Superconductivity in the generalized periodic Anderson model with strong local attraction

S. Robaszkiewicz*
Institut-Laue-Langevin, Boîte Postale 156 X, 38042 Grenoble Cédex, France

R. Micnas* and J. Ranninger
Centre de Recherches sur les Très Basses Températures, Centre National de la Recherche Scientifique, Boîte Postale 166 X, 38042 Grenoble Cédex, France

(Received 29 December 1986)

We study a generalized periodic Anderson model with on-site hybridization between wide- and narrow-band electrons and strong and local coupling with the lattice deformation. Provided that the interaction with the lattice is strong enough, the narrow-band electrons will be turned into small polarons which interact attractively with each other over short distances, leading to the formation of local pairs of narrow-band electrons. This leads to a pinning of the Fermi level which is due to the fact that narrow-band electrons exist only in pair states. By means of a generalized Schrieffer-Wolff transformation we eliminate hybridization and obtain an effective Hamiltonian which describes a contact interaction between local pairs and wide-band electrons as well as the direct hopping of local pairs and interparticle Coulomb interactions. In such a system the two types of mechanisms which can lead to superconductivity have been studied. The first one is due to direct local pair hopping and involves exclusively the narrow-band subsystem giving rise to a superconductivity analogous to superfluidity in ^{4}He. The second one is due to a contact interaction between local pairs and pairs of wide-band electrons. This leads to a superconducting state involving both subsystems where the local pairs of the narrow-band subsystem induce Cooper pairing amongst the electrons of the wide-band subsystem. Consequently, the single-particle spectrum of the wide-band electrons opens up a gap around the position of the narrow band of electrons in pair states. We study the phase diagrams and the superconducting properties of two such coupled subsystems involving bosons and fermions as a function of the position of the narrow band with respect to the wide band (or the relative concentration of narrow and wide-band electrons). We also show that the critical temperature T_c and $T_c/E_g(0)$ [$E_g(0)$ being the energy gap] follow, in general, a strong and nonmonotonic variation. One of the most striking features of this system is that the pairs of narrow-band electrons exist in the normal phase and condense on approaching T_c from above. The existence of such a narrow boson band together with a fermion band in the normal phase leads to characteristic behavior in the specific heat over temperature variation being very similar to that observed in recent studies of nonclassical superconductors.

I. INTRODUCTION

In classical BCS-like (Bardeen-Cooper-Schrieffer–like) superconductors—describing the majority of known superconducting materials—the formation of pairs of electrons at the critical temperature coincides with the formation of a coherent macroscopic quantum state describing superconductivity. It is legitimate to ask the question whether pairs of electrons could not exist independently of such a coherent state; that is to say, a superconducting material which could exhibit pair formation well above T_c. It is known that in the case of strong electron-lattice coupling the electrons change their characteristics completely. They become small polarons, i.e., electrons which carry with them a lattice deformation which is very local and strong. Such entities have the tendency to pair up in the form of local pairs simply due to the very local lattice deformation which provides a short-range attraction between two small polarons. Such particles having Bose character can, in principle, condense and form a superfluid state analogous to ^{4}He II.[1] The macroscopic coherent quantum state associated with it corresponds to a phase-locked state of $k=0$ eigenstates of hard-core bosons on a lattice. As one approaches the critical temperature this quantum coherent state breaks up into hard-core boson wave functions on a lattice which are no longer phase correlated. Thus such superconducting materials should display electron pairs in the normal phase.

The existence of local pairs is now experimentally well established. After the initially discovered cases[2] of Ti_4O_7 and $Na_xV_2O_5$, a large number of other compounds joined their rank. All of those materials for which direct unquestionable proof exists (as concerns local pairs) have not yet shown superconductivity. The possible reasons for this are known. It can be due to the fact that they form half-filled bands of local pairs and hence show a charge-ordered ground state as expected from the theory.[3,4] As examples we quote Ti_4O_7, $Na_xV_2O_5$, and a large group of materials in which cations exist in two valence states differing by $2e$:[5,6] diamagnetic compounds of Sb and Tl,

i.e., Cs_2SbCl_6 and TlF_2; divalent compounds of Ag and Au, e.g., $CsAgCl_3$ and AgF_2; trivalent compounds of Pd and Pt, i.e., $Pd(NH_3)_2Br_3$ and $Pt(NH_3)_2Cl_3$. Other reasons for the nonoccurrence of superconductivity in local-pair systems can be due to their one-dimensional characteristics as in KCP,[7] polypyrrole, and polythiophene,[8] or to structural disorder or nonstoichiometry as in WO_{3-x},[9] or simply the localization of those electrons pairs on impurity centers[10] as in chalcogenide glasses, silicon inversion layers, and amorphous silicon in which such negative-U centers were initially invoked in order to explain their electrical, magnetic, and optical properties.

With the discovery of the so-called exotic superconductors (i.e., all those which do not fit in any unequivocal way to BCS superconductors[11,12]), superconductivity due to local pairs rather than Cooper pairs can be envisaged as a real possibility. In general, these materials are much more complicated (as far as their electronic structure is concerned) than ordinary classical superconductors. They contain invariably several electronic bands, at least one of which is very narrow and frequently of $3d, 4d, 4f, 5f$ character.

Systems in which such local-pair superconductivity can be envisaged are, among others, $A15$, $C15$, Chevrel phases,[11,13–15] the carbides and nitrides,[14,15] and transition-metal dichalcogenides.[16] As specific examples of such systems we mention V_3Si,[13,14,17] Nb_3Ge and Nb_3Al, $PbMo_6S_8$ and $Eu_xMo_6S_8$, NbC and TaC,[14,16] and $2HNbSe_2$ and $2HTaS_2$.[16] All of these materials have narrow electron bands and large values of electron-phonon coupling which result in poor metallic properties in the normal state but rather high values of the superconducting transition temperatures. Similar properties have been observed in some semiconductors and semimetals, such as $BaBi_xPb_{1-x}O_3$,[18] PbTe(Tl),[12,19] $SrTiO_3$,[20] PdH_x,[12] $Li_{1-x}Ti_{2-x}O_4$,[12,21] etc., with superconducting behaviors which are quite different from those of standard BCS ones. Finally, it cannot be excluded that heavy-fermion systems and their exotic superconductivity are not due to local pairing.[1,22,23]

A prerequisite for local pairing is the degree of localization of the electronic wave function. For narrow-band electrons this appears to be feasible provided the commonly used dimensionless coupling constant $\lambda \gtrsim 1$.[1,14] The theory for narrow-band electrons in the presence of strong and local electron-lattice coupling is now quite advanced,[24] predicting many features of the superconducting state which, in fact, are found in a variety of those exotic superconducting materials: nonexponential variation of the specific heat with temperature, large deviations from $2k_BT_c/E_g(0)=0.57$, nonstandard variation of the upper critical field with temperature, $(d^2H_{c2}/dT^2)\,|_{T=T_c}>0$, nonmonotonic variation of T_c with the concentration, extremely high values for H_{c2} and, for the penetration depth, existence of collective modes of the superfluid order-parameter fluctuations, strong effects of magnetic as well as nonmagnetic impurities, etc. All this was derived previously on the basis of a single narrow band and sufficiently strong coupling of the electrons to the lattice such that the only quasiparticles are local pairs.[1]

An attempt has been made to generalize this picture to the situation where the electron-lattice coupling was of intermediate strength, giving rise to coexisting small polarons and a band of resonance states of bipolarons (local pairs) lying at the Fermi level of the polaronic band.[25]

In the present paper we shall address ourselves to a much more realistic situation, namely that in which one has two distinct bands: a wide and a narrow one. Only the narrow-band electrons are assumed to be strongly interacting with the lattice, such that they are unstable towards small-polaron formation and eventually local-pair formation. Moreover, hybridization is assumed to take place between these two types of electrons. For our description we start from a generalized periodic Anderson model plus a strong local interaction of the narrow-band electrons with the lattice. In Sec. II we shall derive an effective Hamiltonian in terms of a mixture of local pairs and wide-band electrons interacting with each other. In general, there are two contributions giving rise to the superconductivity in the system considered. One is due to direct motion of the pairs, which is fairly independent of the wide-band subsystem. The other is due to a coupling between local pairs and pairs of wide-band electrons, which leads to a mutual induction of superconductivity in both subsystems.

In Sec. III we shall set up a mean-field treatment of this effective Hamiltonian and derive the self-consistent equations for the various order parameters describing the superconducting and charge-ordered states for each of the two subsystems (the local pairs and the wide-band electrons). In Sec. IV we discuss the thermodynamic properties of the superconducting state as a function of the relative position of the local pairs level with respect to the wide band of electrons (or, in other words, as a function of the relative concentration of particles of the two subsystems) and the various interaction parameters.

The normal-state properties are analyzed in Sec. V, where we shall show that the corresponding mixture of two lattice gases, one composed of local pairs forming bosons and the other being composed of wide-band electrons—fermions—can give rise to some remarkable features in the temperature variation of the specific heat, the entropy, and the magnetic susceptibility analogous to those recently observed in heavy-fermion systems. The effects of interparticle density-density interactions on the superconducting and normal phases are briefly discussed in Sec. VI. In the discussion and outlook in Sec. VII we review the main features of our system, compare them with those of standard BCS superconductors, and finally give a list of materials to which our model could possibly apply.

II. DERIVATION OF AN EFFECTIVE HAMILTONIAN IN TERMS OF LOCAL PAIRS AND ITINERANT ELECTRONS

In this section we present the basic ingredients of the system which we are going to study: a periodic Anderson model in which the narrow-band electrons are strongly and locally coupled to the lattice.[26] We expect that in such systems the narrow-band electrons will be turned into small polarons which strongly interact in an attrac-

tive way over short distances. This gives rise to the formation of local pairs of narrow-band electrons (bipolarons) formed on effective lattice sites. Depending on the system considered, these effective sites can mean (i) single atomic sites or cation-ligand complexes. As examples we note $BaBi_xPb_{1-x}O_3$,[18] PbTe(Tl),[12,19] PbTe(In),[12] $Pb_{1-x}Sn_xSe$,[27] $In_{1-x}Tl$,[15] Cs_2SbCl_6,[5] KCP,[7] $CsAgCl_3$, and $Pt(NH_3)_2Cl_3$;[5,6] (ii) dimers involving two adjacent metal atoms, examples of which include Ti_4O_7,[2] $Li_{1+x}Ti_{2-x}O_4$,[12,21] $Na_xV_2O_5$,[2] and probably other Magnelli phases; (iii) small clusters of metal atoms, examples of which are Chevrel phases[13-15] $M_xMo_6S_8$ (M = Pb, La, . . . , Cd, Eu), consisting of clusters composed of six Mo atoms on an octahedra, MoN (with clusters of Mo atoms arranged on triangles), and MRh_4B_4 (with clusters of Rh atoms arranged on tetrahedra).

As far as the wide-band electrons are concerned, they couple to the narrow-band ones by way of hybridization. We study the effect of the local-pair formation on this hybridization and show that it leads to an effective coupling between the local pairs and pairs of wide-band electrons which can give rise to superconducting order involving both subsystems: the subsystem of narrow-band electrons and that of wide-band electrons.

