaches the CPA comes in as a technique for evaluating the functional integrals approximately. Although it is a single-site static method, it goes beyond the random-phase approximation (RPA) which includes only quadratic fluctuations about the Hartree-Fock saddle points. Evidently, the theory we shall describe in this paper can also be arrived at by casting the problem into the form of functional integrals over classical isospin fields representing traces over the Nambu space,[33] and approximating them using the CPA. Although some useful insights into the limitations of our approach may be obtained in this way, here we shall not pursue this line of inquiry any further.

Hubbard's classic paper, where he first introduced the alloy-analogy approximation, dealt with a positive-U model and developed the charge-fluctuations-only version of the above theory. As mentioned in the Introduction, he found that, for large enough U, the Hartree-Fock band, given by $\varepsilon_k^{\mathrm{HF}}=\varepsilon_k^0+\frac{1}{2}U\bar{n}$, where ε_k^0 is the lattice Fourier transform of the hopping integral t_{ij}, split into two Hubbard bands: ε_k^0 and ε_k^0+U. Evidently, for a bandwidth $W<U$, there is a gap between the lower and upper bands, as shown schematically in Fig. 1. Since, for one electron per site, the lower band is filled, we have a Mott insulator. The lower band corresponds to states in which sites are singly occupied, and when it is filled, the electrons are localized by correlation. In the large-U limit it is well known on the basis of, more or less, exact theory that the ground state is an antiferromagnetic insulating one. To recover this we must open up the spin sector of the theory. There is a strong circumstantial evidence that the full scheme would give a qualitatively correct account of localized electrons interacting via antiferromagnetic spin interactions both below and above the Néel temperature T_N in the $U\gg W$ limit.[21]

Although current theories of high-temperature super-

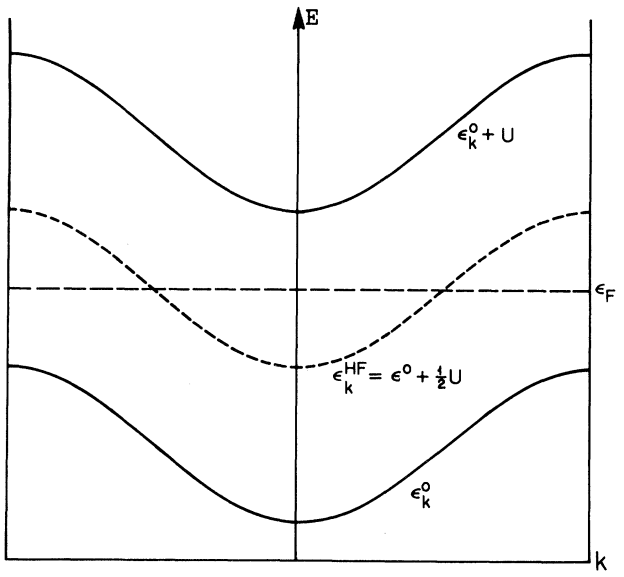

FIG. 1. The Hartree-Fock and the split Hubbard bands for a one-band Hubbard model.

conductivity focus a great deal of attention on the above circumstance, from the point of view of our present concern the more interesting case is that of charge fluctuations in the negative-U Hubbard model. In this sector of the theory, for $|U|$ large enough compared with the bandwidth W, we get the same two Hubbard bands as in the positive-U case but now it is the band corresponding to the double occupancy of sites that is lower in energy. This implies that singly occupied sites may be eliminated from the theory by the canonical transformation mentioned in the Introduction. The result is the effective spin Hamiltonian given in Eq. (2). Note that, for one electron per site, the above picture implies pairs on every other site and hence the state may be metallic. However, in contrast to the Hartree-Fock theory, the current carrying excitations correspond to a charge of $2e$.

When applying the theory at hand to this situation, one must search for the probability factors $P(+)$, $P(-)$, $P(\uparrow)$, $P(\downarrow)$ such that the free energy is minimized. This may lead to a variety of charge-ordering processes, as was found by Robaszkiewicz *et al.*,[5,15] on the basis of the effective spin Hamiltonian given in Eq. (2). Competing with these are transitions into a superconducting state. The central purpose of this paper is to study the latter using a straightforward generalization of the method of random fields described in this section.

Before pursuing the above task, we wish to pause to make a final general comment on the method. Note that the four possible states specified at each site in our method are closely analogous to the four Hubbard states: no electron $|0\rangle$, one spin up electron $|\uparrow\rangle$, one spin down electron $|\downarrow\rangle$, and a singlet pair $|\uparrow\downarrow\rangle$ which span the Hilbert space of a single-orbital Hubbard model on one site. Evidently, $|0\rangle$ and $|\uparrow\downarrow\rangle$ describe spinless charge fluctuations and $|\uparrow\rangle, |\downarrow\rangle$ correspond to spin fluctuations. In an exact theory, the fluctuations between the states $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ are described by the Hubbard operators X_i^{pq}.[33] In our theory only a classical and time-independent representation of these fluctuations survives. Nevertheless, the method can be seen as an attempt to capture, albeit approximately, the essential physics described by the Hubbard operators.[34]

III. THE GOR'KOV EQUATIONS AND THE METHOD OF RANDOM FIELDS

A. The Gor'kov equation

We shall work with the Nambu-style matrix Green's function[2] defined by

$$\underline{G}(i,j;\tau)=-\begin{bmatrix}\langle \mathcal{T}_\tau\{C_{i\uparrow}(\tau)C_{j\uparrow}^\dagger(0)\}\rangle & \langle \mathcal{T}_\tau\{C_{i\uparrow}(\tau)C_{j\downarrow}(0)\}\rangle \\ \langle \mathcal{T}_\tau\{C_{i\downarrow}^\dagger(\tau)C_{j\uparrow}^\dagger(0)\}\rangle & \langle \mathcal{T}_\tau\{C_{i\downarrow}^\dagger(\tau)C_{j\downarrow}(0)\}\rangle\end{bmatrix}. \tag{18}$$

The off-diagonal elements are the usual anomalous propagators of the BCS-Gor'kov theory. They are zero in the normal state and become finite in the superconducting state. Following the arguments which lead to Eq. (4), it can be readily shown that $G(i,j;\tau)$ satisfies the exact equation of motion

$$\sum_l \begin{bmatrix}\left[-\frac{\partial}{\partial\tau}+\mu\right]\delta_{i,l}+t_{i,l} & 0 \\ 0 & \left[-\frac{\partial}{\partial\tau}-\mu\right]\delta_{i,l}-t_{il}\end{bmatrix}\begin{bmatrix}G_{11}(l,j;\tau) & G_{12}(l,j;\tau) \\ G_{21}(l,j;\tau) & G_{22}(l,j;\tau)\end{bmatrix}$$
$$+U\begin{bmatrix}\langle \mathcal{T}_\tau\{C_{i\downarrow}^\dagger(\tau)C_{i\downarrow}(\tau)C_{i\uparrow}(\tau)C_{j\uparrow}^\dagger(0)\}\rangle & \langle \mathcal{T}_\tau\{C_{i\downarrow}^\dagger(\tau)C_{i\downarrow}(\tau)C_{i\uparrow}(\tau)C_{j\downarrow}(0)\}\rangle \\ \langle \mathcal{T}_\tau\{C_{i\uparrow}^\dagger(\tau)C_{i\uparrow}(\tau)C_{i\downarrow}^\dagger(\tau)C_{j\uparrow}^\dagger(0)\}\rangle & \langle \mathcal{T}_\tau\{C_{i\uparrow}^\dagger(\tau)C_{i\uparrow}(\tau)C_{i\downarrow}^\dagger(\tau)C_{j\downarrow}(0)\}\rangle\end{bmatrix}=\delta(\tau)\delta_{i,j}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}. \tag{19}$$

Since we now expect, in the Hartree-Fock approximation to Eq. (19), such anomalous averages as $\langle C_{i\downarrow}^\dagger C_{i\uparrow}^\dagger\rangle$ and $\langle C_{i\uparrow}C_{i\downarrow}\rangle$ to be nonzero, we must decouple the four-point functions keeping all possible two-point averages. On doing this, we find the usual Gor'kov equation,

$$\sum_l \begin{bmatrix}\left[-\frac{\partial}{\partial\tau}+\mu-U\bar{n}_{i\downarrow}\right]\delta_{i,l}+t_{il} & \bar{\Delta}_i\delta_{i,l} \\ \bar{\Delta}_i^*\delta_{i,l} & \left[-\frac{\partial}{\partial\tau}-\mu+U\bar{n}_{i\uparrow}\right]\delta_{i,l}-t_{il}\end{bmatrix}\underline{G}(l,j;\tau)=\delta(\tau)\delta_{i,j}\underline{1}\,, \tag{20}$$

where

$$\bar{\Delta}_i^* \equiv U\langle C_{i\downarrow}^\dagger C_{i\uparrow}^\dagger \rangle = -UG_{21}(i,i;0^+) \tag{21}$$

and the average occupation numbers $\bar{n}_{i\uparrow}$ and $\bar{n}_{i\downarrow}$ are given by Eq. (11). As is conventional, 0^+ denotes a small, positive infinitesimal.

As stressed earlier, our aim is to go beyond the simple approximation above. But, before doing that in the next section, we shall complete our present discussion by solving Eq. (20). This will allow us to clarify some points which will arise later.

In the homogeneous case where $\bar{\Delta}_i = \bar{\Delta}$, $\bar{\Delta}_i^* = \bar{\Delta}^*$ for all i we can take the space and τ Fourier transform of Eq. (20). Introducing $\underline{G}(\mathbf{k};\varepsilon_n)$ by the relation

$$\underline{G}(i,j;\tau) = \frac{1}{\beta}\sum_{n,\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)-i\varepsilon_n\tau}\underline{G}(\mathbf{k};\varepsilon_n) , \tag{22}$$

we find

$$\begin{bmatrix} i\varepsilon_n - \varepsilon_{\mathbf{k}}^0 - U\bar{n}_\downarrow + \mu & \Delta \\ \Delta^* & i\varepsilon_n + \varepsilon_{\mathbf{k}}^0 + U\bar{n}_\uparrow - \mu \end{bmatrix} \underline{G}(\mathbf{k};\varepsilon_n) = \underline{1} . \tag{23}$$

Solving this equation and using Eq. (21) leads to

$$\Delta = -\frac{U}{\beta}\sum_{n,\mathbf{k}} \frac{\Delta}{(i\varepsilon_n - E_{\mathbf{k}})(i\varepsilon_n + E_{\mathbf{k}})} , \tag{24}$$

where

$$E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}}^0 + Un_\uparrow - \mu)^2 + |\Delta|^2} . \tag{25}$$

Carrying out the sum over the Matsubata frequencies by contour integration and replacing the sum over the Brillouin zone by an integration over the density of states

$$n(\varepsilon) = \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}^0 - Un_\downarrow + \mu) , \tag{26}$$

we find the gap equation

$$1 = -U\int_{-\infty}^{\infty} d\varepsilon\, n(\varepsilon) \frac{1}{2\sqrt{\varepsilon^2+|\Delta|^2}} \tanh\tfrac{1}{2}\beta\sqrt{\varepsilon^2+\Delta^2}) . \tag{27}$$

This is the BCS result for our model.