Let us start with the basic Hamiltonian written as a sum of terms:

$$
\begin{aligned}
H &= H_c + H_d + H_{cd} + H_{\rm ph} + H_{d\text{-ph}} \ , \\
H_c &= \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} + \varepsilon_0 - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \tfrac{1}{2} \sum_{ij\sigma\sigma'} V^{cc}_{ij} n^c_{i\sigma} n^c_{j\sigma'} \ , \\
H_d &= \sum_{i\neq j,\sigma} T_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + (E_0 - \mu) \sum_{i\sigma} n^d_{i\sigma} \\
&\quad + U \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + \tfrac{1}{2} \sum_{i\neq j\sigma\sigma'} V^{dd}_{ij} n^d_{i\sigma} n^d_{j\sigma'} \ , \qquad (2.1) \\
H_{cd} &= I \sum_{i\sigma} (d^{\dagger}_{i\sigma} c_{i\sigma} + \text{H.c.}) + \tfrac{1}{2} \sum_{ij\sigma\sigma'} V^{cd}_{ij} n^d_{i\sigma} n^c_{j\sigma'} \ , \\
H_{\rm ph} &= \omega_0 \sum_i b^{\dagger}_i b_i, \quad H_{d\text{-ph}} = -\lambda \sum_{i\sigma} n^d_{i\sigma} (b^{\dagger}_i + b_i) \ ,
\end{aligned}
$$

which denote, in order, the Hamiltonian for the wide-band electrons, the narrow-band electrons, the hybridization and Coulomb interaction between narrow- and wide-band electrons, the phonons, and, finally, the interaction of the phonons with the narrow-band electrons. ε_0 and E_0 denote the site energies of wide- and narrow-band electrons, respectively. $\varepsilon_{\mathbf{k}}$ refers to the dispersion of the wide-band electrons and T_{ij} denotes the hopping integral of the narrow-band electrons. The wide- and narrow-band electrons are denoted by the operators c ($c^{\dagger}$) and d ($d^{\dagger}$), respectively. The number operators for these two types of electrons are denoted $n^c_{i\sigma}$ and $n^d_{j\sigma}$, where i,j refer to the effective lattice sites and σ to the spin of electrons. In the Coulomb interaction V^{dd}_{ij} between the narrow-band electrons at sites i and j, we split off the contribution arising from the on-site interaction $V^{dd}_{ii} \equiv U$, for the sake of clarity in our further analyses. The Coulomb interaction between wide-band electrons is denoted V^{cc}_{ij} and that between wide and narrow-band electrons V^{cd}_{ij}. For the hybridization we take the usual on-site hybridization, denoted I. As far as the phonons are concerned, we restrict ourselves from the outset to an ensemble of independent Einstein oscillations with frequency ω_0. In fact, this is quite realistic since in the case of strong and local coupling mostly the local modes couple to the charge density of the narrow-band electrons.[1] μ denotes the chemical potential.

In the above Hamiltonian we have retained all those terms which are of importance in influencing qualitatively the physical properties which we shall describe below. We have neglected in the above Hamiltonian the interaction of wide-band electrons with phonons which would lead to standard BCS coupling in order to clearly bring out the novel superconducting mechanism which is intrinsic to the model. We shall defer the discussion of such additional electron-phonon mechanisms to the last section.

Given the above starting Hamiltonian, we shall proceed in the following way. We consider ourselves from the outset to be in the limit of small-polaron formation. Hence, as a first step we shall rephrase the above Hamiltonian in terms of small polarons.

We shall find, moreover, small polarons arising from the narrow-band electrons will be unstable to pair formation (bipolarons) provided the electron-phonon coupling λ is large enough. Keeping this in mind we shall eliminate the hybridization between narrow- and wide-band electrons to lowest order by means of a generalized Schrieffer-Wolff transformation and obtain an effective coupling between local pairs of narrow-band electrons and pairs of wide-band electrons. We shall then discuss the various contributions of the effective Hamiltonian obtained in this way for the subsequent treatment of its properties in the superconducting and normal phases.

A. The small-polaron representation

In the case of strong electron-lattice interaction we can eliminate this interaction term to all orders in λ by the standard Lang-Firsov transformation,[28]

$$
\begin{aligned}
&\tilde{H} = UHU^{\dagger}, \quad U = \exp(-S_1) \ , \\
&S_1 = -(\lambda/\omega_0) \sum_{j\sigma} n^d_{j\sigma} (b_j - b^{\dagger}_j) \ ,
\end{aligned} \qquad (2.2)
$$

giving rise to

$$
\begin{aligned}
\tilde{H} &= H_c + \tilde{H}_d + \tilde{H}_{cd} + H_{\rm ph} \ , \\
\tilde{H}_d &= \sum_{i\neq j\sigma} T_{ij} \left[\exp\left[\frac{\lambda}{\omega_0} (\hat{\phi}_j - \hat{\phi}_i) \right] \right] d^{\dagger}_{i\sigma} d_{j\sigma} - (E_0 - \mu - \lambda^2/\omega_0) \sum_{i\sigma} n^d_{i\sigma} + (U - 2\lambda^2/\omega_0) \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + \tfrac{1}{2} \sum_{i\neq j\sigma\sigma'} V^{dd}_{ij} n^d_{i\sigma} n^d_{j\sigma'} \ , \qquad (2.3) \\
\tilde{H}_{cd} &= \sum_{i\sigma} \left\{ I \left[\exp\left[-\frac{\lambda}{\omega_0} \hat{\phi}_i \right] \right] d^{\dagger}_{i\sigma} c_{i\sigma} + \text{H.c.} \right\} + \tfrac{1}{2} \sum_{ij\sigma\sigma'} V^{cd}_{ij} n^d_{i\sigma} n^c_{j\sigma} + \tfrac{1}{2} \sum_{ij\sigma\sigma'} V^{cc}_{ij} n^c_{i\sigma} n^c_{j\sigma'} \ ,
\end{aligned}
$$

where $\hat{\phi}_i = b_i^\dagger - b_i$. We notice that in the polaron picture the hybridization and narrow-band hopping terms become multiplied by operators involving the lattice deformation. In a first approximation one takes the average over those operators over the unperturbed phonon eigenstates of $H_{\rm ph}$.[28] This gives rise to

$$\left\langle \exp\left[\pm \frac{\lambda}{\omega_0} \hat{\phi}_i \right] \right\rangle_0 \equiv \mathrm{Tr}\left[\rho \exp\left[\pm \frac{\lambda}{\omega_0} \phi_i \right] \right] = \exp(-g^2/2) ,$$

$$\left\langle \exp\left[\frac{\lambda}{\omega_0} (\hat{\phi}_i - \hat{\phi}_j) \right] \right\rangle_0 = \left\langle \exp\left[\frac{\lambda}{\omega_0} \hat{\phi}_i \right] \right\rangle_0 \left\langle \exp\left[-\frac{\lambda}{\omega_0} \hat{\phi}_j \right] \right\rangle_0 = e^{-g^2} , \tag{2.4}$$

$$g^2 = \frac{\lambda^2}{\omega_0^2} \coth\left[\frac{\omega_0}{2k_B T} \right], \quad \rho = \exp(-H_{\rm ph}/k_B T)/\mathrm{Tr}[\exp(-H_{\rm ph}/k_B T)] .$$

We observe a strong exponential reduction of the hopping integral for narrow-band electrons and of the hybridization constant,

$$T_{ij} \to \tilde{T}_{ij} = T_{ij} \exp(-g^2), \quad I \to \tilde{I} = I \exp(-g^2/2) , \tag{2.5}$$

which in the limit of interest ($k_B T \ll \omega_0$) are temperature-independent quantities. Moreover, the center of the narrow band of electrons is shifted downwards and the on-site Coulomb interaction between them is reduced,

$$E_0 \to \tilde{E}_0 = E_0 - E_p, \quad U \to \tilde{U} = U - 2E_p , \tag{2.6}$$

where $E_p = \lambda^2/\omega_0$ is the polaron ionization energy—the energy necessary to liberate a self-trapped narrow-band electron from its surrounding lattice deformation.

Provided the electron-phonon interaction is strong enough that the interpolaron interaction is attractive ($\tilde{U} < 0$) and $|\tilde{U}| > \tilde{T}_{ij}$, $\tilde{I}$ polarons are unstable to local-pair formation. In this case all the single-polaron operators will disappear from the Hamiltonian, which in the end will contain only operators designating bound-polaron pairs.

B. Generalized Schrieffer-Wolff transformation

Our next aim will be to rephrase the initial Hamiltonian—the periodic Anderson model in the presence of a strong local interaction between the narrow-band electrons and the lattice—in terms of a picture in which these electrons occur exclusively in the form of bound states of pairs of them. It is therefore natural to eliminate the hybridization term to lowest order, which will give us an effective hybridization between pairs of narrow- and wide-band electrons. The generalized Schrieffer-Wolff transformation which will do that is highly reliable in our case. This is because—to a first approximation—we can take the zero-bandwidth limit for the narrow-band electrons ($\tilde{T}_{ij} \to 0$) due to the strong reduction of the bare hopping integral [$T_{ij} \to \tilde{T}_{ij} \ll T_{ij}$, Eq. (2.5)], and because of the smallness of the renormalized hybridization constant: $I \to \tilde{I} \ll I$ and $\tilde{T}_{ij} \ll \tilde{I}$.

The canonical transformation $U = e^{-S_2}$ which will eliminate the hybridization to lowest order is determined by[29,30]

$$[S_2, H_0] + H_1 = 0 , \tag{2.7}$$

where we have already set equal to zero the strongly reduced narrow-band electron hopping integral.

In Eq. (2.7) we use the notation where

$$\tilde{H} = H_0 + H_1 + H_C, \quad H_1 = \tilde{I} \sum_{i\sigma} (c_{i\sigma}^\dagger d_{i\sigma} + \mathrm{H.c.}) , \tag{2.8}$$

$$H_0 = (\tilde{E}_0 - \mu) \sum_{i\sigma} n_{i\sigma}^d + \tilde{U} \sum_i n_{i\uparrow}^d n_{i\downarrow}^d + \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} + \varepsilon_0 - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} ;$$

H_C denotes all the Coulomb-interaction terms proportional to V_{ij}^{cc}, V_{ij}^{cd}, and V_{ij}^{dd} ($i \neq j$).

The condition (2.7) determines S_2 to be equal to

$$S_2 = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}i\sigma\alpha} [\tilde{I}/(\varepsilon_{\mathbf{k}} + \varepsilon_0 - \varepsilon_\alpha)] (c_{\mathbf{k}\sigma}^\dagger n_{i,-\sigma}^\alpha d_{i\sigma}^\alpha e^{i\mathbf{k}\cdot\mathbf{R}_i} - \mathrm{H.c.}) ,$$

$$\varepsilon_\alpha = \tilde{E}_0 + \tilde{U}, \quad n_{i,-\sigma}^\alpha = n_{i,-\sigma}^d \quad \text{for } \alpha = + ,$$

$$\varepsilon_\alpha = \tilde{E}_0, \quad n_{i,-\sigma}^\alpha = 1 - n_{i,-\sigma}^d \quad \text{for } \alpha = - . \tag{2.9}$$

After eliminating the hybridization term, to lowest order we obtain the following Hamiltonian:

$$\mathcal{H} = e^{S_2} \tilde{H} e^{-S_2} = H_0 + H_C + H_2 + [S_2, H_C] + \cdots . \tag{2.10}$$

The term $[S_2, H_C]$ in the effective Hamiltonian (2.10) amounts to a small correction to the unrenormalized Coulomb interaction H_C and we shall in the following neglect it. This is justified in the large-$\tilde{U}$ limit: $|\tilde{U}| \gg V_C$ [$V_C = V_{ij}^{dd}$ ($i \neq j$), V_{ij}^{cc}, V_{ij}^{cd}], where the terms arising from the commutator $[S_2, H_C]$ have a coupling strength of the order of $\tilde{I} V_C / |\tilde{U}|$ which is much smaller than V_C.