For simplicity, here and later, we will work with a square density of states of bandwidth W. Evidently, W should be though of as $2zt$, where z is the number of nearest neighbors, even though W does not arise from a nearest-neighbor hopping model. By this we do not mean to focus on two-dimensional systems, but use this form only to simplify the algebra and to approximate the rise and fall of a generic d-band density of states.[35]

For this model density of states, the gap equation becomes

$$1 = -U\int_{-W/2}^{W/2} \frac{d\varepsilon}{2W} \frac{1}{\sqrt{(\varepsilon-\mu)^2+|\Delta|^2}} \times \tanh[\tfrac{1}{2}\beta\sqrt{(\varepsilon-\mu)^2+|\Delta|^2}] \tag{28}$$

and the chemical potential μ is determined by

$$n = \frac{2}{\beta}\sum_{n,\mathbf{k}} e^{i\varepsilon_n\delta} G_{11}(\mathbf{k};\varepsilon_n) = \int_{-W/2}^{W/2} \left[1 - \frac{\varepsilon-\mu}{\sqrt{(\varepsilon-\mu)^2+|\Delta|^2}} \times \tanh[\tfrac{1}{2}\beta\sqrt{(\varepsilon-\mu)^2+|\Delta|^2}]\right] \frac{d\varepsilon}{W} . \tag{29}$$

To highlight an important difference between this and the usual BCS result, we note that, for $T=0$, Eqs. (28) and (29) can be solved analytically. After some straightforward algebra we find

$$\Delta = \frac{W}{2}\sqrt{n(2-n)}\left[\left[\frac{e^{-2W/U}+1}{e^{-2W/U}-1}\right]-1\right]^{1/2} . \tag{30}$$

For a half-filled band, this relation is plotted in Fig. 2. Evidently, for $|U|/W \ll 1$ and $n=1$, we have the BCS-like result that $\Delta = We^{-W/|U|}$. For $|U|/W \gg 1$, $\Delta = \frac{1}{2}|U|$. The former case is characteristic of pairing with the assistance of the Pauli exclusion principle, namely, of Cooper pairs. However, in the opposite limit, we may recognize $\frac{1}{2}U$ as the binding energy per particle in a "molecule" which would form even in free space without the Fermi sea of other electrons. The smooth transition between these two limits was the subject of Leggett's investigation.[1] The point at stake in this paper is that, for $T>0$, the transition is not smooth. As in the BCS theory, Eqs. (28) and (29) yield $k_B T_c \cong \Delta(0)$. In fact, for $|U|/W \gg 1$ and $n=1$, we have $k_B T_c \cong \frac{1}{2}\Delta(0) = \frac{1}{4}U$. On the other hand, the arguments of Rubaszkiewicz *et al.*[5] and Nozières and Schmitt-Rink[6] convincingly lead to the conclusion that, for $|U|/W \gg 1$, $k_B T_c$ decreases with increasing $|U|$ ($k_B T_c \cong W^2/|U|$). Thus, for some value of $|U|/W$, the BCS mean-field theory, as encapsulated by Eqs. (28) and (29), must break down. Our principal concern here is where and how this happens.

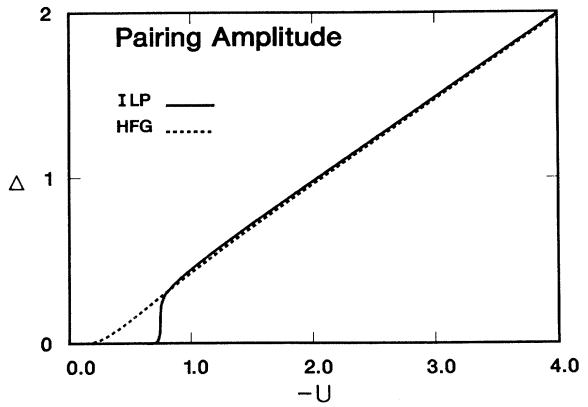

FIG. 2. The zero-temperature gap as a function of the interaction constant U: as given by the Hartree-Fock-Gor'kov theory (dashed line) and ILP state (solid line) for a band filling $n=1$. In this and subsequent figures all energies are in units of the bandwith W.

B. Beyond the Gor'kov decoupling

It is now a straightforward matter to apply the method of random fields, as developed in Sec. II, to improve upon the Gor'kov approximation given in Eq. (20). Evidently, we must consider the generalization of Eq. (7) for the case of the matrix Green's function $\underline{\tilde{G}}(i,j;\varepsilon_n)$. Namely, by removing the average sign $-$ from $\overline{n}_{i,\sigma}$ and $\overline{\Delta}_i$ and transforming it into the Matsundera-frequency space, we may rewrite Eq. (20) as

$$\sum_l \begin{bmatrix} i\varepsilon_n+\mu-Un_{i\downarrow})\delta_{i,l}+t_{il} & \Delta_i\delta_{i,l} \\ \Delta_i^*\delta_{i,l} & (i\varepsilon_n-\mu+Un_{i\uparrow})\delta_{i,l}-t_{il} \end{bmatrix} \underline{\hat{G}}(l,j;\varepsilon_n)=\underline{1}\delta_{i,j} , \tag{31}$$

where $n_{i\sigma}$ and Δ_i are now independent random variables. As we explained earlier, our approximation for the Green's function is the average

$$\underline{G}(i,j;\varepsilon_n)=\langle \underline{\hat{G}}(i,j;\varepsilon_n)\rangle \tag{32}$$

with respect to some suitably chosen ensemble.

At this stage of theory, it makes no sense to consider more general fluctuations in $n_{i,\sigma}$ then the four states $n_{i,\sigma}^{\uparrow}$, $n_{i,\sigma}^{\downarrow}$, $n_{i,\sigma}^{+}$, $n_{i,\sigma}^{-}$ depicted in Eqs. (12) and (13), together with fluctuations in the pair field. The qualitatively different feature of the theory is the fluctuating pairing potential Δ_i. It is a complex number which we take to be of the form

$$\Delta_i=|\Delta_i|e^{i\theta} . \tag{33}$$

For simplicity, we assume that only the θ phase fluctuates. Thus, the ensemble with respect to which the average in Eq. (32) is to be taken is described by the distribution

$$P(\{\nu_i,\theta_i\})=\prod_i P_i(\nu_i,\theta_i) . \tag{34}$$

Following the arguments in Sec. II, we carry out the averaging using the CPA. The coherent potential matrix Green's function is defined by

$$\sum_l \begin{bmatrix} [i\varepsilon_n+\mu-\Sigma_{11}^i(\varepsilon_n)]\delta_{i,l}+t_{il} & -\Sigma_{12}^i(\varepsilon_n)\delta_{i,l} \\ -\Sigma_{21}^i(\varepsilon_n)\delta_{i,l} & [i\varepsilon_n-\mu-\Sigma_{22}^i(\varepsilon_n)]\delta_{i,l}-t_{il} \end{bmatrix} \underline{G}^c(l,j;\varepsilon_n)=\underline{1}\delta_{i,j} . \tag{35}$$

To determine the coherent potential

$$\underline{\Sigma}^i(\varepsilon_n)=\begin{bmatrix} \Sigma_{11}^i(\varepsilon_n) & \Sigma_{12}^i(\varepsilon_n) \\ \Sigma_{21}^i(\varepsilon_n) & \Sigma_{22}^i(\varepsilon_n) \end{bmatrix} , \tag{36}$$

we replace it by the "impurity" potential

$$\underline{V}_i^{\nu}(\theta)=\begin{bmatrix} Un_{i\uparrow}^{\nu} & |\Delta_i|e^{i\theta} \\ -|\Delta_i|e^{-i\theta} & Un_{i\downarrow}^{\nu} \end{bmatrix} , \tag{37}$$

find the corresponding impurity Green's function

$$\underline{G}^{\nu_i,\theta_i}(i,i;\varepsilon_n)=\left[\underline{1}-\left[\underline{V}_i^{\nu_i}(\theta_i)-\underline{\Sigma}^i(\varepsilon_n)\right]\underline{G}^c(i,i;\varepsilon_n)\right]^{-1}\underline{G}^c(i,i;\varepsilon_n) , \tag{38}$$

and require that the CPA condition

$$\sum_{\nu_i}\int_{-\pi}^{\pi} d\theta_i P_i(\nu_i;\theta_i)\underline{G}^{\nu_i\theta_i}(i,i;\varepsilon_n)=\underline{G}^c(i,i;\varepsilon_n) \tag{39}$$

is fulfilled. Evidently, Eq. (39) is the fundamental equation of our inhomogeneous CPA.

We shall use the above theory as the basis for some formal manipulation. However, we can contemplate actually solving Eq. (39) only in the homogeneous limit. In that case, $P_i(\nu_i,\theta)=P(\nu_i,\theta)$ and therefore $\underline{\Sigma}^i(\varepsilon_n)=\underline{\Sigma}(\varepsilon_n)$. Consequently,

$$\underline{G}^c(i,i;\varepsilon)=\int_{\mathrm{BZ}}\frac{dk^3}{(2\pi)^3}\underline{G}^c(\mathbf{k};\varepsilon_n) , \tag{40}$$

where $\underline{G}^c(\mathbf{k};\varepsilon_n)$ satisfies the equation

$$\begin{bmatrix} i\varepsilon_n-(\varepsilon_k^0-\mu)-\Sigma_{11}(\varepsilon_n) & -\Sigma_{12}(\varepsilon_n) \\ -\Sigma_{21}^*(\varepsilon_n) & i\varepsilon_n+(\varepsilon_k^0-\mu)-\Sigma_{22}(\varepsilon_n) \end{bmatrix} \underline{G}^c[\mathbf{k},(\varepsilon_n)]=\underline{1} \tag{41}$$

and the CPA condition reads

$$\sum_{\nu}\int d\theta\, P(\nu,\theta)\underline{G}^{\nu,\theta}(i,i;\varepsilon_n)=\underline{G}^{c}(i,i;\varepsilon_n)\ . \tag{42}$$

The formula for the impurity Green's function $\underline{G}^{\nu,\theta}(i,i;\varepsilon)$ is that given in Eq. (38) with $\underline{V}^{\nu}(\theta)$ and $\underline{\Sigma}$ replacing $\underline{V}_i^{\nu}(\theta_i)$ and Σ^i. In short, in a homogeneous state, Eqs. (40)–(42) and (38) are a complete statement of the theory for the one-particle Green's function.

C. The incoherent local pair state

In order to illustrate how the above theory works, we shall now consider the simple example where the phase of the pairing potential θ_i is the only fluctuating quantity. Namely, we set the occupation variables equal to their average value which is taken to be the same on all sites. We also take the magnitude of Δ_i to be $\overline{\Delta}$ for all i. Thus, we study the limit where

$$n_{i,\sigma}=\overline{n}_{\sigma}\ ,\quad \Delta_i=\overline{\Delta}e^{i\theta_i}\ , \tag{43}$$

$$P_i(\theta_i)=\frac{1}{2\pi}\ . \tag{44}$$

Clearly, the theory in Sec. III B, together with Eqs. (43) and (44), completely defines the mathematical problem that we are to solve.