$H_2 \equiv \frac{1}{2}[S_2, H_1]$ can then be written as the following sum of terms:

$$H_2 = H_{\rm charge} + H_{\rm hopping} + H_{\rm direct} + H_{\rm exchange} ,$$

$$H_{\rm charge} = -\sum_i I_0 (\rho_i^+ Q_i^- + Q_i^+ \rho_i^-) - \tfrac{1}{2} \sum_{i \neq j} I_{ij} [\rho_i^- (c_{j\uparrow}^\dagger c_{i\uparrow}^\dagger + c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger) + \mathrm{H.c.}] ,$$

$$H_{\rm hopping} = \sum_{i\sigma} (2W_0 + I_0 n_{i,-\sigma}^d) n_{i\sigma}^d + \sum_{i \neq j,\sigma} 2W_{i-j} d_{i\sigma}^\dagger d_{j\sigma} + \tfrac{1}{2} \sum_{i \neq j,\sigma} I_{i,-j} (n_{i-\sigma}^d + n_{j-\sigma}^d) d_{i\sigma}^\dagger d_{j\sigma} , \tag{2.11}$$

$$H_{\text{direct}}=-2W_0\sum_{i\sigma}n_{i\sigma}^{c}-\tfrac{1}{2}I_0\sum_i(2\rho_i^z+1)(2Q_i^z+1)$$
$$-\sum_{i\neq j,\sigma}W_{i,-j}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})-\tfrac{1}{2}\sum_{i\neq j,\sigma}I_{i,-j}\{[(2\hat{\rho}_i^z+1)+(2\hat{\rho}_j^z+1)]c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.}\}\ ,$$
$$H_{\text{exchange}}=I_0\sum_i(S_i^+\sigma_i^-+S_i^-\sigma_i^+ +2S_i^z\sigma_i^z)+\tfrac{1}{2}\sum_{i\neq j}I_{i,-j}S_i^+(c_{j\downarrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{j\uparrow})+S_i^-(c_{j\uparrow}^{\dagger}c_{i\downarrow}+c_{i\uparrow}^{\dagger}c_{j\downarrow})$$
$$+\tfrac{1}{2}\sum_{i\neq j}I_{i,-j}S_i^z(c_{j\uparrow}^{\dagger}c_{i\uparrow}+c_{i\uparrow}^{\dagger}c_{j\uparrow}-c_{j\downarrow}^{\dagger}c_{i\downarrow}-c_{i\downarrow}^{\dagger}c_{j\downarrow})\ .$$

The various coupling constants are defined by

$$I_0=-\frac{1}{N}\sum_{\mathbf{k}}I_{\mathbf{k}},\quad W_0=-\frac{1}{N}\sum_{\mathbf{k}}W_{\mathbf{k}}\ ,$$
$$I_{i,-j}=-\frac{1}{N}\sum_{\mathbf{k}}I_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\ ,$$
$$W_{i,-j}=-\frac{1}{N}\sum_{\mathbf{k}}W_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\ , \tag{2.12}$$
$$I_{\mathbf{k}}=\tilde{I}^2\left[\frac{1}{\varepsilon_{\mathbf{k}}+\varepsilon_0-\tilde{E}_0-\tilde{U}}+\frac{1}{\tilde{E}_0-\varepsilon_{\mathbf{k}}-\varepsilon_0}\right]\ ,$$
$$W_{\mathbf{k}}=\tfrac{1}{2}\tilde{I}^2\frac{1}{\varepsilon_{\mathbf{k}}+\varepsilon_0-\tilde{E}_0}\ .$$

The charge operators $\boldsymbol{\rho}$ and $\mathbf{Q}$ for narrow- and wide-band electrons, as well as the spin operators $\mathbf{S},\boldsymbol{\sigma}$ for these two types of electrons, are defined by

$$\rho_i^z=\tfrac{1}{2}(n_{i\uparrow}^d+n_{i\downarrow}^d-1),\quad Q_i^z=\tfrac{1}{2}(n_{i\uparrow}^c+n_{i\downarrow}^c-1)\ ,$$
$$\rho_i^+=d_{i\uparrow}^{\dagger}d_{i\downarrow}^{\dagger},\quad Q_i^+=c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\ ,$$
$$\rho_i^-=d_{i\downarrow}d_{i\uparrow},\quad Q_i^-=c_{i\downarrow}c_{i\uparrow}\ , \tag{2.13}$$
$$S_i^z=\tfrac{1}{2}(n_{i\uparrow}^d-n_{i\downarrow}^d),\quad \sigma_i^z=\tfrac{1}{2}(n_{i\uparrow}^c-n_{i\downarrow}^c)\ ,$$
$$S_i^+=d_{i\uparrow}^{\dagger}d_{i\downarrow},\quad \sigma_i^+=c_{i\uparrow}^{\dagger}c_{i\downarrow}\ ,$$
$$S_i^-=d_{i\downarrow}^{\dagger}d_{i\uparrow},\quad \sigma_i^-=c_{i\downarrow}^{\dagger}c_{i\uparrow}\ .$$

The physical meaning of the various terms in H_2 [Eq. (2.11)] is as follows.

The first term (H_{charge}) represents the transverse component of the charge-charge coupling between the two subsystems which is crucial for the superconducting mechanism which we want to study in this paper. It may be useful to rewrite this term in k space for the narrow-band electrons,

$$H_{\text{charge}}=\frac{1}{2N}\sum_{i\mathbf{k}\mathbf{k}'}(I_{\mathbf{k}}+I_{-\mathbf{k}'})$$
$$\times(c_{\mathbf{k}'\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}d_{i\downarrow}d_{i\uparrow}e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{R}_i}+\text{H.c.})\ ,$$

from which we notice the superconducting-like coupling of the local pairs $d_{i\uparrow}^{\dagger}d_{i\downarrow}^{\dagger}$ to the Cooper pairs of the wide-band electrons $c_{\mathbf{k}'\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}$.

The second term (H_{hopping}) represents the shift in the site energy and renormalization of on-site interaction between the narrow-band electrons—a contribution which will be absorbed into H_0. The last two terms of H_{hopping} represent the hybridization-induced (correlated) hopping of narrow-band electrons.

The third term (H_{direct}) presents the shift in the site energy of the wide-band electrons and the longitudinal part of the charge-charge coupling between the two subsystems and the hybridization-induced hopping of wide-band electrons.

Finally, the last term (H_{exchange}) describes the magnetic exchange interaction between the two subsystems.

C. The limit of strong local attraction

Our main objective here is to study the limit of strong attraction between polarons formed by the narrow-band electrons. In this limit we can neglect in the Hamiltonian (2.11) all terms proportional to I_{ij} ($i\neq j$) being much smaller than I_0 ($I_0<0$ for $\tilde{U}<0$). One can see this from Eq. (2.12), where one can replace $\varepsilon_{\mathbf{k}}+\varepsilon_0$ by $\varepsilon_F\simeq\tilde{E}_0+\tilde{U}/2$, provided $|\tilde{U}|\gg\tilde{E}_0\gg 2D$—the bandwidth of the wide-band electrons (the energy is measured from the bottom of the width band). We shall point out that the pinning of the Fermi energy at $\tilde{E}_0+\tilde{U}/2$ holds for any density of narrow-band electrons only in the case of $\tilde{U}<0$. For $\tilde{U}>0$ this pinning at $\tilde{E}+\tilde{U}/2$ only occurs for an exactly half-filled narrow band.[31]

The same argument as developed above for I_{ij} holds also for W_{ij} and, hence, the hybridization-induced hopping of wide- and narrow-band electrons is very small. For wide-band electrons this hybridization-induced hopping can therefore be neglected against the direct hopping contained in $\sum_{k\sigma}\varepsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$. On the contrary, for narrow-band electrons this contribution presents the lowest-order nonvanishing term for narrow-band electron hopping, since previously the direct hopping $\sim\tilde{T}_{ij}$ was taken to be negligibly small compared to the hybridization term $\sim\tilde{I}$ [see Eq. (2.5)].

Let us now come to the derivation of the effective Hamiltonian which we obtain in the large-negative-$\tilde{U}$ limit in which all narrow-band electrons are in bound states of pairs. In this case we can restrict ourselves to the subspace of effective sites which are either empty or occupied by two polarons, i.e., $n_{i\uparrow}^d+n_{i\downarrow}^d=0$ or 2, and the sites containing single polarons will be excluded. For this purpose let us rewrite our effective Hamiltonian $\mathcal{H}$, (2.10), after the omission of terms discussed above, and regrouping the remainder, in the following way:

$$\mathcal{H}=\bar{H}_0+H_{\text{I}}+H_{\text{II}}+H_{\text{III}}\ ,$$
$$\bar{H}_0=(\tilde{E}_0-\mu+2W_0)\sum_{i\sigma}n_{i\sigma}^d+(\tilde{U}+2I_0)\sum_i n_{i\uparrow}^d n_{i\downarrow}^d$$
$$+(\varepsilon_0-\mu-2W_0)\sum_{i\sigma}n_{i\sigma}^c+\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}\ ,$$

$$H_{\rm I}=-\sum_i I_0(Q_i^+\rho_i^- +{\rm H.c.})$$
$$-\tfrac{1}{2}I_0\sum_i (n_{i\uparrow}^d+n_{i\downarrow}^d)(n_{i\uparrow}^c+n_{i\downarrow}^c)+H_C\ , \qquad (2.14)$$
$$H_{\rm II}=\sum_{i\neq j,\sigma} 2W_{ij}(d_{i\sigma}^\dagger d_{j\sigma}+{\rm H.c.})\ ,$$
$$H_{\rm III}=I_0\sum_i \mathbf{S}_i\cdot\boldsymbol{\sigma}_i\ .$$

In the limit of strong on-site attraction ($\tilde{U}<0$, $|\tilde{U}|\gg W_{ij}, I_0, V_{ij}^{cc}, V_{ij}^{cd}, V_{ij}^{dd}$), it is sufficient to consider $H_{\rm I}$, $H_{\rm II}$, and $H_{\rm III}$ as perturbations and to work to the lowest nontrivial order in $\{I_0/|\tilde{U}|, W_{ij}/|\tilde{U}|,\ldots\}$, i.e., to first order in $H_{\rm I}$ and to second order in $H_{\rm II}$. The spin operators $\mathbf{S}_i$, involving single-electron occupation of sites, are eliminated in the subspace considered and $H_{\rm III}$ does not contribute to the effective Hamiltonian, which in its final form is

$$H_{\rm eff}=H_{\rm eff}^c+H_{\rm eff}^d+H_{\rm eff}^{cd}\ ,$$
$$H_{\rm eff}^c=(\bar{\varepsilon}_0-\mu)\sum_{i\sigma} n_{i\sigma}^c+\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$$
$$+\tfrac{1}{2}\sum_{ij\sigma\sigma'} V_{ij}^{cc}n_{i\sigma}^c n_{j\sigma'}^c\ ,$$
$$H_{\rm eff}^d=(\Delta_0-\mu)\sum_i (2\rho_i^z+1) \qquad (2.15)$$
$$-\sum_{i\neq j} J_{ij}[\tfrac{1}{2}(\rho_i^+\rho_j^- +\rho_j^+\rho_i^-)-\rho_i^z\rho_j^z]$$
$$+\tfrac{1}{2}\sum_{i\neq j} V_{ij}^{dd}(2\rho_i^z+1)(2\rho_j^z+1)\ ,$$
$$H_{\rm eff}^{cd}=|I_0|\sum_i(\rho_i^+c_{i\downarrow}c_{i\uparrow}+{\rm H.c.})$$
$$+\tfrac{1}{2}\sum_{ij} V_{ij}(2\rho_i^z+1)(n_{j\uparrow}^c+n_{j\downarrow}^c)\ ,$$

with the following definitions:

$$\bar{\varepsilon}_0=\varepsilon_0-2W_0\ ,$$
$$\Delta_0=\tilde{E}_0-\tfrac{1}{2}(|\tilde{U}|+2|I_0|)+2W_0\ ,$$
$$V_{ij}=(V_{ii}^{cd}+|I_0|)\delta_{ij}+V_{ij}^{cd}(1-\delta_{ij})\ , \qquad (2.16)$$
$$J_{ij}=\frac{2W_{ij}^2}{|\tilde{U}|+2|I_0|}\ .$$

In the subspace in which the Hamiltonian equation (2.15) is defined, the charge operators $\{\boldsymbol{\rho}_i\}$ given by (2.13) obey the Pauli spin-$\frac{1}{2}$ commutation relations, i.e.,

$$[\rho_i^-,\rho_j^+]_-=(1-2\rho_i^+\rho_i^-)\delta_{ij}=-2\rho_i^z\delta_{ij}\ ,$$
$$[\rho_i^{+\,(-)},\rho_j^{+\,(-)}]_-=0,\quad \rho_i^+\rho_i^-=\rho_i^z+\tfrac{1}{2}\ , \qquad (2.17)$$

and the following relations are fulfilled:

$$n_{i\uparrow}^d+n_{i\downarrow}^d=2\rho_i^z+1,\quad n_{i\uparrow}^d n_{i\downarrow}^d=\tfrac{1}{2}+\rho_i^z$$
$$[(n_{i\uparrow}-n_{i\downarrow})^2=0]\ . \qquad (2.18)$$

In the following we shall take the bottom of the wide band to have zero energy, i.e., $\min(\varepsilon_{\mathbf{k}}+\bar{\varepsilon}_0)=0$. In that case Δ_0 measures the relative position of the local-pair level with respect to the bottom of the band of the wide-band electrons (see Fig. 1).

Expression (2.15) represents the effective Hamiltonian in final form, which we shall use in the subsequent analyses of its superconducting and normal-state properties. This Hamiltonian was derived step by step from our starting Hamiltonian (2.1) describing a generalized Anderson Hamiltonian in the presence of strong coupling between the narrow-band electrons and the lattice. In this derivation rather stringent conditions on various parameters were required. In particular, the applicability of the Schrieffer-Wolff transformation requires that the initial bandwidth of narrow-band electrons, $\sim\tilde{T}_{ij}$ (before this transformation), must not only be smaller than $\tilde{I}$ but also smaller than the effective coupling I_0 which results from this transformation. Moreover, neglecting all the terms $\sim I_{ij}$ in expression (2.11) requires $2D\ll\tilde{E}_0\ll|\tilde{U}|$ [see Eq. (2.12)].

We want to stress that these conditions are sufficient conditions rather than necessary ones and that, in general, we can expect the structure of the Hamiltonian (2.15) to hold in a much wider range of parameters and, in particular, in the case $\tilde{T}>\tilde{I}$. That this is true can easily be seen when treating our starting Hamiltonian (2.1) in the limit of zero hybridization, $\tilde{I}=0$. In that case the Hamiltonian (2.15) can be derived with $J_{ij}\simeq 2\tilde{T}_{ij}^{\,2}/|\tilde{U}|$.[1,3,4,32]

Hence, in the following we shall treat the various coupling constants occurring in $H_{\rm eff}$ as parameters permitting J_{ij} to be either bigger or smaller than I_0, which will distinguish between two distinct physical situations as far as the superconductivity is concerned.

To conclude this section on the derivation of an effective Hamiltonian in the large-negative-$\tilde{U}$ limit, a few comments might be in order to compare this situation with the one for large positive $\tilde{U}$. In that case, if one assumes $n>1$ and takes $-E_0$ and $E_0+\tilde{U}$ to be larger than the bandwidth (i.e., the limit in which the Schrieffer-Wolff transformation is applicable for $\tilde{U}>0$), the Hamiltonian

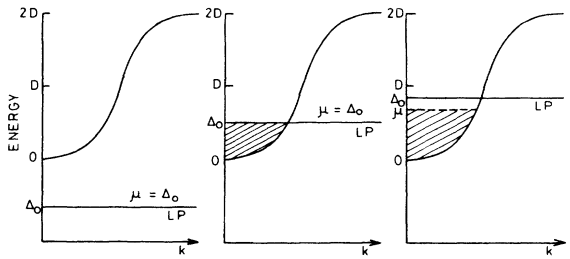

FIG. 1. The relative position of the local-pair (LP) level Δ_0 with respect to the bottom of the wide band of electrons in the absence of any interaction effects. $\Delta_0=\tilde{E}_0-\frac{1}{2}|\tilde{U}|$, μ denotes the chemical potential. (a) $\Delta_0<0$. In the ground state only LP states are occupied. (b) $0<\Delta_0=\mu$. In the ground state, both the single-particle states of wide-band electrons and the local-pair states are occupied. (c) $\mu<\Delta_0$. In the ground state only the single-particle states of wide-band electrons are occupied.

(2.11) and (2.12) can be reduced to

$$H_{\text{eff}}=\sum_{\mathbf{k}\sigma}(\varepsilon_{\mathbf{k}}+\bar{\varepsilon}_0-\mu)c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+H_{\text{exchange}}+\text{const}\ , \tag{2.19}$$

where H_{exch} is given by the corresponding expression in (2.10), with $\mathbf{S}_i$ being spin-$\frac{1}{2}$ operators. This is nothing but the Kondo-lattice Hamiltonian,[30,33] which is the sum of the usual Kondo Hamiltonians for each site plus extra terms proportional to $J_{i,-j}$ which describe correlated conduction-electron hopping and spin exchange on different sites. Contrary to $\tilde{U}<0$, in the case $\tilde{U}>0$, the density of both types of electrons is fixed at $n_2=(1/N)\sum_{i\sigma}\langle n^d_{i\sigma}\rangle=1$, $n_1=n-1$, for any $-E_0$, $E_0+\tilde{U}\gg 2D$, and $k_BT\ll D$. The appropriate coupling constants will be of the form

$$\begin{aligned} I_0&\sim\tilde{I}^2/(\varepsilon_F-\tilde{E}_0)+I^2/(\tilde{E}_0+\tilde{U}-\varepsilon_F)\ ,\\ W_0&\sim-\frac{\tilde{I}^2}{2}\Big/(\varepsilon_F-\tilde{E}_0)\ , \end{aligned} \tag{2.20}$$

where ε_F is the Fermi energy.

III. DETERMINATION OF THE FREE ENERGY

In this section we shall treat the effective Hamiltonian, Eq. (2.15), within the framework of a mean-field approximation and determine the corresponding free energy at finite temperature. Apart from homogeneous solutions for the mean-field ground state of our system, we also envisage symmetry-breaking solutions with a certain periodicity on the lattice. For this reason it is advantageous to introduce the following average values:

$$\begin{aligned} \rho^x_0&\equiv\frac{1}{N}\sum_i\langle\rho^x_i\rangle,\quad \rho^z_0=\tfrac{1}{2}(n_2-1)=\frac{1}{N}\sum_i\langle\rho^z_i\rangle\ ,\\ \rho^x_{\mathbf{Q}}&\equiv\frac{1}{N}\sum_i\langle\rho^x_i\rangle e^{i\mathbf{Q}\cdot\mathbf{R}_i},\quad \rho^z_{\mathbf{Q}}=\frac{1}{N}\sum_i\langle\rho^z_i\rangle e^{i\mathbf{Q}\cdot\mathbf{R}_i}\ ,\\ x_0&\equiv\frac{1}{N}\sum_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\rangle=\frac{1}{N}\sum_i\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}\rangle\ ,\\ x_{\mathbf{Q}}&\equiv\frac{1}{N}\sum_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k}+\mathbf{Q}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\rangle=\frac{1}{N}\sum_i\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}\rangle e^{i\mathbf{Q}\cdot\mathbf{R}_i}\ ,\\ n_1&=\frac{1}{N}\sum_{\mathbf{k}\sigma}\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle=\frac{1}{N}\sum_{i\sigma}\langle c^{\dagger}_{i\sigma}c_{i\sigma}\rangle\ ,\\ n_{\mathbf{Q}}&=\frac{1}{N}\sum_{\mathbf{k}\sigma}\langle c^{\dagger}_{\mathbf{k}+\mathbf{Q},\sigma}c_{\mathbf{k}\sigma}\rangle=\frac{1}{N}\sum_{i\sigma}\langle c^{\dagger}_{i\sigma}c_{i\sigma}\rangle e^{i\mathbf{Q}\cdot\mathbf{R}_i}\ . \end{aligned} \tag{3.1}$$

where $\mathbf{Q}$ is half a reciprocal-lattice vector and ρ^x_0 and $\rho^x_{\mathbf{Q}}$ as well as x_0 and $x_{\mathbf{Q}}$ denote the superconducting order parameters for local pairs and wide-band electrons, respectively. $\rho^z_{\mathbf{Q}}$ and $n_{\mathbf{Q}}$ are the corresponding charge-order parameters, and n_1 and n_2 denote average densities of wide- and narrow-band electrons, respectively. In the following we shall restrict ourselves exclusively to the uniform and two-sublattice-type orderings. In such a case the relevant thermal averages are translationally invariant in each sublattice, from which follows

$$\begin{aligned} \langle\rho^x_i\rangle&=\rho^x_0+\exp(i\mathbf{Q}\cdot\mathbf{R}_i)\rho^x_{\mathbf{Q}}\ ,\\ \langle\rho^z_i\rangle&=\rho^z_0+\exp(i\mathbf{Q}\cdot\mathbf{R}_i)\rho^z_{\mathbf{Q}}\ ,\\ \langle c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}\rangle&=x_0+\exp(i\mathbf{Q}\cdot\mathbf{R}_i)x_{\mathbf{Q}}\ ,\\ \sum_{\sigma}\langle c^{\dagger}_{i\sigma}c_{i\sigma}\rangle&=n_1+\exp(i\mathbf{Q}\cdot\mathbf{R}_i)n_Q\ . \end{aligned} \tag{3.2}$$

Following the Bogoliubov approach[4,34] and performing the corresponding factorization of the Hamiltonian (2.15) using relations (3.2), we obtain the following mean-field Hamiltonian:

$$\begin{aligned} H^{\text{MF}}&=C+H^{(d)}_0+H^{(c)}_0\ ,\\ C/N&=J_0(\rho^x_0)^2+J_{\mathbf{Q}}(\rho^x_{\mathbf{Q}})^2-K_0(\rho^z_0)^2-K_{\mathbf{Q}}(\rho^z_{\mathbf{Q}})^2-2\,|I_0|\,x_0\rho^x_0-2\,|I_0|\,x_{\mathbf{Q}}\rho^x_{\mathbf{Q}}\\ &\quad-V_0(\rho^z_0+\tfrac{1}{2})n_1-V_{\mathbf{Q}}\rho^z_{\mathbf{Q}}n_{\mathbf{Q}}-\tfrac{1}{2}V^{cc}_0n^2_1-\tfrac{1}{2}V^{cc}_{\mathbf{Q}}n^2_{\mathbf{Q}}-(\mu-\Delta_0-V^{dd}_0-\tfrac{1}{2}V_0n_1)\ ,\\ H^{(d)}_0&=-2\sum_i[(J_0\rho^x_0-|I_0|\,x_0)-(J_0\rho^x_{\mathbf{Q}}+|I_0|\,x_{\mathbf{Q}})e^{i\mathbf{Q}\cdot\mathbf{R}_i}]\rho^x_i\\ &\quad+2\sum_i[(K_0\rho^z_0+\tfrac{1}{2}V_0n_1)+(K_{\mathbf{Q}}\rho^z_{\mathbf{Q}}+\tfrac{1}{2}V_{\mathbf{Q}}n_{\mathbf{Q}})e^{i\mathbf{Q}\cdot\mathbf{R}_i}]\rho^z_i-2(\mu-\Delta_0-V^{dd}_0)\sum_i\rho^z_i\ ,\\ H^{(c)}_0&=\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c^{c}_{\mathbf{k}\sigma}+|I_0|\,\rho^x_0\sum_{\mathbf{k}}(c_{\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}+\text{H.c.})+|I_0|\,\rho^x_{\mathbf{Q}}\sum_{\mathbf{k}}(c_{-\mathbf{k}-\mathbf{Q}\downarrow}c_{\mathbf{k}\uparrow}+\text{H.c.})\\ &\quad+(V_{\mathbf{Q}}\rho^z_{\mathbf{Q}}+V^{cc}_{\mathbf{Q}}n_{\mathbf{Q}})\sum_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma}c_{\mathbf{k}\sigma}-[\mu-\tfrac{1}{2}V_0(2\rho^z_0+1)-V^{cc}_0n_1-\bar{\varepsilon}_0]\sum_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\ . \end{aligned} \tag{3.3}$$

In Eq. (3.3) the following notation, together with Eq. (2.16), is used:

$$\begin{aligned} J_{\mathbf{q}}&=\sum_{j\,(\neq i)}J_{ij}\exp[i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)]\ ,\\ K_{\mathbf{q}}&=\sum_{j\,(\neq i)}K_{ij}\exp[i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)]\ , \end{aligned}$$

$$\begin{aligned} V_{\mathbf{q}}&=\sum_j V_{ij}\exp[i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)]\ ,\\ V^{cc}_{\mathbf{q}}&=\sum_j V^{cc}_{ij}\exp[i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)]\ ,\\ K_{ij}&=J_{ij}+2V^{dd}_{ij}\ , \end{aligned} \tag{3.4}$$

where K_{ij} denotes the effective density-density interaction for local pairs and V_{ij} [Eq. (2.16)] that between local pairs and wide-band electrons.