Before moving on to do that, however, we wish to comment on the physical nature of this incoherent local pair state that we are about to decribe. Recall that the phase of the complex order parameter $\psi=|\psi|e^{i\theta}$ in the Ginzburg-Landau theory is the conjugate variable to the number of Cooper pairs in the system.[34] Thus, loosely speaking, we may interpret the local phase of the order parameter $\langle C_{i\uparrow}C_{i\downarrow}\rangle=U^{-1}\overline{\Delta}e^{i\theta_i}$ as the conjugate variable to the local occupation number N_i which denotes the number of pairs (bosons) at the site i. In an exact theory there is a pair occupation number operator $\hat{N}_i$ whose eigenvalues are 0 and 1 due to the exclusion principle operating between the fermions which make up the pairs. We would like to stress that $\hat{N}_i$ above is not that operator but some suitably coarse-grained version of it corresponding to the coarse-gained phase θ_i. Nevertheless, on some time scale, long compared to the hopping time $\hbar/W$ for the individual electrons but one which is not infinite, we may make the following argument: when the phases $\{\theta_i\}$ are well defined and are the same, $P(\theta_i)=\delta(\theta_i-\bar{\theta})$, the occupation numbers $\{N_i\}$ are ill defined, i.e., they fluctuate wildly, and we cannot tell how many pairs are at the site i. We say that, in this state, the local order parameters are coherent and the bosons are overlapping. Thus, we interpret this situation as corresponding to the presence of a Bose-Einstein condensate of pairs. Unless the pairs are localized, this state is superconducting. On the other hand, when the phases $\{\theta_i\}$ are random, i.e., $P(\theta_i)=1/2\pi$, the occupation numbers are well defined and, for a given residence time, we can tell how many bosons are at a site. In this state, the local phases are incoherent and it is reasonable to construe that we are describing an ensemble of bosons in their normal state. This state is not superconducting but differs from the standard normal state of the electrons in that a significant fraction of the electrons are bound in pairs.

Clearly, the above ILP state may be associated with the state expected for $T_c<T<T_p$ according to the arguments in the Introduction. In short, for $T<T_c$, there is a coherent order parameter all through the lattice and we may regard the state as a Bose-Einstein condensate of pairs. Above T_c the order parameter is incoherent from site to site. This describes pairs in their normal state. Above T_p, the pairs are broken up by thermal fluctuations.

The calculation we are about to describe refers to the case of random phases. The question whether there will be pairs in the normal state or no pairs at all will be decided by the calculation. In other words, our self-consistent scheme will converge either to a solution for which $\overline{\Delta}=0$ or to one with $\overline{\Delta}\neq 0$. Obviously, in the latter case we have normal pairs.

Because the occupation numbers $n_{i,\sigma}$ take their Hartree-Fock values $\overline{n}_{i,\sigma}$, it is best to define the Green's function $\underline{G}^{c}(\mathbf{k};\varepsilon_n)$ in Eq. (40) by

$$\begin{bmatrix} i\varepsilon_n-(\varepsilon_{\mathbf{k}}^{\mathrm{HF}}-\mu)-\Sigma_{11}(\varepsilon_n) & -\Sigma_{12}(\varepsilon_n) \\ -\Sigma_{21}(\varepsilon_n) & i\varepsilon_n+(\varepsilon_k^{\mathrm{HF}}-\mu)-\Sigma_{22}(\varepsilon_n)\end{bmatrix}\underline{G}^{c}(\mathbf{k};\varepsilon_n)=\underline{1}\ . \tag{45}$$

Then, for the distribution $P(\theta)$ in Eq. (44), the CPA equations, which determine the self-energy matrix $\underline{\Sigma}(i,i;\varepsilon_n)$, take the following form:

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta\,\underline{G}^{\theta}(i,i;\varepsilon_n)=\underline{G}^{c}(i,i;\varepsilon_n)\ . \tag{46}$$

Moreover, the "impurity" Green's function is given by

$$G^{\theta}(i,i;\theta)=\underline{D}^{\theta}(i,i;\varepsilon_n)\underline{G}^{c}(i,i;\varepsilon_n)\ , \tag{47}$$

where

$$G^{c}(i,i;\varepsilon_n)=\sum_{\mathbf{k}}^{\mathrm{BZ}}\underline{G}^{c}(\mathbf{k};\varepsilon_n)\ , \tag{48}$$

$$\underline{D}^{(\theta)}(i,i;\varepsilon_n)=\{\underline{1}-[\underline{V}-\underline{\Sigma}(\varepsilon_n)]\underline{G}^{c}(i,i;\varepsilon_n)\}^{-1}\ , \tag{49}$$

and

$$\underline{V}=\begin{bmatrix}0 & -\overline{\Delta}e^{i\theta}\\ -\overline{\Delta}e^{i\theta} & 0\end{bmatrix}\ . \tag{50}$$

Finally, using Eq. (47), we may rewrite Eq. (46) as

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta\,\underline{D}^{(\theta)}(i,i;\theta)=\underline{1}\ . \tag{51}$$

To solve the above equation we note that a general 2×2 matrix in the Nambu isospin space, like the Green's function $\underline{G}^{c}$ or the self energy $\underline{\Sigma}$ will be of the form

$$\underline{G}^{c}=G_0^{c}\underline{1}+G_1^{c}\underline{\tau}^1+G_2^{c}\underline{\tau}^2+G_3^{c}\underline{\tau}^3\ , \tag{52}$$

where $\underline{1}$, $\underline{\tau}^1$, $\underline{\tau}^2$, and $\underline{\tau}^3$ are the usual complete set of 2×2 Pauli matrices

$$\begin{bmatrix}1&0\\0&1\end{bmatrix},\quad\begin{bmatrix}1&0\\0&1\end{bmatrix},\quad\begin{bmatrix}0&-i\\i&0\end{bmatrix},\quad\begin{bmatrix}1&0\\0&-1\end{bmatrix},$$

respectively. Clearly,

$$\underline{V}(\theta)=\overline{\Delta}\underline{\tau}^1\cos\theta-\overline{\Delta}\underline{\tau}^2\sin\theta \tag{53}$$

and, hence, varying θ implies a rotation in the 1-2 subspace. Consequently, in a state which is locally gauge invariant, such as the one described by $P_i(\theta)=1/2\pi$, the 1-2 components G_1^c, G_2^c, and Σ_1^c and Σ_2^c must vanish. Thus, we can assume at the outset that

$$\underline{G}^c(i,i;\varepsilon_n)=\begin{bmatrix}G_{11}^c(i,i;\varepsilon_n)&0\\0&G_{22}^c(i,i;\varepsilon_n)\end{bmatrix}. \tag{54}$$

The, Eqs. (45) and (48) imply that

$$\Sigma^c(\varepsilon_n)=\begin{bmatrix}\Sigma_{11}(\varepsilon_n)&0\\0&\Sigma_{22}(\varepsilon_n)\end{bmatrix}. \tag{55}$$

Using Eq. (49), this leads to

$$\underline{D}^{(\theta)}(i,i;\varepsilon)=[(1+\Sigma_{11}^cG_{11}^cG_{11}^c)(1+\Sigma_{22}^cG_{22}^c)-\overline{\Delta}^2G_{11}^cG_{22}^c]^{-1}\begin{bmatrix}1+\Sigma_{22}^cG_{22}^c&\overline{\Delta}e^{i\theta}G_{22}^c\\\overline{\Delta}e^{i\theta}G_{11}^c&1+\Sigma_{11}G_{11}^c\end{bmatrix} \tag{56}$$

and our fundamental equation, Eq. (51), becomes

$$(1+\Sigma_{11}^cG_{11}^c)(1+\Sigma_{22}^cG_{22}^c)-\overline{\Delta}^2G_{11}^cG_{22}^c)^{-1}\begin{bmatrix}1+\Sigma_{22}^cG_{22}^c&0\\0&1+\Sigma_{11}^cG_{11}^c\end{bmatrix}=\begin{bmatrix}1&0\\0&1\end{bmatrix}. \tag{57}$$

We have solved these equations at a number of complex energies z following a very efficient iterative procedure described in Appendix B. Instead of using some characteristic band structure for $\varepsilon_k^{\rm HF}$, we made use of the square density of states employed in Sec. III C. Namely, for a self-energy matrix $\Sigma(z)$, we calculated the corresponding Green's function by evaluating, numerically, the following integral:

$$\underline{G}^c(i,i;z)=\int_{-W/2-\mu}^{W/2-\mu}\frac{d\varepsilon}{W}\begin{bmatrix}\dfrac{1}{z-\varepsilon-\Sigma_{11}(z)}&0\\0&\dfrac{1}{z-\varepsilon-\Sigma_{22}(z)}\end{bmatrix}. \tag{58}$$

Once $\Sigma(z)$ and, hence, $\underline{G}^c(i,i;z)$ have been determined on a large number of z points, a further self-consistency cycle begins, to determine the magnitude of the pairing potential $\overline{\Delta}$. For an assumed value of $\overline{\Delta}$ we find the impurity Green's function $\underline{G}^\theta(i,i;\varepsilon_n)$ and calculate the corresponding local pairing potential by evaluating the Matsubara sum

$$\Delta(\theta)=-\frac{U}{\beta}\sum_n e^{i\varepsilon_n\delta}G_{12}^\theta(i,i;\varepsilon_n)\,. \tag{59}$$

Since it follows from Eq. (56) that D_{12}^θ, and $\Delta(\theta)$ are proportional to $\overline{\Delta}e^{i\theta}$, we can cancel $\overline{\Delta}e^{i\theta}$ on both sides of Eq. (59) and find

$$1=-\frac{U}{\beta}\sum_n e^{i\varepsilon_n\delta}\{[1+\Sigma_{11}(\varepsilon_n)G_{11}^c(i,i;\varepsilon_n)][1+\Sigma_{22}(\varepsilon_n)G_{22}^c(i,i;\varepsilon_n)]-\overline{\Delta}^2G_{11}^c(i,i;\varepsilon_n)G_{22}^c(i,i;\varepsilon_n)\}^{-1}[G_{22}^c(i,i;\varepsilon_n)]^2\,. \tag{60}$$

Thus, on evaluating the right-hand side of this equation for a starting value of $\overline{\Delta}$, it is compared to 1. If it is not 1, within a prescribed accuracy $\overline{\Delta}$ is modified and the whole process, including solving Eq. (51), is repeated until convergence is achieved.

Method of solution apart, Eq. (60) may be recognized as the local gap equation in the present approximation. Recall, however, that because the phase is random, the state described is not superconducting even if Eq. (60) has a solution for which $\overline{\Delta}\neq0$.

Our solution for $\overline{\Delta}$ as a function of U is plotted in Fig. 2. In this and subsequent figures we express our results in units of the bandwidth W. Clearly for values of U having a magnitude greater than some critical value U_c, where $U_c\sim0.8W$, the ILP state with a finite "gap" $\overline{\Delta}$ is a solution. Below U_c, the above algorithm converges to $\overline{\Delta}=0$. This curve is the principal result of this section.