For the sake of simplicity, we shall restrict ourselves from now on to the study of systems which can be considered as being composed of two equivalent sublattices for which we have $\varepsilon_{\mathbf{k}}=-\varepsilon_{\mathbf{k}+\mathbf{Q}}$, $\mathbf{Q}$ being the reciprocal-lattice vector linking the two sublattices. After a straightforward diagonalization of the mean-field Hamiltonian (3.3), we obtain the following eigenvalues for $H_0^{(d)}$:

$$E_1^{\pm}=\pm\Delta_1, \quad E_2^{\pm}=\pm\Delta_2 ,$$
$$\Delta_1^2=[\mu-\Delta_0-V_0^{dd}-(K_0\rho_0^z+K_{\mathbf{Q}}\rho_{\mathbf{Q}}^z)-\tfrac{1}{2}(V_0n_1+V_{\mathbf{Q}}n_{\mathbf{Q}})]^2+[(J_0\rho_0^x-|I_0|x_0)-(J_0\rho_{\mathbf{Q}}^x+|I_0|x_{\mathbf{Q}})]^2 , \tag{3.5}$$
$$\Delta_2^2=[\mu-\Delta_0-V_0^{dd}-(K_0\rho_0^z-K_{\mathbf{Q}}\rho_{\mathbf{Q}}^z)-\tfrac{1}{2}(V_0n_1-V_{\mathbf{Q}}n_{\mathbf{Q}})]^2+[(J_0\rho_0^x-|I_0|x_0)+(J_0\rho_{\mathbf{Q}}^x+|I_0|x_{\mathbf{Q}})]^2 ,$$

and the following eigenvalues for $H_0^{(c)}$:

$$\omega_{1,4}(\mathbf{k})=\pm A_1(\mathbf{k}), \quad \omega_{2,3}(\mathbf{k})=\pm A_2(\mathbf{k}) , \tag{3.6}$$

where

$$A_{1,2}(\mathbf{k})=\{\varepsilon_{\mathbf{k}}^2+\bar{\mu}^2+Y^2+X^2+X_{\mathbf{Q}}^2\pm 2[\varepsilon_{\mathbf{k}}^2(\bar{\mu}^2+X_{\mathbf{Q}}^2)+\bar{\mu}^2Y^2+X_{\mathbf{Q}}^2X^2+2\bar{\mu}YXX_{\mathbf{Q}}]^{1/2}\}^{1/2} ,$$
$$X=|I_0|\rho_0^x, \quad X_{\mathbf{Q}}=|I_{\mathbf{Q}}|\rho_{\mathbf{Q}}^x, \quad Y=V_{\mathbf{Q}}\rho_{\mathbf{Q}}^z+V_{\mathbf{Q}}^{cc}n_{\mathbf{Q}}, \quad \bar{\mu}=\mu-\tfrac{1}{2}V_0n_2-V_0^{cc}n_1-\bar{\varepsilon}_0 .$$

We are now in a position to evaluate the free energy, for which we obtain (β denoting $1/k_BT$):

$$F_0/N=-(2\beta)^{-1}\ln[4\cosh(\beta\Delta_1)\cosh(\beta\Delta_2)]-(\beta)^{-1}\sum_{\mathbf{k}}\ln\{4\cosh[\beta A_1(\mathbf{k})/2]\cosh[\beta A_2(\mathbf{k})/2]\}$$
$$+\mu(n_1+n_2)-\bar{\mu}-(\mu-\Delta_0-V_0^{dd}-\tfrac{1}{2}V_0n_1)+J_0(\rho_0^x)^2+J_{\mathbf{Q}}(\rho_{\mathbf{Q}}^x)^2-K_0(\rho_0^z)^2-K_{\mathbf{Q}}(\rho_{\mathbf{Q}}^z)^2$$
$$-2|I_0|x_0\rho_0^x-2|I_0|X_{\mathbf{Q}}\rho_{\mathbf{Q}}^x-V_0(\rho_0^z+\tfrac{1}{2})n_1-V_{\mathbf{Q}}\rho_{\mathbf{Q}}^zn_{\mathbf{Q}}-\tfrac{1}{2}V_0^{cc}n_1^2-\tfrac{1}{2}V_{\mathbf{Q}}^{cc}n_{\mathbf{Q}}^2 . \tag{3.7}$$

In the remainder of this paper we shall examine the phase diagram and thermodynamic properties of the model as a function of Δ_0 (the relative position of the local-pair level with respect to the bottom of the band of the wide-band electrons), the total number of particles per site (n), and the various coupling constants.

IV. HOMOGENEOUS SUPERCONDUCTING PHASE

We shall begin this study with the case of the homogeneous superconducting phase for which $\rho_{\mathbf{Q}}^x=x_{\mathbf{Q}}=0$ and $\rho_{\mathbf{Q}}^z=n_{\mathbf{Q}}=0$, which implies absence of charge order. In this case the eigenvalues of H_0^d and H_0^c are given by

$$\Delta\equiv\Delta_1=\Delta_2, \quad A(\mathbf{k})\equiv A_1(\mathbf{k})=A_2(\mathbf{k}) , \tag{4.1}$$

with

$$\Delta^2=(\mu-\Delta_0-K_0\rho_0^z-V_0^{dd}-\tfrac{1}{2}V_0n_1)^2+(J_0\rho_0^x-|I_0|x_0)^2,$$
$$A^2(\mathbf{k})=(\varepsilon_{\mathbf{k}}-\bar{\mu})^2+(I_0\rho_0^x)^2 , \tag{4.2}$$
$$\bar{\mu}=\mu-\bar{\varepsilon}_0-\tfrac{1}{2}V_0(2\rho_0^z+1)-V_0^{ce}n_1 .$$

The resulting expression for the free energy then becomes

$$F_0/N=-\frac{1}{\beta}\ln 2\cosh(\beta\Delta)-\frac{2}{\beta N}\sum_{\mathbf{k}}\ln 2\cosh[\beta A(\mathbf{k})/2]+\mu(n_1+n_2)-\bar{\mu}-(\mu-\Delta_0-\tfrac{1}{2}V_0^{dd}-\tfrac{1}{2}V_0n_1)$$
$$+J_0(\rho_0^x)^2-K_0(\rho_0^z)^2-2|I_0|x_0\rho_0^x-V_0(\rho_0^z+\tfrac{1}{2})n_1-\tfrac{1}{2}V_0^{cc}n_1^2 . \tag{4.3}$$

Upon minimizing this free energy with respect to the variables ρ_0^x, x_0, and μ, we obtain the following self-consistent equations:

$$\rho_0^x=[(J_0\rho_0^x-|I_0|x_0)/2\Delta]\tanh(\beta\Delta) ,$$
$$x_0=-\frac{1}{2N}\sum_{\mathbf{k}}\frac{|I_0|\rho_0^x}{A(\mathbf{k})}\tanh\left[\frac{\beta A(\mathbf{k})}{2}\right] , \tag{4.4}$$
$$n=n_1+n_2 ,$$

where

$$n_2-1=2\rho_0^z=[(\mu-\Delta_0-K_0\rho_0^z-V_0^{dd}-\tfrac{1}{2}V_0n_1)/\Delta]\tanh(\beta\Delta),$$
$$n_1-1=\frac{-1}{N}\sum_{\mathbf{k}}\frac{\varepsilon_{\mathbf{k}}-\bar{\mu}}{A(\mathbf{k})}\tanh\left[\frac{\beta A(\mathbf{k})}{2}\right] .$$

We shall now analyze the superconducting phase in the absence of any density-density coupling terms. In Sec. VI we shall show that, provided $K_{ij},V_{ij},V_{ij}^{cc}\ll D$ (D being the half-bandwidth), their effective does not change the qualitative features of the superconducting phase.

In order to appreciate the characteristic difference in

the superconducting properties due to the two distinct mechanisms involved here, we shall study the ground-state and finite-temperature phase diagrams first, for each of the mechanisms $J_0 \neq 0, I_0 = 0$ and $I_0 \neq 0, J_0 = 0$ separately, and, finally, when they both are at work ($J_0 \neq 0, I_0 \neq 0$).

A. $J_0 \neq 0, I_0 = 0$

In the absence of hybridization our system is described as an ensemble of $n_2/2$ hard-core bosons and n_1 fermions on a lattice. This case presents a generalization of a system studied earlier in which only bosons exist.[1,3,4] In the present case the number of bosons is no longer a constant, but will vary as a function of temperature such that both fermions and bosons are in thermal equilibrium, their total number, n being constant.[35]

The self-consistent equations (4.4) then reduce to

$$\Delta = \frac{J_0}{2}\tanh(\beta\Delta) ,$$
$$n_2 - 1 = 2\rho_0^z = [(\mu - \Delta_0)/\Delta]\tanh(\beta\Delta) , \tag{4.5}$$
$$n_1 - 1 = -\frac{1}{N}\sum_{\mathbf{k}} \tanh[\beta(\varepsilon_{\mathbf{k}} - \bar{\mu})/2] .$$

with $\Delta^2 = (\mu - \Delta_0)^2 + J_0(\rho_0^x)^2$.

In the following we make use of a model square density of states for the wide-band electron states,

$$N(\varepsilon) = \begin{cases} 1/2D & \text{for } 0 \le \varepsilon_{\mathbf{k}} + \bar{\varepsilon}_0 \le 2D , \\ 0 & \text{otherwise} , \end{cases} \tag{4.6}$$

with D denoting an effective half-bandwidth.

The self-consistent equations (4.5) can be solved analytically at $T=0$. These results are summarized in Figs. 2–4. In Fig. 2(a) we plot the ground-state phase diagram for n versus Δ_0/D for a fixed value of $J_0/2D = 0.25$. For comparison, we plot in Fig. 2(b) the same diagram in the absence of any superconducting coupling between the local pairs, $J_0 = 0$. In Figs. 3(a)–3(c) we plot the ground-state phase diagrams for $J_0/2D$ versus Δ_0/D for three values of n, 0.5, 1, and 2. The regions of local-pair superconductivity are determined by

$$-(J_0/2D)(n-1) < \Delta_0/D < J_0/2D + n .$$

Finally, in Figs. 4(a)–4(d) we plot the zero-temperature variation of n_1 and n_2 as a function of Δ_0/D for four values of n (1, 1.5, 2, and 2.5) and $J_0/2D = 0.05$. We also give in the same figure the variation of the superconducting order parameter ρ_0^x at zero temperature as a function of Δ_0/D.

Notice that, for $n \le 1$, ρ_0^x steadily increases upon increasing the number of local pairs, reaching a saturation value when the number of local pairs has attained its maximum value: $n_2 = n$. For $1 < n \le 2$, ρ_0^x has a maximum for $n_2 = 1$ (half-filled band of local pairs). Upon increasing n_2 above unity, ρ_0^x decreases, reaching a saturation value $\rho_0^x = \frac{1}{2}\sqrt{n(2-n)}$ when n_2 has become equal to n.

For $n=2$, $\rho_0^x = 0$ when n_2 reaches the two limiting values $n_2 = 0$ and 2 [Fig. 4(c)]. The reason for this behavior is clear since, indeed, neither for $n_2 = 0$ nor for $n_2 = 2$ can we have superconductivity. In the first case this is because there are no local pairs in the system and, in the second, because all the available sites are occupied by lo-

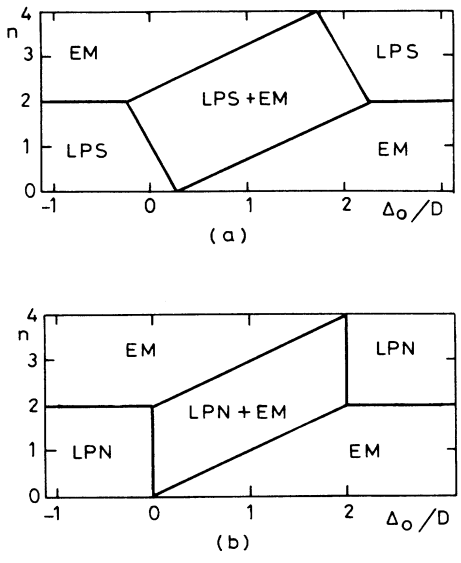

FIG. 2. Ground-state phase diagram for $J_0 \neq 0, I_0 = 0$ as a function of the total number of particles n, vs Δ_0/D for two characteristic values (a) $J_0/2D = 0.25$ and (b) $J_0/D = 0$. Notation: LPS (superconducting state of local pairs), EM (metallic state of wide-band electrons), and LPN (nonmetallic state of local pairs).