It should be noted that, for $|U/W|\gg1$, $\overline{\Delta}\cong\frac{1}{2}U$ as on the BCS solution. Note, however, that the ILP state described above is not superconducting. Although it can be shown that $T_p\sim U$ is a characteristic temperature of the problem, it is not T_c where the superconducting state yields to the normal state. In fact, it is the temperature where thermal fluctuations break up pairs. Thus, in the ILP state, which is stable for $T_c<T<T_p$, we have a normal liquid of charged bosons, i.e., electron pairs. The existence of this remarkable state is the most striking geature of the strong pairing alternative to the usual BCS scenario.

To investigate the ILP state further, we have calculated the quasiparticle density of states

$$N(\varepsilon)=-\pi^{-1}\,\mathrm{Im}\langle\hat{G}_{11}(i,i;-i\varepsilon+0^+)\rangle\,.$$

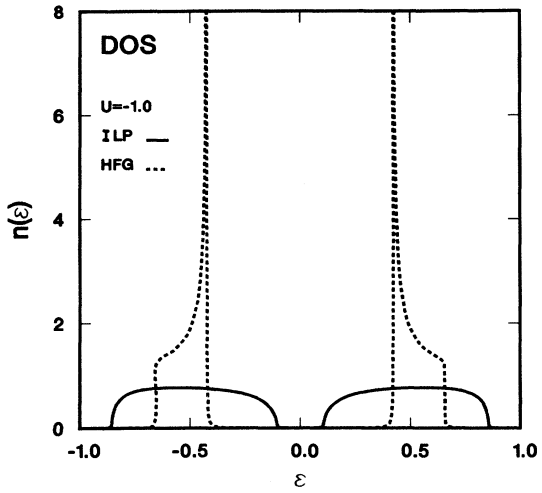

FIG. 3. The quasiparticle density of states as predicted by the Hartree-Fock-Gor'kov (dashed line) and ILP (solid line) approximations for $n=1$.

For $U=-1.0W$ this is shown in Fig. 3 together with the BCS density of states $N^{\rm BCS}(\varepsilon)$. Evidently, the $\sqrt{\varepsilon}$ singularity of $N^{\rm BCS}(\varepsilon)$ has been smoothed out by the phase fluctuations but a definite gap remains. This is an example of the general remark that a "pairing gap" need not mean superconductivity. Strikingly, in the present case it merely means a normal fluid of pairs. Note, moreover, that the observation of this gap in the nonsuperconducting state would be an unequivocal experimental proof that a system is is in the ILP state.

Given the above interpretation of the ILP state, it is interesting to ask what fraction of the electrons can be said to have turned into bosonic pairs. The answer to this question turns out not to be altogether straightforward. Clearly, the operators $b_i \equiv C_{i\uparrow}C_{i\downarrow}$ and $b_i^\dagger \equiv C_{i\downarrow}^\dagger C_{i\uparrow}^\dagger$ create and annihilate pairs at the site i. Although both b_i and $b_i^\dagger$ commute with b_j and $b_j^\dagger$ for $i \neq j$ as good bosonic operators should, on the same site the commutator

$$[b_i^\dagger, b_i] = C_{i\uparrow}^\dagger C_{i\uparrow} + C_{i\downarrow}^\dagger C_{i\downarrow} - 1 = \hat{n} - 1 \tag{61}$$

takes on the bosonic value 1 only if the site is doubly occupied. For empty and singly occupied sites, $b_i^\dagger, b_i$ do not behave like bose creation and annihilation operators. In fact, the operator

$$\sum_i b_i^\dagger b_i = \sum_i C_{i\uparrow}^\dagger C_{i\uparrow} C_{i\downarrow}^\dagger C_{i\downarrow} \tag{62}$$

merely counts the number of double occupied sites which is finite even if there are no bound pairs.

On the other hand, the expectation values $\langle b_i^\dagger \rangle$ and $\langle b_i \rangle$ behave more in line with expectations. It follows from Eq. (21) that, at $T=0$, $\langle b_i \rangle = \Delta/|U|$. Thus, $\Delta/|U|$ may be interpreted as the order parameter of a conventional Bose-Einstein condensate. In the ILP state,

$$\langle b_i \rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \langle b_i \rangle_{\theta_i} = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\, \Delta_0 e^{i\theta} = 0 \ . \tag{63}$$

Reassuringly, this result is consistent with our interpretation that, in the ILP state, the bosons form a normal liquid. Moreover, it suggests that we take

$$N_i^B = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \langle b^\dagger \rangle_\theta \langle b \rangle_\theta = \left[\frac{\bar{\Delta}_i}{U}\right]^2 \tag{64}$$

as the average number of pairs at the site i. Thus, in the homogeneous ILP state, the average number of bosons per site is

$$\bar{N}^B = \left[\frac{\bar{\Delta}}{U}\right]^2 . \tag{65}$$

We have solved the fundamental equations of the ILP state for a number of electrons per site n (band filling). We show our results in Fig. 4 for $U=-8W$. The curve for such a large $|U|$ perfectly fits the formula

$$\left[\frac{\bar{\Delta}}{U}\right]^2 = \tfrac{1}{4} n(2-n) \ . \tag{66}$$

Thus, for small n using Eqs. (65) and (66), we find $\bar{N}^B \cong \frac{1}{2}n$. Namely, in this dilute limit all the electrons are bound into pairs. As n increases towards 1.0, N^B falls below $\frac{1}{2}n$. We may interpret this behavior as the consequence of repulsive interactions between the pairs on neighboring sites. In other words, in the dense system some electrons do not form pairs because the repulsion between pairs outweighs the gain in pairing. The fact that the pair-pair interaction appears to be repulsive is reassuring since it is necessary for stabilizing a Bose-Einstein condensate.

Another interesting feature of the $\bar{N}_B$ versus n curve in Fig. 4 is its particle-hole symmetry. Evidently, for $n>1$ it is the holes that are pairing and, hence, $n \sim 2$ is the dilute hole-pairs limit.

In short, for large enough $|U|$, pairing will occur at $T < T_p \sim \frac{1}{4}|U|$ without Bose-Einstein condensation. In the next section we begin our investigations of what hap-

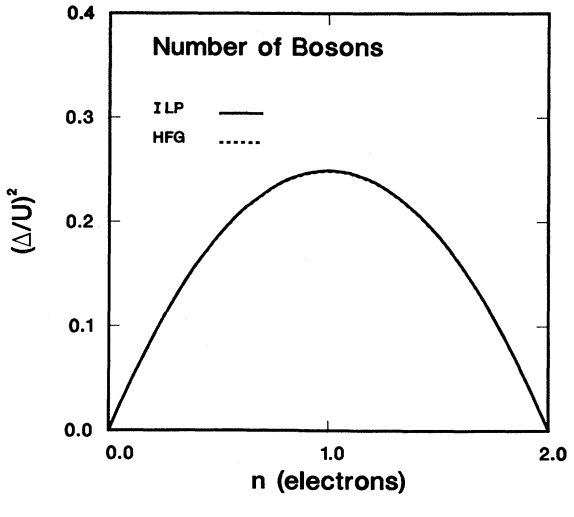

FIG. 4. The number of bosons, $N^B=(\Delta/U)^2$, as a function of band filling n in the Hartree-Fock-Gor'kov (dashed-line) and ILP (solid line) theories. Note the curves lie on top of one another.

pens when we lower the temperature towards $T=0$ by a comparative study of the BCS and ILP ground-state free energies.

IV. THE PAIRING ENERGY OF THE BCS AND THE ILP STATE

To begin, we note that, by integrating the Maxwell relation

$$-\left[\frac{\partial\Omega}{\partial\mu}\right]_T=\bar{N}(\mu)=k_BT\sum_{i,\sigma}\sum_n e^{+i\varepsilon_n\delta}G_{\sigma\sigma}(i,i;\varepsilon_n) \tag{67}$$

for a particular gap $\{\Delta_0 e^{i\theta_i}\}$ and occupation number $\{n_i\}$ configuration, we obtain the following general formula for the grand potential $\Omega(\mu)$:

$$\Omega_s(\mu)=-\frac{2}{\beta}\sum_n e^{i\varepsilon_n\delta}\frac{1}{2}\ln\left[\frac{\|i\varepsilon_n\hat{1}-\hat{H}^{\rm HF}\|}{\|i\varepsilon_n\hat{1}+\hat{H}^{\rm HF}\|}+\frac{1}{2}\ln\left\|\begin{matrix}i\varepsilon_n\hat{1}-\hat{H}^{\rm HF} & \hat{\Delta}\\ \hat{\Delta} & i\varepsilon_n\hat{1}+\hat{H}^{\rm HF}\end{matrix}\right\|\right]+\tfrac{1}{2}U\sum_i n_i^2-\frac{1}{2U}\sum_i|\Delta_i|^2\,, \tag{68}$$

where the quantities with a caret label matrices in the site representation such as

$$\hat{H}^{\rm HF}=H_{ij}^{\rm HF}=(\varepsilon_0+\tfrac{1}{2}U\bar{n}_i)\delta_{i,j}-t_{ij}\,,$$

$\hat{\Delta}=\bar{\Delta}e^{i\theta_i}\delta_{i,j}$, and $\hat{1}=\delta_{i,j}$ $\|\hat{o}\|$ denotes the operation of taking the determinant of the matrix $\hat{o}$. In the normal state the analogous grand potential is given by

$$\Omega(\mu)=-\frac{2}{\beta}\sum_n e^{i\varepsilon_n\delta}\ln\|i\varepsilon_n\hat{1}-\hat{H}^{\rm HF}\|+\frac{1}{2U}\sum_i n_i^2\,. \tag{69}$$

Naturally, taking the derivative of Eq. (68) with respect to μ leads to Eq. (67). More interestingly, minimizing Eq. (68) with respect to Δ_i yields the gap equation

$$\Delta_i=-U\frac{1}{\beta}\sum_n e^{i\varepsilon_n}\hat{G}_{12}(i,i;\varepsilon_n) \tag{70}$$

which also follows from Eq. (31).

We shall be interested in the condensation energy per lattice site

$$\Delta\Omega=[\Omega_s(\mu)-\Omega_n(\mu)]/\mathcal{N}\,, \tag{71}$$

where $\mathcal{N}$ is the number of lattice sites. For the BCS state, $\theta_i=\bar{\theta}$ and $n_i=\bar{n}$ for all i and we find

$$\begin{aligned}\Delta\Omega^{\rm BCS}(\mu)=-\frac{2}{\beta}\sum_n e^{i\varepsilon_n\delta}[&\tfrac{1}{2}\ln\|\hat{G}^{-1}(\varepsilon_n)\|\\&-\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}-\hat{H}^{\rm HF}\|\\&+\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}+\hat{H}^{\rm HF}\|]\\&-\frac{1}{2U}|\Delta|^2\,,\end{aligned} \tag{72}$$

where the Green's-function matrix $\hat{G}(\varepsilon_n)$ is the appropriate solution of Eq. (31). Converting the Matsubata sum over n into a contour integration in the usual way,[2] the above expression reduces, for our model density of states, to

$$\begin{aligned}\Delta\Omega^{\rm BCS}(\mu,T)=-k_BT\int_{-(W/2)-\mu}^{(W/2)-\mu}\frac{d\varepsilon}{W}[&(|\sqrt{\varepsilon^2+|\Delta^2|}-|\varepsilon|)/k_BT\\&+2\ln(1+e^{-(\sqrt{\varepsilon^2+|\Delta^2|})/k_BT})-2\ln(1+e^{-\varepsilon/k_BT}]-\frac{1}{2U}|\Delta|^2\,.\end{aligned} \tag{73}$$

For $T=0$, only the first term contributes and the integration can be carried out analytically. The result is

$$\Delta\Omega^{\rm BCS}(\mu=0,T=0)=\frac{W}{4}[1-\sqrt{1+(4|\Delta|^2/W)}]+|\Delta|^2\left[\frac{2}{U}-\frac{1}{2W}\ln\left[\frac{1+\sqrt{1+(4|\Delta|^2/W)}}{-1+\sqrt{1+(4|\Delta|^2/W)}}\right]\right] \tag{74}$$

for a half-filled band, i.e., $\mu=0$. Note that $\Delta\Omega^{\rm BCS}(\mu,T=0)$ in Eq. (74) has a minimum at Δ give by Eq. (30) which is the solution of the appropriate gap equation. In Fig. 5 we compare this result for $\Delta\Omega^{\rm BCS}(\mu=0,T=0)$ with the corresponding quantity for the ILP state.

To find $\Omega^{\rm ILP}$ we note that, for a fixed pairing field $\{\Delta_0 e^{i\theta}\}$ in place of Eq. (72), we have

$$\Delta\tilde{\Omega}(\mu,T)=-2k_BT\sum_n e^{i\varepsilon_n\delta}[\tfrac{1}{2}\ln\|\tilde{G}^{-1}(\varepsilon_n)\|+\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}-\hat{H}^{\rm HF}\|-\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}+\hat{H}^{\rm HF}\|]-\frac{1}{2U}|\Delta|^2\,. \tag{75}$$

We now rewrite $\underline{G}^{-1}(\varepsilon_n)$ using

$$\underline{\tilde{G}}(\varepsilon_n)=\underline{\tilde{G}}^{c}(\varepsilon_n)+\underline{\tilde{G}}^{c}(\varepsilon_n)[\underline{\hat{V}}-\underline{\hat{\Sigma}}(\varepsilon_n)]\underline{\tilde{G}}(\varepsilon_n) \tag{76}$$

as follows:

$$[\underline{\tilde{G}}(\varepsilon_n)]^{-1}=[\underline{\hat{G}}^{c}(\varepsilon_n)]^{-1}-[(\underline{\hat{V}}-\underline{\hat{\Sigma}}(\varepsilon_n)]=[\underline{\hat{G}}^{c}(\varepsilon_n)]^{-1}\{\underline{\hat{1}}-\underline{\hat{G}}^{c}(\varepsilon_n)[\underline{\hat{V}}-\underline{\hat{\Sigma}}(\varepsilon_n)]\}\ . \tag{77}$$

Then,

$$\Delta\tilde{\Omega}(\mu,T)=-\frac{2}{\mathcal{N}}\sum_n e^{i\varepsilon_n\delta}[\tfrac{1}{2}\ln\|(\underline{\hat{G}}^{c})^{-1}\|-\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}-\hat{H}^{\mathrm{HF}}\|-\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}+\hat{H}^{\mathrm{HF}}\|+\tfrac{1}{2}\ln\|\underline{1}-\underline{\hat{G}}^{c}(\underline{\hat{V}}-\underline{\hat{\Sigma}})\|]-\frac{1}{2U}|\Delta|^2 \tag{78}$$

and, hence,

$$\Delta\Omega^{\mathrm{ILP}}(\mu,T)=\Delta\Omega^{c}(\mu,T)+\frac{1}{\mathcal{N}}\sum_i\int_{-\pi}^{\pi}d\theta_i P_i(\theta_i)\Delta\Omega(\mu,T,\theta_i)\ , \tag{79}$$

where to simplify the notation we introduced

$$\Delta\Omega^{c}(\mu,T)=-2k_BT\sum_n e^{i\varepsilon_n\delta}\{\tfrac{1}{2}\ln\|[\underline{\hat{G}}^{c}(\varepsilon_n)]^{-1}\|-\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}-\hat{H}^{\mathrm{HF}}\|-\tfrac{1}{2}\ln\|i\varepsilon_n\hat{1}+\hat{H}^{\mathrm{HF}}\|\}-\frac{1}{2U}|\Delta|^2 \tag{80}$$

and

$$\Delta\Omega(\mu,T,\theta)=-\frac{2k_BT}{\mathcal{N}}\sum_n e^{i\varepsilon_n\delta}\tfrac{1}{2}\ln\|\underline{1}-\underline{G}^{c}(i,i;\varepsilon_n)[\underline{V}(\theta_i)-\underline{\Sigma}^{c}(\varepsilon_n)]\|\ . \tag{81}$$

Equation (79) is the principal result of the above discussion and is the basis of all the arguments to be deployed presently.

In this section our interest focuses on the ILP state studied in Sec. III 3 C. In this case, $P_i(\theta_i)=1/2\pi$ for all i. To simplify matters we also take the limit of a half-filled band $\mu=0$ and $T=0$. Then the sum over the Matsundera frequencies in Eq. (79) becomes an integral over the real axis. Explicitly, for the square density of states used in Eq. (73), we find

$$\Delta\Omega^{\mathrm{ILP}}(\mu=0,T=0)=\int_{-W/2}^{W/2}\frac{d\varepsilon}{W}\oint_c dz\left[\frac{1}{2}\ln\left[1-\frac{\Sigma_{11}^{c}(z)}{z-(\varepsilon-\mu)}\right]+\frac{1}{2}\ln\left[1-\frac{\Sigma_{22}(z)}{z+\varepsilon-\mu}\right]\right]$$
$$+\frac{1}{2}\oint dz\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\ln\|\underline{1}-\underline{G}^{c}(z)[\underline{V}(\theta)-\underline{\Sigma}^{c}(z)]\|\ . \tag{82}$$

We have evaluated this expression for a large number of values for $\bar{\Delta}$ in Eq. (50) by using the contour, in the complex energy plane, shown in Fig. 6. The results are compared to $\Delta\Omega^{\mathrm{BCS}}(\mu=0,T=0)$ in Fig. 5.

Evidently even though the minimum of $\Delta\Omega^{\mathrm{ILP}}$ occurs at larger values of $\bar{\Delta}$ than the minimum of $\Delta\Omega^{\mathrm{BCS}}$, $\Delta\Omega^{\mathrm{ILP}}$ is always above $\Delta\Omega^{\mathrm{BCS}}$. Thus, the ground state is the Hartree-Fock-Gor'kov, i.e., the BCS ground state. However, at finite temperature we must associate extra entropy with the random phases in the ILP state and, hence, eventually the ILP state will have the lower free energy. In the next section we develop a method for determining the temperature where this happens.

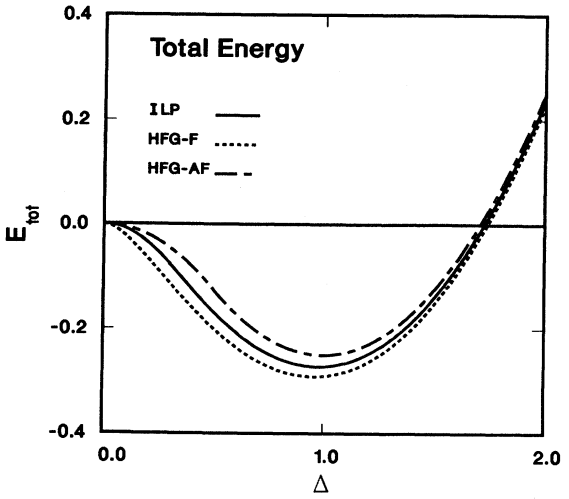

FIG. 5. The ground-state energy of the Hartree-Fock-Gor'kov state (dashed line) and ILP state (solid line) and the antiferrosuperconducting state (dot-dashed line) for $U=-2.0W$ and $n=1$.

V. THE SUPERCONDUCTING TRANSITION TEMPERATURE T_c

We determine T_c by finding the temperature at which the ILP state becomes unstable to development of phase

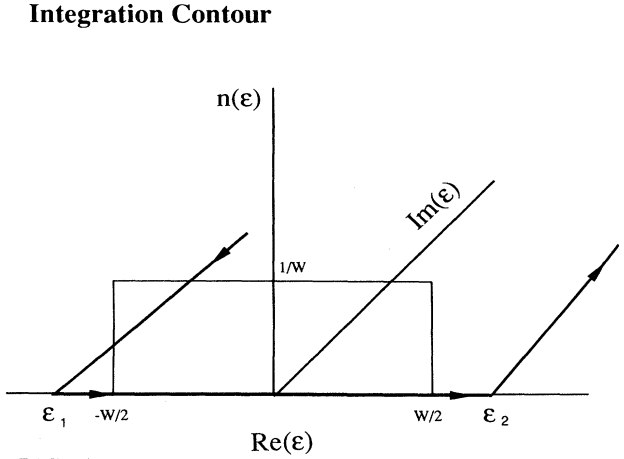

FIG. 6. The complex energy contour used to evaluate the various energy integrals numerically.

coherence between sites. The strategy is to consider a small deviation $\delta P_i(\theta)$ from $P_i(\theta)=1/2\pi$ and calculate the corresponding change in the average gap $\langle \Delta_i(\theta)\rangle$ self-consistently. The first temperature where there is a $\langle \Delta_i(\theta)\rangle \neq 0$ solution is the transition temperature. For reasons which will be evident presently, we shall also allow the magnitude of the gap $\bar{\Delta}$ to change with the development of coherence described by $\delta P_i(\theta)$. In short, we consider two contributions: Δ_1 and Δ_2 to

$$\langle \Delta_i(\theta)\rangle = \int_{-\pi}^{\pi} d\theta\, P(\theta)\Delta_i(\theta) \ . \tag{83}$$

Namely,

$$\langle \Delta_i \rangle = \Delta_{1,i} + \Delta_{2,i} \ , \tag{84}$$

where

$$\begin{aligned} \Delta_{1,i} &= \Delta_0 \int_{-\pi}^{\pi} d\theta\, \delta P_i(\theta) e^{i\theta} \ , \\ \Delta_{2,i} &= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta\, \delta\bar{\Delta}_i(\theta) e^{i\theta} \ , \end{aligned} \tag{85}$$

and Δ_0 is the ILP gap.