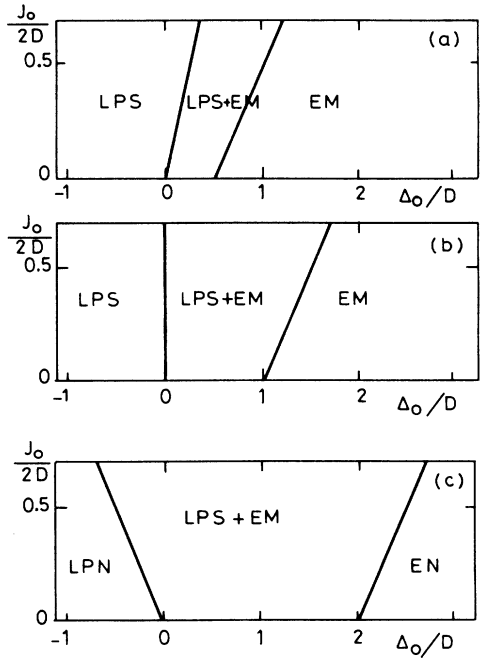

FIG. 3. Ground-state phase diagram for $J_0 \neq 0, I_0 = 0$ as a function of $J_0/2D$, vs Δ_0/D for three different values of n. (a) $n = 0.5$, (b) $n = 1$, and (c) $n = 2$. The same notation as in Fig. 2 is used, with EN denoting the nonmetallic state of the wide-band electrons.

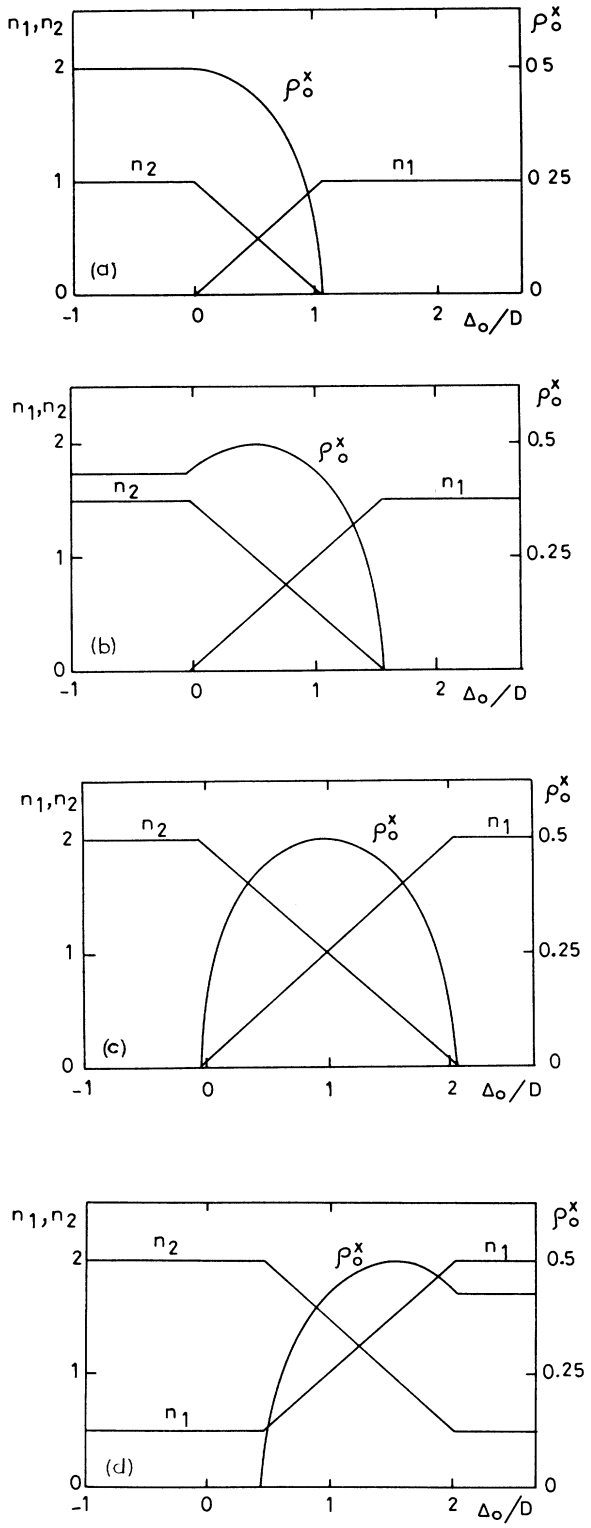

FIG. 4. Variation of n_1 (number of wide-band electrons), n_2 (number of narrow-band electrons in local-pair states), and the superconducting order parameter ρ_0^x for local pairs as a function of Δ_0/D at zero temperature and $J_0/2D=0.05, I_0=0$. (a) n $(=n_1+n_2)=1$, (b) $n=1.5$, (c) $n=2$, and (d) $n=2.5$.

cal pairs and hence they cannot move.

The transition at $\Delta_0=J_0/2+nD$ between the superconducting state with $n_2\neq 0$ and the nonordered state with $n_1=n$ is always second order. The same is true for $n=2$ at $\Delta_0=-J_0/2$ between the superconducting phase and the nonordered one with $n_2=2$. On the other hand, the transition for $n<2$ at $\Delta_0=-(J_0/2)(n-1)$ between the superconducting phase with $n_2=n$ and the superconducting phase with $n_2<n$ and $n_1>0$ is always of higher order.

Let us consider next the finite-temperature phase diagram. Upon eliminating the chemical potential in the last of the two equations (4.5), we obtain (within the temperature regime where the superconducting order is stable) the following equation determining the temperature dependence of the number of local pairs:

$$\Delta_0-2D-\frac{J_0}{2}(n_2-1) = \frac{1}{\beta}\ln\left[\frac{1-\exp[-(n-n_2)\beta D]}{\exp[(2-n+n_2)\beta D]-1}\right]-\frac{J_0}{2}n_2 . \quad (4.7)$$

From Eq. (4.5) we obtain, for the chemical potential,

$$\mu=\Delta_0+\frac{J_0}{2}(n_2-1) , \quad (4.8)$$

the temperature dependence of which is hence determined by the variation of n_2 with temperature.

The critical temperature T_c is obtained by taking the limit $\rho_0^x\to 0$ in Eqs. (4.5), yielding

$$k_B T_c=J_0[n_2(T_c)-1]/\ln\{n_2(T_c)/[2-n_2(T_c)]\} . \quad (4.9)$$

Equation (4.9) together with the solution of Eq. (4.7) determines T_c. In Fig. 5 we plot the numerical solutions of these equations, i.e., T_c as a function of Δ_0/D for several values of n and $J_0/2D=0.05$. It is interesting to notice the gradual changeover of the phase diagram as one departs from $n=2$ upon decreasing the number of particles. For $n=2$ the superconducting region is well confined between two limiting values of Δ_0/D: $-\frac{1}{2}J_0<\Delta_0<\frac{1}{2}J_0+2D$. For $n<2$, on the contrary, the superconducting phase extends over the entire region of $\Delta_0/D<\frac{1}{2}J_0+nD$, for sufficiently low temperatures. On the right-hand side of the phase diagram ($\frac{1}{2}J_0+nD\gtrsim\Delta_0$),

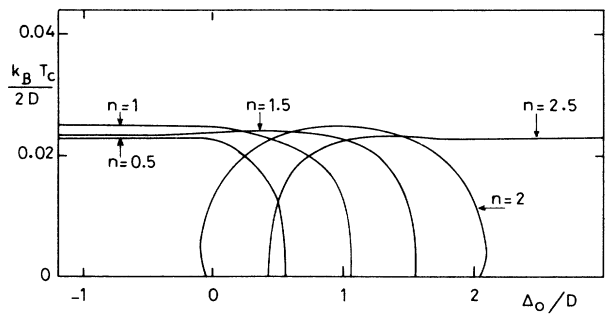

FIG. 5. The superconducting critical temperature as a function of Δ_0/D for five values of n ($=0.5$, 1, 1.5, 2, and 2.5) and $J_0/2D=0.05$, $I_0=0$. n denotes the total number of particles.

T_c drops off sharply like

$$T_c \sim -J_0/\ln n_2(0)$$
$$= -J_0/\ln\{(\tfrac{1}{2}J_0+nD-\Delta_0)/[(\tfrac{1}{2}J_0+D)]\}$$

as Δ_0 increases, tending to zero at $\Delta_0=\frac{1}{2}J_0+nD$. On the left-hand side of the phase diagram, T_c tends to a saturation value

$$T_c^*=J_0(n-1)/\ln[n/(2-n)]$$

as the number of local pairs tends to a saturation value as Δ_0/D decreases.

The overall picture of T_c which evolves is that upon increasing the number of local pairs (upon decreasing Δ_0/D) T_c first sharply rises before it either goes through a maximum and then decreases towards a finite saturation value T^* (the behavior for $n>1$) or continues to increase and saturates at T_c^* (the behavior for $n\leq 1$). Only for $n=2$, $T_c=0$ for any Δ_0 below $-\frac{1}{2}J_0$.

B. $J_0=0$, $I_0\neq 0$

In the case $J_0\neq 0$, $I_0=0$ studied previously, the system of local pairs was self-sufficient to produce a superconducting state. In the case $J_0=0$, $I_0\neq 0$, which we are going to study now, superconductivity can only occur provided both subsystems (the local pairs and the wide-band electrons) participate in its formation.[36] This happens in the following way. Due to hybridization of localized and wide-band electrons, the pair state of localized electrons induces pairing of the wide-band electrons on the same site. This spontaneous creation of wide-band electron pairs occurs randomly on any individual lattice site. At any given moment we find that a given site is either empty or occupied by a pair of electrons which are either localized or wide-band electrons. What leads to an ordered superconducting state of these pairs is the itinerancy of the wide-band electrons which lead to effective superconducting interactions of the form $Q_i^+Q_j^-+\text{H.c.}$ for the wide-band electrons and $\rho_i^+\rho_j^-+\text{H.c.}$ for the local pairs. Superconductivity is then controlled by two order parameters, $\rho_0^x=(1/N)\sum_i\langle\rho_i^+\rangle$ and $x_0=(1/N)\sum_i\langle Q_i^+\rangle$, both of which are finite in the superconducting state and which jointly tend to zero as the critical temperature is approached.

As before, we write the free-energy and self-consistent equations determining the order parameters and the chemical potential:

$$F_0/N=-(1/\beta)\ln(2\cosh\{\beta[(\mu-\Delta_0)^2+(I_0x_0)^2]^{1/2}\})$$
$$-\frac{2}{\beta N}\sum_{\mathbf{k}}\ln\left[2\cosh\left\{\frac{\beta}{2}[(\varepsilon_{\mathbf{k}}-\bar{\mu})^2+(I_0x_0)^2]^{1/2}\right\}\right]+\mu n-(2\mu-\Delta_0)-2|I_0|\rho_0^x x_0\ ,$$
$$\rho_0^x=-\{|I_0|x_0/2[(\mu-\Delta_0)^2+(I_0x_0)^2]^{1/2}\}\tanh\{\beta[(\mu-\Delta_0)^2+(I_0x_0)^2]\}\ ,$$
$$x_0=-\left[\frac{1}{2N}\right]\sum_{\mathbf{k}}\{(|I_0|\rho_0^x)/[(\varepsilon_{\mathbf{k}}-\bar{\mu})^2+(I_0\rho_0^x)^2]^{1/2}\}\tanh\left[\frac{\beta}{2}[(\varepsilon_{\mathbf{k}}-\bar{\mu})+(I_0\rho_0^x)^2]^{1/2}\right]\ , \tag{4.10}$$
$$n_2-1=\frac{\mu-\Delta_0}{[(\mu-\Delta_0)^2+(I_0x_0)^2]^{1/2}}\tanh\{\beta[(\mu-\Delta_0)^2+(I_0x_0)^2]^{1/2}\}\ ,$$
$$n_1-1=-\frac{1}{N}\sum_{\mathbf{k}}\frac{\varepsilon_{\mathbf{k}}-\bar{\mu}}{[(\bar{\mu}-\Delta_0)^2+(I_0\rho_0^x)^2]^{1/2}}\tanh\left[\frac{\beta}{2}[(\bar{\mu}-\Delta_0)^2+(I_0\rho_0^x)^2]^{1/2}\right]\ .$$