In a sensible mean-field theory, the natural choice for $P_i(\theta)$ is

$$P_i(\theta_i) = \frac{1}{Z_i} e^{-\beta \Delta\Omega_i(\theta_i)} \ , \tag{86}$$

where $\Delta\Omega(\theta_i)$ is as given in Eq. (81) and Z_i is the normalization constant; for a more careful derivation see Ref. 26. Recall that, in the ILP state, $\Delta\Omega_i(\theta_i)$ was independent of θ_i and, hence, $P_i(\theta)=\frac{1}{2\pi}$ for all i. To lowest order in the deviation from the ILP state,

$$\begin{aligned} \delta P_i(\theta_i) &= -\frac{1}{Z_0}\left[\frac{\delta Z_i}{Z_0} + \beta \delta\Delta\Omega_i(\theta_i)\right] \\ &= -\frac{\beta}{2\pi}[\delta\Delta\Omega_i(\theta_i) - \langle \delta\Delta\Omega_i(\theta_i)\rangle] \ , \end{aligned} \tag{87}$$

where

$$\langle \delta\Delta\Omega_i(\theta_i)\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\, \delta\Delta\Omega_i(\theta) \ . \tag{88}$$

Thus,

$$\Delta_{1,i} = -\Delta_0 \frac{\beta}{2\pi}\int_{-\pi}^{\pi} d\theta\, \delta\Delta\Omega_i(\theta) e^{i\theta} \ . \tag{89}$$

Similarly, we note that

$$\bar{\Delta} = -e^{-i\theta}\frac{U}{\beta}\sum_n e^{i\varepsilon_n\delta}\tilde{G}^{\theta}_{12}(ii;\varepsilon_n) \ , \tag{90}$$

where the impurity Green's function $\tilde{G}^{\theta}_{12}(i,i;\varepsilon_n)$ is given by Eq. (76). Consequently,

$$\Delta_{2,i} = -\frac{U}{2\pi\beta}\sum_n e^{i\varepsilon_n\delta}\int_{-\pi}^{\pi} d\theta\, \tilde{G}^{\theta}_{12}(i,i;\varepsilon_n) e^{-i\theta} \ . \tag{91}$$

We now expand the right-hand sides of Eqs. (89) and (91) to lowest order in $\Sigma^c_{12}(i,i;\varepsilon_n)$. In the ILP state, Σ^c_{12} was zero. However, in the slightly coherent state, it is given by

$$\begin{aligned} \Sigma^c_{12}(i,i;\varepsilon_n) = &\sum_j \int_{-\pi}^{\pi} d\theta\, \lambda_{12}(i,j;\varepsilon_n;\theta)\delta P_j(\theta) \\ &+ \sum_j \int_{-\pi}^{\pi} d\theta\, \gamma_{12}(i,j;\varepsilon_n;\theta)\delta\Delta_{0,j}(\theta) \end{aligned} \tag{92}$$

with a similar expression for $\Sigma^c_{21}(i,i;\varepsilon_n)$, where λ_{12} and γ_{12} are a pair of linear response functions to be determined presently. By expanding both sides of the CPA equation, Eq. (39), to lowest order in Σ^c_{21} and using Eq. (92), one can derive a set of Bethe-Salpeter-like equations for the response functions defined in Eq. (92). Using these the expansions of Eqs. (89) and (91) can be turned into a set of self-consistency equations for $\Delta_{1,i}$ and $\Delta_{2,i}$. In general, they describe an arbitrary inhomogeneous perturbation about the ILP state. They can be readily solved by taking the lattice Fourier transform of all the relevant equations and the results describe the finite wave vector, $\mathbf{q}$, fluctuations about the ILP state. As an interesting case, we have investigated the zone-boundary ($\mathbf{q}=\frac{1}{2}\mathbf{K}$, where $\mathbf{K}$ is a reciprocal-lattice vector) fluctuations. If these have negative energy, the system would have been unstable to a transition into an antiferrosuperconducting state where the order parameter takes on two different values on two interpenetrating sublattices.[36] We study this interesting case briefly in Appendix C. However, our present concern is with the homogeneous case where $\Delta_{1,i}=\Delta_1$ and $\Delta_{2,i}=\Delta_2$ for all i. In this limit, after some lengthy but straightforward algebra, we find the following basic equations for Δ_1 and Δ_2:

$$\begin{aligned} &(1-\beta\Delta^2 J)\Delta_1 - \beta\Delta^2\Xi\Delta_2 = 0 \ , \\ &U\Xi\Delta_1 + (1-M)\Delta_2 = 0 \ , \end{aligned} \tag{93}$$

where

$$J = \frac{1}{\beta}\sum_n e^{i\varepsilon_n\delta}\frac{-X_{12}(\varepsilon_n)}{\mathcal{D}(\varepsilon_n)[1+\Sigma^c_{11}(\varepsilon_n)G^c_{11}(i,i;\varepsilon_n)]} \ , \tag{94}$$

$$\Xi = \frac{1}{\beta}\sum_n e^{i\varepsilon_n\delta}\frac{-X_{12}(\varepsilon_n)}{\mathcal{D}(\varepsilon_n)} \ , \tag{95}$$

$$\begin{aligned} M = -U\frac{1}{\beta}\sum_n e^{i\varepsilon_n\delta}[&-X_{12}(\varepsilon_n) \\ &+ G^c_{11}(i,i;\varepsilon_n)G^c_{22}(i,i;\varepsilon_n)] \ , \end{aligned} \tag{96}$$

$$\begin{aligned} \mathcal{D}(\varepsilon_n) = &[1+\Sigma^c_{11}(i,i;\varepsilon_n)G^c_{11}(i,i;\varepsilon_n)] \\ &\times[1+\Sigma^c_{22}(i,i;\varepsilon_n)]G^c_{22}(i,i;\varepsilon_n) \\ &-\Delta_0^2 G^c_{11}(i,i;\varepsilon_n)G^c_{22}(i,i;\varepsilon_n) \ , \end{aligned} \tag{97}$$

and

$$\begin{aligned} X_{12}(\varepsilon_n) = \int d^3k [&G^c_{11}(\mathbf{k};\varepsilon_n)G^c_{22}(\mathbf{k};\varepsilon_n) \\ &- G^c_{11}(i,i;\varepsilon_n)G^c_{22}(i,i;\varepsilon_n)] \ . \end{aligned} \tag{98}$$

Evidently, the ILP state becomes unstable to a lining up of the local phases at the temperature $k_B T_c = 1/\beta_c$, where

$$(1-\beta_c\bar{\Delta}^2 J)(1-M) + \beta_c U\bar{\Delta}^2\Xi^2 = 0 \ . \tag{99}$$

Consequently, the principal formal result of this section is

$$k_B T_c = \bar{\Delta}^2 J - U\bar{\Delta}^2 \Xi^2 (1-M)^{-1} , \tag{100}$$

or

$$[1-M(T=T_c)]=0 .$$

Equation (99) depends on the temperature in two distinct ways. Firstly, there is the explicit factor β. This comes from the temperature dependence of $\delta P_i(\theta)$ and its physical origin is the entropy associated with the random phases of the pairing fields $\bar{\Delta} e^{i\theta}$. The second kind of temperature dependence is through the Matsubata frequencies in the definitions of the response functions J, Ξ, M, and X_{12} given in Eqs. (94)–(96) and (98). This is due to thermal excitations of electron-hole pairs. It turns out that, at temperatures $T \sim T_c$, the above entropy of electron-hole pairs can be safely neglected. As evidence for this, we show the solution of the BCS gap equation, Eqs. (28) and (29) in Fig. 7 for various values of U. We note, in anticipation of our results, that, for each U, $T_c \ll T_c^{\rm BCS}$, and, hence, $\Delta^{\rm BCS}(T \sim T_c)$ is practically $\Delta^{\rm BCS}(T=0)$. We took advantage of this fortunate circumstance and evaluated J, Ξ, M, D, and X_{12} at $T=0$ using the $T=0$, ILP state solution discussed in the previous section. To do this we converted the Matsubata sums into a contour integrals and evaluated them numerically taking a sufficiently dense set of points to ensure convergence.

We have calculated T_c using Eq. (100) for a half-filled band, $n=1$, for various values of U. The results are shown in Fig. 8 together with $T_c^{\rm BCS}$. As expected, for large enough $|U|$, the ILP state is stable to temperatures much below $T_c^{\rm BCS}$. In fact, even at $U=-1.0W$, T_c is small enough that the entropy contribution of the electron-hole pairs is negligible. Further support for this conclusion is provided by Fig. 2 where, for $U=-1.0W$, the gap is $\sim 0.45W$ and, hence, much larger than $k_B T_c \sim 0.04W$ at $U=-1.0W$ in Fig. 8.

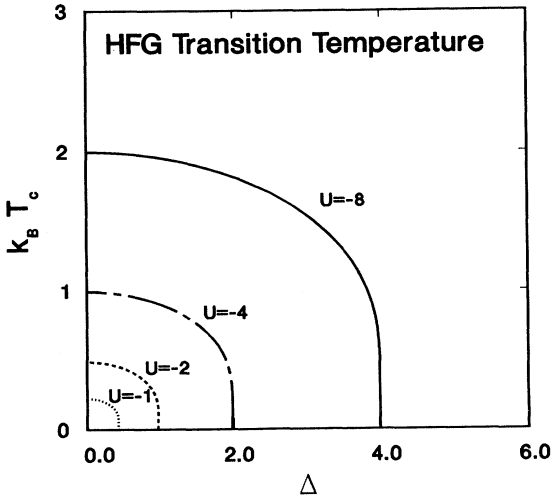

FIG. 7. The temperature dependence of the Hartree-Fock-Gor'kov gap for $n=1$ and various values of the interaction constant U.

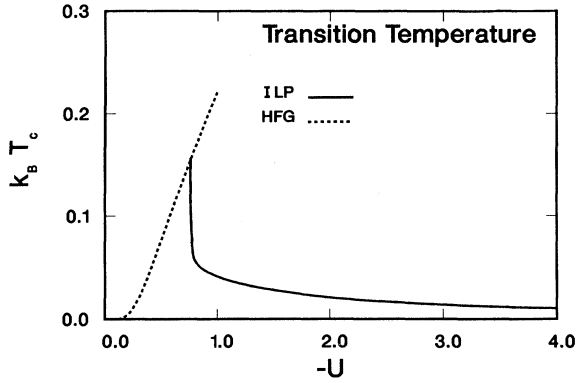

FIG. 8. The instability temperature T_c of the ILP state (solid line) and BCS state (dashed line) for $n=1$. This is our prediction for the superconducting transition temperature.

In light of our discussion in the Introduction, it is also a very satisfactory feature of Fig. 8 that T_c decreases with increasing U for $|U|/W \gg 1$. In fact, analyzing our numerical solutions, we find that, for $|U|/W \gg 1$, the formula

$$k_B T_c \cong \frac{1}{6}\frac{W^2}{|U|}\left[\frac{\Delta^2}{U^2}\right] \tag{101}$$

fits them very well. This relation is, then, the principal result of this section.

Remarkably, Eq. (101) displays the dependence of $k_B T_c$ on $W^2/|U|$ we have anticipated in Sec. I on the basis of Bose-Einstein condensation of bound pairs. The central point is that the arguments leading to $k_B T_c \sim W^2/|U|$ implied a large-$|U|$ ($|U|/W \gg 1$) expansion. Hence, we may conclude that our method of random fields successfully extrapolates between the small-$|U|$ BCS, and large-$|U|$ ILP limits. Moreover, it does so without transforming away, as other approaches do, the naturally occurring electronic degrees of freedoms in favor of pseudospins or effective bosons.