Let us first consider the ground-state properties of this system. Taking the limit $T\to 0$ in Eqs. (4.10), we obtain, with the use of the square density of states, Eq. (4.6),

$$\rho_0^x=-\frac{|I_0|x_0}{2[(\mu-\Delta_0)^2+(I_0x_0)^2]^{1/2}}\ ,$$
$$\frac{2x_0}{|I_0|\rho_0^x}=-\frac{1}{2D}\ln\left[\frac{2D-\mu+[(2D-\mu)^2+(I_0\rho_0^x)^2]^{1/2}}{\mu+[\mu^2+(I_0\rho_0^x)^2]^{1/2}}\right]\ ,$$
$$n_2-1=\frac{\mu-\Delta_0}{[(\mu-\Delta_0)^2+(I_0\rho_0^x)^2]^{1/2}}\ , \tag{4.11}$$
$$n_1-1=-\frac{1}{2D}\{[(2D-\mu)^2+(I_0\rho_0^x)^2]^{1/2}-[\mu^2+(I_0\rho_0^x)^2]^{1/2}\}\ ,$$
$$F_0/N(\beta\to\infty)=E_{\mathrm{GS}}=[(\mu-\Delta_0)^2+(I_0x_0)^2]^{1/2}-\frac{1}{2D}\int_0^{2D}d\varepsilon[(\varepsilon-\mu)^2+(I_0\rho_0^x)^2]^{1/2}+\mu n-(2\mu-\Delta_0)-2|I_0|\rho_0^x x_0\ .$$

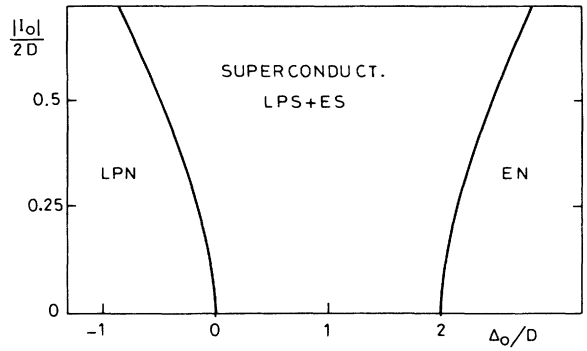

FIG. 6. Ground-state phase diagram for $n=2$, $J_0=0$ (n being the total number of particles), as a function of $|I_0|/2D$, vs Δ_0/D. LPS+ES denotes the superconducting state involving both local pairs and wide-band electrons. LPN and EN indicate the nonmetallic states of local pairs and wide-band electrons, respectively.

The ground-state (GS) chemical potential explicitly reads

$$\frac{\mu}{D}-1=-\omega\{[1+I_0^2(\rho_0^x/D)^2-\omega^2]/(1-\omega^2)\}^{1/2}\ ,$$

$$\omega=-[1-(2\rho_0^x)^2]^{1/2}+2-n \quad \text{for } n\neq 2\ ,$$

and

$$\left[\frac{\mu}{D}-1\right]^2=[1-(2\rho_0^x)^2][1+(I_0/2D)^2] \quad \text{for } n=2\ .$$

Numerical solution of these equations show that the superconducting state is always the ground state for all values of I_0/D and Δ_0/D for any value of n except $n=2$. For $n=2$, Eqs. (4.11) indicate second-order phase boundaries between the superconducting and normal phases which are insulating. In Fig. 6 we plot the ground-state phase diagram as a function of $|I_0|/2D$ versus Δ_0/D, for $n=2$. In Figs. 7(a)–7(c) we present the zero-temperature behavior of n_1, n_2, ρ_0^x, and x_0 for $|I_0|/2D=0.5$ and three different values for n.

Let us now investigate the phase diagram at finite temperature. For this purpose we shall evaluate T_c as a function of Δ_0/D assuming that the phase transition between the superconducting and the normal phase is second order. From Eq. (4.10) we obtain the following self-consistent equations for $T_c=1/k\beta_c$ and the chemical potential:

$$\frac{I_0^2}{8D}\left[\int_0^{2D} d\varepsilon \frac{\tanh[(\beta_c/2)(\varepsilon-\mu)]}{\varepsilon-\mu}\right]\frac{\tanh[\beta_c(\mu-\Delta_0)]}{\mu-\Delta_0}=1\ , \tag{4.12}$$

$$n-2=\tanh[\beta_c(\mu-\Delta_0)]-\frac{1}{D\beta_c}\ln\left[\frac{\cosh[\beta_c(2D-\mu)/2]}{\cosh(\beta_c\mu/2)}\right].$$

The numerical solutions of these equations are plotted for T_c versus Δ_0/D in Figs. 8(a) and 8(b) for two characteristic values of $|I_0|/2D$ (0.1, 0.5) and $n=0$, 5, 1, 1.5, and 2.

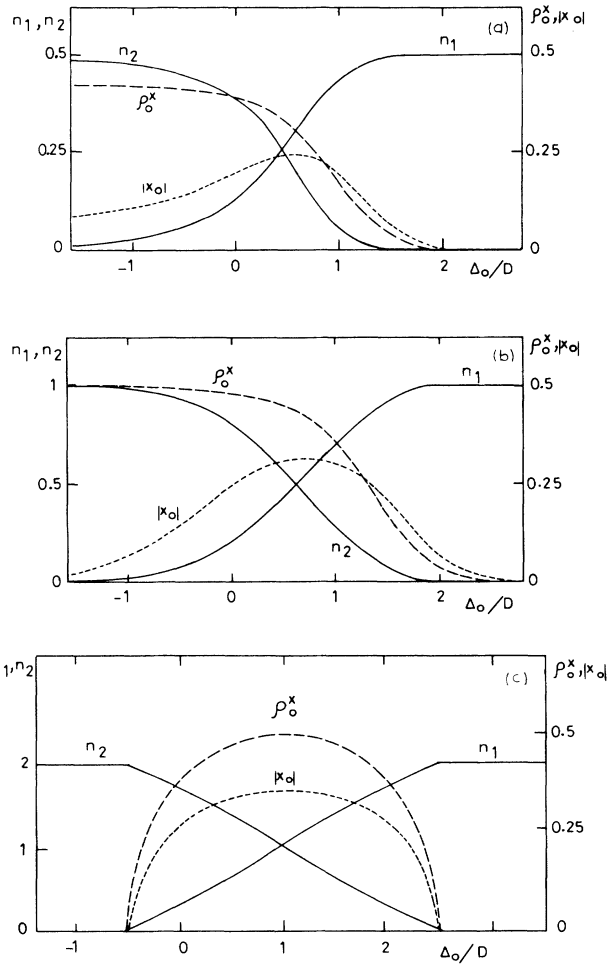

FIG. 7. Variation of n_1 (number of wide-band electrons), n_2 (number of narrow-band electrons in local-pair states), and the superconducting order parameters ρ_0^x and x_0 for local pairs and wide-band electrons as a function of Δ_0/D at zero temperature and $J_0=0$, $|I_0|/2D=0.5$. (a) n $(=n_1+n_2)=0.5$, (b) $n=1$, and (c) $n=2$.

From Figs. 7 and 8, we notice that, except for the case $n=2$, for which the superconducting phase is restricted to a finite interval in Δ_0/D, for any $n<2$ the superconducting state extends over the entire region of the parameter Δ_0/D. For large values of Δ_0/D we find that the number of local pairs is exponentially small but finite, which leads to exponentially small superconducting order parameters ρ_0^x and x_0. Upon decreasing Δ_0/D below some definite value of Δ_0/D, the number of local pairs very quickly changes from infinitesimally small values to finite values with a corresponding rise of the values for ρ_0^x and x_0. Depending on the value of n, we find that, upon decreasing Δ_0/D, ρ_0^x either monotonically increases and then saturates at a finite value, or first goes through a maximum and then saturates at a finite value. The first type of behavior occurs for $n<1$ and the second for $1<n<2$ with a maximum at a value for Δ_0/D where $n_1\simeq n_2$.

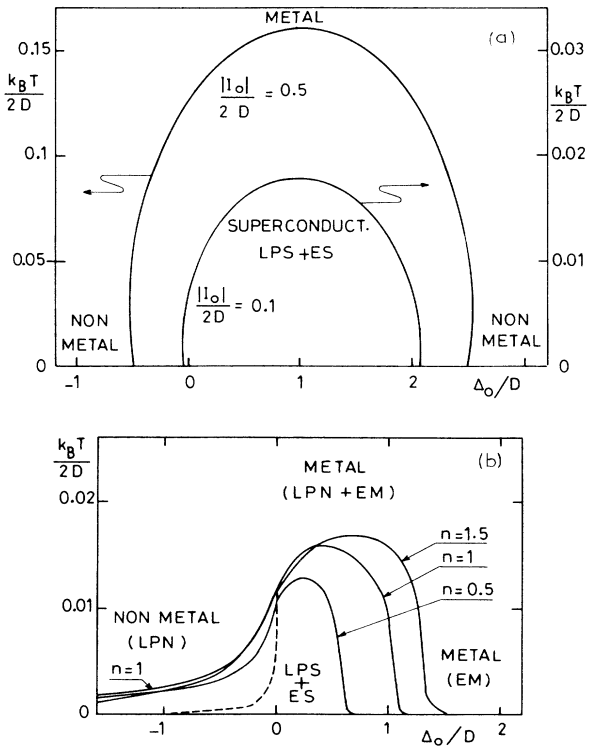

FIG. 8. Finite-temperature phase diagram as a function of Δ_0/D. (a) For two values of $|I_0|/2D$ (0.5, 0.1) and n (total number of particles)=2; (b) for $|I_0|/2D=0.1$ and $n=0.5$, 1, and 1.5. The dashed line (which on the scale presented is indistinguishable for all three cases of n) corresponds to T_c calculated by a perturbational approach for $\Delta_0 \lesssim 0$, see Eq. (4.20). LPS+ES denotes the superconducting state involving both local pairs and wide-band electrons. LPN stands for the nonmetallic state of only local pairs and EM indicates the metallic state of only wide-band electrons.

It is worthwhile to compare the two cases $J_0 \neq 0$, $I_0=0$ and $J_0=0$, $I_0 \neq 0$. In the first case superconductivity is due to coherent hopping of the bosons (local pairs) on the lattice. The hopping of bosons presents an intrinsic mechanism in this case. On the contrary, in the case $J_0=0$, $I_0 \neq 0$ direct boson hopping is absent. Bosons now move via an intermediate state where they have dissociated into pairs of wide-band electrons. Due to this, a superconducting order among the bosons involving coherent hopping of them induces an analogous coherent state among the wide-band electrons. Consequently, in the case $J_0=0$, $I_0 \neq 0$ a gap opens in the single-particle spectrum of the wide-band electrons, being equal to $E_g=2\min[(\varepsilon_k-\bar{\mu})^2+(I_0\rho_0^x)^2]^{1/2}$.

It is instructive to compare Figs. 4,5 and 7,8 far as T_c and the superconducting order parameter for the local pairs, ρ_0^x, are concerned. The superconducting order parameter at zero temperature for $n=2$ shows very similar behavior in the two cases. Starting from zero at some value of Δ_0/D for which n becomes zero, ρ_0^x goes through a maximum at $n_1=n_2=1$ upon increasing Δ_0/D and finally decreases to zero at some value of Δ_0/D for which n_2 becomes zero. For $n<2$ the right-hand parts of Figs. 4 and 7 are rather similar as far as ρ_0^x is concerned, except that, for $J_0 \neq 0$, $I_0=0$, ρ_0^x sharply drops to zero at $\Delta_0/D \sim n+J_0/2D$, while, for $J_0=0$, $I_0 \neq 0$, ρ_0^x starts to drop near $\Delta_0/D \sim n$, and $\Delta_0/D \sim n+J_0/2D$ then tends to zero asymptotically as Δ_0/D is further increased. Upon decreasing Δ_0/D below n, ρ_0^x and n_2 again show very similar behavior for both cases $J_0 \neq 0$, $I_0=0$ and $J_0=0$, $I_0 \neq 0$, except that for the first case both ρ_0^x and n_2 saturate at some given value of Δ_0/D, while for the second case this saturation value is approached asymptotically.