The factor Δ^2/U^2 in Eq. (101) deserves several comments. Firstly, in Sec. III C, we have interpreted it as the number of bosons $\bar{N}_B$. For comparison, we recall that Nozières and Schmitt-Rink[6] found

$$k_B T_c = (W^2/|U|)\bar{N}_B^{2/3}$$

in the large-$|U|$ and noninteracting Bose limit. Robaszkiewicz *et al.*[5] also found the same result by using the effective spin Hamiltonian in Eq. (2) and the RPA approximation. Although near the half-filled band, $n=1$, where the pairs are strongly interacting, we do not expect the free-boson factor $\bar{N}_B^{2/3}$, in the dilute limit the lack of such behavior must be considered as a shortcoming of the theory. We speculate that our calculation does not reproduce this result because we have neglected the charge and spin fluctuations in our application of the method of random fields. We shall remedy this omission in a future publication.

As our second comment, we observe that the above dependence of $k_B T_c$ on the band filling n, via Eq. (66), is the same as that of $\Delta_{\rm BCS}^2/U^2$, where $\Delta_{\rm BCS}$ is given in Eq.

(30). This fact can be readily understood by noting that, for large $|U|$ [$(W/|U| \ll 1)$], the amplitude of the pairing field $\Delta(\theta)=\bar{\Delta}e^{i\theta}$ does not fluctuate much in the ILP state and, hence, it takes on a value very close to that of the Hartree-Fock-Gor'kov solution. This behavior is analogous to the U dependence of $\bar{\Delta}$ displayed in Fig. 2. In other words, for the strong pairing force, the amplitude of the pairing field, and hence the number of pairs, does not depend much on the state of intersite phase coherence of the pairing field.

Thirdly, we note that the above situation arises because, for $W/|U| \ll 1$, the J term dominates on the right-hand side of Eq. (100). This is understandable because J can be shown to be a response function related to phase-phase correlations. In our calculations, when $W/|U|$ increases to unity and beyond, the second term, which is due to amplitude fluctuations, becomes comparable to the first [$(1-M)$ becomes small]. Also, in this regime Eq. (66) no longer holds. In fact, as the rise of T_c in Fig. 8 shows, the system appears to undergo a transition as a function of $|U|/W$. The physics of this transition is most interesting: the number of bound pairs in the normal state is decreasing and their role in forming the condensate is taken over by Cooper pairs. Somewhat surprisingly, when this happens T_c rises. Clearly, the maximum T_c in this model is governed by the balance of these competing processes.

By bound pairs we mean pairs of electrons which would bind even if there were only two electrons on the entire lattice. On the other hand, Cooper pairs form only with the help of the exclusion principle. Evidently, when a bound pair forms on a site there is a gain of U in potential energy. However, there is a loss in kinetic energy. To estimate this, we note that, for large $|U|$ $(>t)$, the effective hopping integral for a pair is $2t \times t/U$; z times this is the kinetic energy of a bound pair, which can be contrasted to $2tz$, the kinetic energy of two independent pairs. More generally, in the strongly attractive limit, $|U| \gg zt$, we have bound pairs, but for $|U| \ll t$, a lone pair of electrons would not bind in three dimensions. Consequently, for $|U| \ll zt$, pairs form only by the Cooper mechanism as in the BCS theory. Clearly, the transition from the former of these regimes to the latter is the physics behind the phase transition noted to take place near $|U| \sim zt = W$. Interestingly, from this point of view, the case of two dimensions is rather special and is attracting considerable attention.[37]

To highlight the intricate process at work, we note that, near the critical value of $|U_c|/W$, the amplitude $\bar{\Delta}$ is rapidly collapsing in the ILP state. This is demonstrated in Fig. 2. Evidently, this is the consequence of the fact that the attractive force described by U is losing its ability to bind. Thus, the number of pairs which exist in the ILP state prior to condensation is rapidly decreasing. Nevertheless, as noted above, at the same time as $\bar{\Delta}$ falls, $k_B T_c$ rises rapidly, due to the second term in Eq. (100), towards the $k_B T_c^{\mathrm{BCS}}$ value.

This implies that exclusion-principle-assisted Cooper pairs are formed to compensate for the losses of real pairs. It may be helpful to observe that the above process is rather analogous to the formation of magnetic moments in metals. In good moment systems, like Fe, local moments exist below and above the Curie temperature and they are about the same size whether they are lined up or not. By contrast in highly itinerant metals, like Ni or Cr, moments seem to exist only if assisted by long-range order.

VI. CONCLUSIONS

We have studied pairing, condensation, and superconductivity using a one-band Hubbard model with an attractive interaction between the electrons. It may be helpful if we began our summary by recapitulating the physical picture in the strong-coupling limit. Within the framework described by the Hamiltonian given in Eq. (1), for $|U| > zt$ the single occupied sites can be eliminated and the model becomes that of interacting bosons hopping from site to site with the probability amplitude $2t^2/U^2$. Evidently, the state of such a system may be gas, liquid, superfluid, or crystalline. Although the corresponding phase diagram has been studied in some detail by Micnas *et al.*,[15] even here there are many open questions. Of particular interest is the relative stability of the highly quantum crystalline state and the superfluid phase. This problem is especially intriguing in two dimensions where both phases are subject to the Kosterlitz-Thouless analysis.

In the present work, our aim was to develop a theory which, while retaining the language of the electronic degrees of freedom in the spirit of the BCS theory, is able to describe the strong-coupling regime where, hitherto, only effective boson or pseudo-spin Hamiltonians could be used. The approximation scheme we have proposed consists of applying the method of random fields in conjunction with the Gor'kov decoupling procedure. When fully implemented, including charge, spin as well as pairing field fluctuations, it has been designed to treat all the phases we have mentioned above within what might be called a mean-field approximation. To illustrate the method we have treated the pairing field fluctuations only. This restricted the applicability of our actual calculations to a study of the normal metal to superconductor phase transition. Our principle results are summarized in Eq. (100). We argued that they are consistent with the notion that this phase transition is equivalent to a normal Bose liquid to superfluid transition of bound electron pairs.

Of course, for $|U| \ll zt = W$, the theory reduces to the BCS predictions for the present model. These are given, for reference, in Eqs. (30) and (74).

Finally, our most interesting results concern the intermediate regime $|U| \sim zt = W$. Here, our theory describes the transition from bound pairs to Cooper pairs as $|U|$ approaches W from above. This transition is depicted in Fig. 8 near $|U| \sim -1.0W$. Also, in Eq. (100) it corresponds to $k_B T_c$ being dominated by J for $|U| \gg W$. While near $|U| \sim W$, the main contribution is due to M being close to unity in the second term. The response function J describes site-to-site phase coherence of the pairing field. We have interpreted the development of

such coherence as an indication that the Bose-Einstein condensation of preexisting pairs is taking place. As $|U|$ approaches W, such pairs no longer form. This is signaled by the collapse of the gap amplitude $\bar{\Delta}$ in the ILP state shown in Fig. 2. As $\bar{\Delta}^{\rm ILP}$ goes to zero, $\bar{\Delta}^2 J$ goes to zero. It is the strength of the theory that, when this happens, Eq. (100) still describes $k_B T_c$ but now the second term, which corresponds to the production of Cooper pairs, dominates. As usual, such pairs condense when they are formed and $k_B T_c$ recovers its BCS value. Thus, the theory interpolates smoothly between the two extremes.

Although the present theory may not be the final word on the nature of this crossover, for instance, taking fully into account the thermal fluctuations of electron-hole pairs would smooth out the sharp rise in Fig. 8, it highlights the significance of working with electronic variables if we are to identify the competing physical processes in the crossover regime. Evidently, it is in this regime that the maximum T_c is determined.

In conclusion, we wish to comment on the relevance of the negative-U Hubbard model to high-temperature superconductivity. Clearly, the model we studied is too simple to describe the chemically derived picture of Wilson[38] or the bipolaron mechanism of Alexandrov *et al.*[14] However, such qualitative features as the existence of bosonic pairs above T_c and their competition with Cooper pairing must be a generic feature of any model with strong local pairing correlations. Thus, it is sensible to think about experiments which would identify such pairs in the normal state. For instance, if the pairs are singlets, their existence in the normal state implies a reduction of the local susceptibility. This effect may show up in NMR experiments. Indeed, some evidence that it does already has been reported.[39]

ACKNOWLEDGMENTS

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APPENDIX A: EFFECTIVE HAMILTONIANS

Let us rewrite the Hubbard Hamiltonian in Eq. (1) as follows:

$$H = T_1 + T_2 + T_3 + T + V_4 \ , \tag{A1}$$

where

$$\begin{aligned}
T_1 &= \sum_{i,j,\sigma} t_{ij}(1-\hat{n}_{i,-\sigma}) C^{\dagger}_{i,\sigma} C_{j,\sigma}(1-\hat{n}_{j,-\sigma}) \ , \\
T_2 &= \sum_{i,j,\sigma} t_{ij}(1-\hat{n}_{i,-\sigma}) C^{\dagger}_{i,\sigma} C_{j,\sigma}\hat{n}_{j,-\sigma} \ , \\
T_3 &= \sum_{i,j,\sigma} t_{ij}\hat{n}_{i,-\sigma} C^{\dagger}_{i,\sigma} C_{j,\sigma}(1-\hat{n}_{i,-\sigma}) \ , \\
T_4 &= \sum_{i,j\sigma} t_{ij}\hat{n}_{i,-\sigma} C^{\dagger}_{i,\sigma} C_{j,\sigma}\hat{n}_{j,-\sigma} \ , \\
V &= \tfrac{1}{2} U \sum_{i,\sigma} \hat{n}_{i,\sigma}\hat{n}_{i,-\sigma} \ ,
\end{aligned} \tag{A2}$$

and study its canonical transform

$$H_{\rm eff} = e^{iS} H e^{-iS} \ .$$

To lowest order in s we find

$$\begin{aligned}
H_{\rm eff} &= H + i[S,H] + \cdots \\
&= T_1 + T_2 + T_3 + T_4 + V \\
&\quad + i[S_1,T_1] + i[S_1,T_2] + i[S_1,T_3] \\
&\quad + i[S_i,T_4] + i[S_1,V] \ .
\end{aligned} \tag{A3}$$

Let us chose the, hitherto, arbitrary operator S such that

$$T_2 + T_3 + i[S,V] = 0 \ . \tag{A4}$$

Using the original form of H, given in Eqs. (A1) and (A2), it is easy to show that Eq. (A4) implies that

$$S = -\frac{i}{U}(T_2 - T_3) \ . \tag{A5}$$

Substituting this result into Eq. (A3) we find the following.

(i) For $U = |U|$ in the subspace of no doubly occupied sites,

$$H_{\rm eff} = T_1 + V + \sum_{i,j} J_{ij}(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4}) \ ,$$

where $T_{ij} = 4t_{ij}^2/|U|$.

(ii) For $U = -|U|$ in the subspace of no singly occupied sites,

$$H_{\rm eff} = -\sum_{i,j} J_{ij}(S_i^+ S_i^- - S_i^z S_j^z) - B\sum_i (2S_i^{z+1}) \ ,$$

where $T_{ij} = 4t_{ij}^2/|U|$, $B = \mu - \varepsilon_0 + \frac{1}{2}|U|$, and $S_i^z = \frac{1}{2}(\hat{n}_i - 1)$ with $\hat{n}_i = \hat{n}_{i\downarrow} + \hat{n}_{i\uparrow}$.

APPENDIX B

In this appendix we describe a very efficient iteration scheme for solving the CPA equation, Eq. (51), in the discretized form

$$\sum_{\theta} P(\theta)\underline{D}^{(\theta)} = \underline{1} \ .$$

Using Eq. (49), it is straightforward to rewrite this as

$$\sum_{\theta} P(\theta)\underline{X}_c^{(\theta)} = \underline{0} \ ,$$

where

$$\underline{X}_c^{(\theta)} = [(\underline{\Sigma} - \underline{V}^{(\theta)})^{-1} - \underline{G}^c]^{-1} \ .$$

Note now that

$$\underline{X}_c = \sum_{\theta} P(\theta) X_c^{(\theta)} = [(\underline{\Sigma}_c^n - \underline{\Sigma}_c^{n+1})^{-1} - \underline{G}^c(\underline{\Sigma}_c^n)]^{-1}$$

is solved when $\underline{\Sigma}_c^n = \underline{\Sigma}_c^{n+1}$, where $\underline{\Sigma}_c^n$ and $\underline{\Sigma}_c^{n+1}$ are the self-energy at the end of the nth and $(n+1)$th iteration. Finally, we recast the above form into the following relation:

$$\underline{\Sigma}_c^n = \underline{\Sigma}_c^{n+1} + [\underline{X}_c^{-1} - \underline{G}^c(\underline{\Sigma}_c^n)] \ .$$

We iterate the above recursion relation numerically starting with the average-t-matrix approximation (ATA) for Σ_c, i.e.,

$$\underline{\Sigma}_c^{n=0-} = \underline{\Sigma}^{\rm ATA} \ ,$$

where the self-energy $\underline{\Sigma}^{\mathrm{ATA}}$ was generated from the averaged t matrix,

$$\underline{t}^{\mathrm{ATA}}=\sum_{\theta}P(\theta)(\underline{1}-\underline{V}^{(\theta)}\underline{G}_0)\underline{V}^{(\theta)}$$

and the relation

$$\underline{\Sigma}^{\mathrm{ATA}}=-(\underline{t}^{-1}_{\mathrm{ATA}}+\underline{G}_0)^{-1}\ .$$

APPENDIX C: ANTIFERROSUPERCONDUCTIVITY

For simplicity consider two interpenetrating "lattices" as shown in Fig. 9. Assuming that the gap Δ takes on different values, Δ_{I} and Δ_{II}, respectively, on the two sublattices the finite-temperature Gor'kov equation is given by

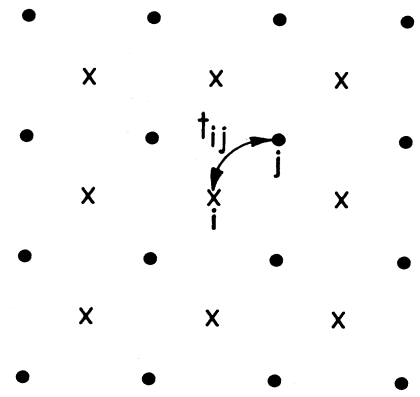

FIG. 9. The two interpenetrating sublattices of the antiferrosuperconductivity considered in Appendix C.

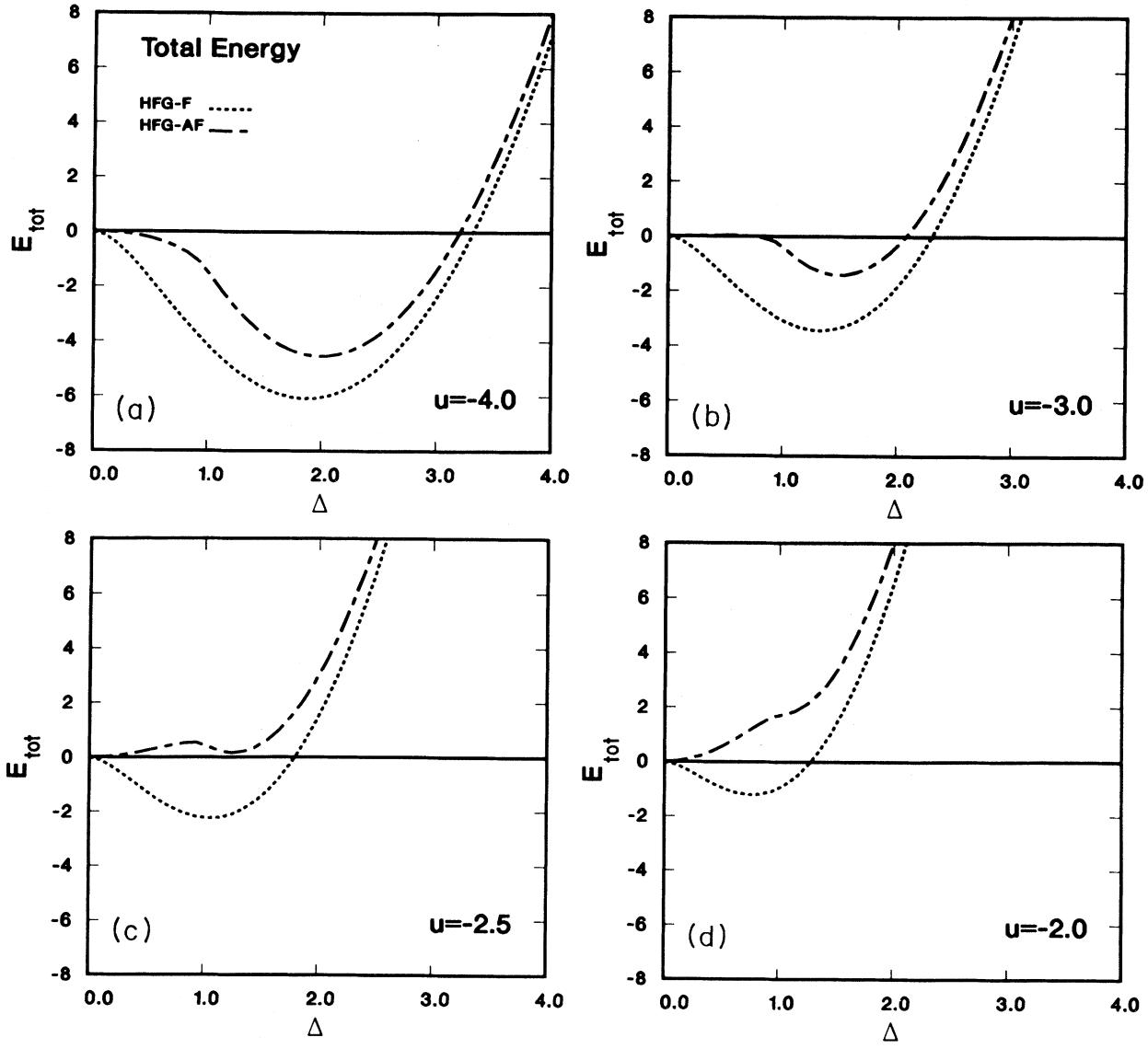

FIG. 10. A comparison of the ground-state energies of the ferromagnetic (dashed line) and antiferromagnetic (dot-dashed line) superconducting states as functions of the gap Δ for $n=1$.

$$\begin{bmatrix} i\varepsilon_n-\varepsilon_0+\mu & \Delta_{\rm I} & t(k) & 0 \\ \Delta^* & i\varepsilon_n-\varepsilon_0+\mu & 0 & -t(k) \\ t(k) & 0 & i\varepsilon_n-\varepsilon_0+\mu & \Delta_{\rm II} \\ 0 & -t(k) & \Delta_{\rm II}^* & i\varepsilon_n-\varepsilon_0+\mu \end{bmatrix} \times \begin{bmatrix} G_{11}^{\rm I,I} & G_{12}^{\rm I,I} & G_{11}^{\rm I,II} & G_{12}^{\rm I,II} \\ G_{21}^{\rm I,I} & G_{22}^{\rm I,I} & G_{21}^{\rm I,II} & G_{22}^{\rm I,II} \\ G_{11}^{\rm II,I} & G_{12}^{\rm II,I} & G_{11}^{\rm II,II} & G_{12}^{\rm II,II} \\ G_{21}^{\rm II,I} & G_{22}^{\rm II,I} & G_{21}^{\rm II,II} & G_{22}^{\rm II,II} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} .$$

This leads to the coupled gap equations

$$\Delta_{\rm I}^* = -\frac{U}{\beta}\sum_{k,n} e^{i\varepsilon_n\delta} G_{21}^{\rm I,I}(k,i\varepsilon_n) ,$$

$$\Delta_{\rm II}^* = -\frac{U}{\beta}\sum_{k,n} e^{i\varepsilon_n\delta} G_{21}^{\rm II,II}(k,i\varepsilon_n) .$$

Surprisingly, as well as the conventional case of $\Delta_{\rm I}=\Delta_{\rm II}$, the above equations also have a solution for $\Delta_{\rm I}=-\Delta_{\rm II}$. In analogy with the terminology of ferroelectricity and antiferroelectricity, we shall refer to the cases $\Delta_i=\Delta_{\rm II}=\Delta^{\rm F}$ and $\Delta_{\rm I}=\Delta_{\rm II}=\Delta^{\rm HF}$ as ferro- and antiferrosuperconductivity, respectively. The possibility of this latter solution has been noted by Allen.[40]

Proceeding in the usual manner, we find for $T=0$ that

$$\Delta^{\rm F} = -U\Delta^{\rm F}\sum_{\rm k}\left[\frac{1}{4\sqrt{[\varepsilon_0+t(k)]^2+|\Delta^F|^2}} + \frac{1}{4\sqrt{[\varepsilon_0-t(k)]^2+|\Delta^F|^2}}\right]$$

and

$$\Delta^{\rm AF} = -U\Delta^{\rm AF}\sum_{k}\frac{1}{2\sqrt{\varepsilon_0^2+|\Delta^{\rm AF}|^2}} .$$

Although the antiferrosuperconducting gap $\Delta^{\rm AF}$ always works out to be greater than $\Delta^{\rm F}$ for the same U and intersublattice hopping integral t, the latter state has lower energy. Explicitly, we find the condensation energies to be

$$\delta E^{\rm F} = -\sum_{\rm k}\{|\sqrt{[\varepsilon_0+t(k)]^2+|\Delta|^2}|-|[\varepsilon_0+t(k)] + |\sqrt{[\varepsilon_0-t(k)]^2+|\Delta|^2}| - |[\varepsilon_0-t(k)]^2\} - \frac{2}{U}|\Delta|^2 ,$$

$$\delta E^{\rm AF} = -\sum_{\rm k}\{|\sqrt{[\varepsilon_0^2+|\Delta|]^2}+t(k)|-|[\varepsilon_0+t(\mathbf{k})] + \sqrt{[\varepsilon_0^2+|\Delta|]^2}-|[\varepsilon_0+t(\mathbf{k})]\}$$

for a normal-state dispersion relation $\varepsilon_k^0=\varepsilon_0-t\cos(ka)$. We have evaluated these expressions for various values of U. The results are shown in Fig. 10. Evidently, $\delta E^{\rm F}<\delta E^{\rm AF}$ for all U. Thus, we conclude that the antiferrosuperconduting soluting corresponds to a metastable state. Whether the same could be said in cases of more general models remains to be investigated.

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