Let us next consider the variation of T_c as a function of Δ_0/D. For $n=2$ the behavior of T_c for the two cases $J_0 \neq 0$, $I_0=0$ and $J_0=0$, $I \neq 0$ is very similar and shows a small reentrance region [cf. Figs. 5 and 8(a)].

For $n<2$ we shall first discuss the case $J_0 \neq 0$, $I_0=0$ (see Fig. 5). Upon approaching $\Delta_0/D \simeq n+J_0+2D$ from below, T_c rapidly drops to zero. Upon decreasing Δ_0/D below $\Delta_0/D \lesssim n$, T_c first goes through a maximum and then drops and approaches a saturation value below $\Delta_0/D=0$ provided $1<n<2$. For $n<1$, T_c monotonically increases and approaches a saturation value as Δ_0/D is lowered. This behavior can easily be understood. T_c is maximal if the concentration of local pairs is equal to $\frac{1}{2}$ ($n_2=1$). For $n<1$ all particles are in states of local pairs for $\Delta_0/D<-J_0(n-1)/2$. Upon increasing Δ_0/D above zero, the number of electrons in the local-pair states is diminished, while the number of wide-band electrons is increased. Since here the superconductivity is exclusively due to the local pairs, T_c monotonically decreases as Δ_0/D increases from negative to positive values and becomes identically zero at $\Delta_0/D \simeq n+J_0/2D$, at which point the number of local pairs has dropped to zero. The case $1<n<2$ is somewhat different. For $\Delta_0/D<-J_0(n-1)/2$ there are $n_2=n$ electrons in pair states. Upon increasing Δ_0/D this number of electrons in pair states decreases, reaching a value of 1 at some Δ_0/D between 0 and n, and then further decreases to zero at $\Delta_0/D=n+J_0/2D$. Hence, upon increasing Δ_0/D from values below zero to $\Delta_0/D=n+J_0/2D$, we first notice a rise in T_c until Δ_0/D reaches the value for which $n_2=1$ and then drops to zero.

Let us now discuss the behavior of T_c for the case $J_0=0$, $I_0 \neq 0$ for $0<n<2$ [see Fig. 8(b)]. Upon approaching $\Delta_0/D=n$, we again find a very rapid drop of T_c, but contrary to the case $J_0 \neq 0$, $I_0=0$, T_c only tends to zero asymptotically as Δ_0/D is increased. Upon decreasing Δ_0/D below n, T_c first rises, goes through a maximum, and then drops off, slowly tending to zero as $\Delta_0/D \to -\infty$.

Our mean-field results seem to be quite plausible in the region $0<\Delta_0/D<n$. In contrast, the relative large values for T_c which we obtain for $J_0=0$, $I_0 \neq 0$ and $\Delta_0/D<0$ are rather surprising, given the fact that in this regime the number of wide-band electrons is very small. In order to test this result we adopt an approach which in this regime is superior to a mean-field treatment (if $|I_0| \ll D$ and is based on a perturbation approach). The idea is that in

this regime of Δ_0/D all the electrons are in local-pair states and thus the motion of those pairs can only come about by their dissociations into a virtual pair of wide-band electrons with an energy above one of the local pairs.

Let us for this purpose consider our Hamiltonian (2.15) in the absence of any density-density interparticle interaction as well as of the direct hopping term, and which, for clarity, we repeat here:

$$H=H_0+H_1 ,$$
$$H_0=(\Delta_0-\mu)\sum_i (2\rho_i^z+1)+\sum_{k\sigma}(\varepsilon_k-\bar{\mu})c_{k\sigma}^{\dagger}c_{k\sigma} , \tag{4.13}$$
$$H_1=|I_0|\sum_i (Q_i^{+}\rho_i^{-}+\rho_i^{+}Q_i^{-}) .$$

Our aim is to reformulate this Hamiltonian in terms of an effective hopping of local pairs via virtual excitations into wide-band states. For this purpose we eliminate, to first order, the contact interaction H_1 between local pairs and pairs of wide-band electrons. The unitary transformation which will do this is given by

$$U=e^{-S},S=\frac{I_0}{N}\sum_{jqp}\frac{e^{iq\cdot R_j}}{\bar{\varepsilon}_p+\bar{\varepsilon}_{q-p}-2\Delta_0}\rho_j^{-}c_{p\uparrow}^{\dagger}c_{q-p\downarrow}^{\dagger}-\text{H.c.} . \tag{4.14}$$

After the transformation of the Hamiltonian (4.13) one obtains a series of terms which are, in general, products of local pair operators ρ_i and wide-band electrons. In the regime of interest, i.e., $\Delta_0/D<0$, this rather complicated form of the transformed Hamiltonian is very much simplified and finally yields

$$\bar{H}=\bar{H}_0+\bar{H}_1 ,$$
$$\bar{H}_0=\sum_{k\sigma}(\varepsilon_k-\bar{\mu})c_{k\sigma}^{\dagger}c_{k\sigma}+2(\Delta_0-\mu-\tfrac{1}{2}\tilde{A})\sum_i\rho_i^z$$
$$+N(A(0)+\Delta_0-\mu) ,$$
$$\bar{H}_7=\tfrac{1}{2}\sum_{i\neq j}A(R_{ij})(\rho_i^{+}\rho_j^{-}+\rho_j^{+}\rho_i^{-})$$
$$=\frac{1}{2N}\sum_q\left[A_q-\frac{1}{N}\sum_k A_k\right](\rho_q^{+}\rho_q^{-}+\text{H.c.}) , \tag{4.15}$$

with

$$A(R_{ij})=\frac{1}{N}\sum_k e^{-k\cdot R_{ij}}A_k,$$
$$A_k=|I_0|^2\frac{1}{N}\sum_p\frac{n_p+n_{k+p}-1}{\bar{\varepsilon}_k+\bar{\varepsilon}_{k+p}-2\Delta_0} ,$$
$$\tilde{A}=\left[\frac{I_0}{N}\right]^2\sum_{kp}\frac{n_p+n_{k+p}-1-2n_pn_{k+p}}{\bar{\varepsilon}_p+\bar{\varepsilon}_{k+p}-2\Delta_0} , \quad \bar{\varepsilon}_k=\varepsilon_k+\varepsilon_0 . \tag{4.16}$$

In this derivation of the effective Hamiltonian we have, moreover, averaged over the wide-band electron degrees of freedom, which is justified as long as correlations between them can be neglected. For $\Delta_0/D<0$ this condition is trivially satisfied. This effective Hamiltonian describes long-range hopping of the local pairs—or, in pseudospin language, an indirect (Rudermann-Kittel-Kasuya-Yosida–type) interaction.

The essential new feature appearing in the Hamiltonian (4.15) is the self-energy correction $\sum_k A_k$, which is absent in the mean-field treatment of the contact interaction [Eq. (2.15)] applied in the bulk of this section. We shall see that this self-energy correction substantially modifies the behavior of T_c as a function of Δ_0/D. For this purpose we evaluate T_c on the basis of a mean-field treatment of the transformed Hamiltonian (4.15), which yields

$$k_BT_c=-\tilde{J}_0(n-1)/\ln[n/(2-n)] ,$$
$$\tilde{J}_0=|I_0|^2[A_{k=0}-A(0)] . \tag{4.17}$$

Evaluating $A_{k=0}$ and

$$A(R_{ij}=0)=\frac{1}{N}\sum_k A_k$$

with the use of the square density of states for the wide-band electrons, we obtain

$$A(0)=-\frac{1}{D}\left[\frac{x+1}{x}\ln(1+x)-\left[1+\frac{2}{x}\right]\ln\left[1+\frac{x}{2}\right]\right] ,$$
$$A_{k=0}=-\frac{1}{4D}\ln(x+1), \quad x=2D/|\Delta_0| . \tag{4.18}$$

A simple numerical analysis of $\tilde{J}_0$ as a function of Δ_0/D shows a very sharp drop of J_0 as Δ_0/D is lowered below zero, giving values for T_c well below those predicted by the mean-field treatment of the contact interaction. In Fig. 8(b) we plot this result (dashed line) for T_c, which finally leads to a picture for $n<2$ which is in fact, very similar to that obtained for $n=2$, i.e., a sharp dropoff of T_c as one approaches values of Δ_0/D where either the concentration of local pairs or wide-band electrons becomes very small.

The ratio of $2T_c/E_g(0)$ is a quantity frequently referred to in order to show to what extent a system is a classical BCS superconductor for which this value equals 0.57. For our system there is no gap in the single-particle excitation spectrum for wide-band electrons for the case $J_0\neq 0$, $I_0=0$ since they are not superconducting. Hence the quantity $2T_c/E_g(0)$ is infinite. In contrast, for the case $J_0=0$, $I_0\neq 0$, $2T_c/E_g(0)$ varies considerably as the relative proportion of local pairs and wide-band–electron pairs is varied. We plot this variation of $2T_c/E_g(0)$ as a function of Δ_0/D in Fig. 9 and notice that its value approaches the BCS value in the limit of predominantly wide-band electrons in the system. $T_c/E_g(0)$ is larger than the classical value for some intermediate values of Δ_0/D, where both the number of local pairs and the number of wide-band electrons are comparable. Finally, the value for $2T_c/E_g(0)$ drops to zero in the limit of predominantly local pairs.

C. $J_0\neq 0$, $I_0\neq 0$

We shall now discuss the finite-temperature phase diagram for the general case $J_0\neq 0$, $I_0\neq 0$. Again, let us sup-

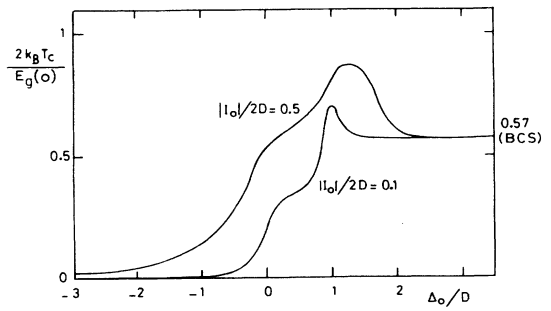

FIG. 9. $2k_BT_c/E_g(0)$ as a function of Δ_0/D for $J_0=0$ and two values of $|I_0|/2D$ (0.5, 0.1) and $n=1$. $E_g(0)$ denotes the gap in the single-particle spectrum of the wide-band electrons at zero temperature.

pose that the phase transition between the low-temperature superconducting state and the high-temperature normal state is of second order. Then, taking the limits ρ_0^x and $x_0\to 0$ in the set of Eq. (4.4), we obtain

$$\frac{1}{2}\left[J_0+\frac{I_0^2}{2N}\sum_{\mathbf{k}}\frac{\tanh(\beta_c/2)(\varepsilon_{\mathbf{k}}-\bar{\mu})}{\varepsilon_{\mathbf{k}}-\bar{\mu}}\right]\times\frac{\tanh[\beta_c(\mu-\Delta_0)]}{\mu-\Delta_0}=1\ ,$$

$$n-2=\tanh[\beta_c(\mu-\Delta_0)]-\frac{1}{N}\sum_{\mathbf{k}}\tanh\left[\frac{\beta_c(\varepsilon_{\mathbf{k}}-\bar{\mu})}{2}\right]\ . \tag{4.19}$$

Using the square density of states for the wide-band electrons, Eq. (4.19) can be rewritten in the form

$$\frac{1}{2}\left[J_0+\frac{|I_0|^2}{4D}S\right]B=1\ ,$$

$$n-2=\tanh[\beta_c(\mu-\Delta_0)]-\frac{1}{D\beta_c}\ln\left[\frac{\cosh[\beta_c(2D-\mu)/2]}{\cosh(\beta_c\mu/2)}\right]\ , \tag{4.20}$$

$$S=\int_0^{2D}d\varepsilon\frac{\tanh[(\beta_c/2)(\varepsilon-\mu)]}{\varepsilon-\mu}\ ,\quad B=\frac{\tanh[\beta_c(\mu-\Delta_0)]}{\mu-\Delta_0}\ .$$

In general, these equations can only be solved numerically and we present those results for T_c as a function of Δ_0/D in Fig. 10 for several values of n ($=1$, 1.5, and 2), $J_0/2D=0.05$, and (a) $|I_0|/2D=0.025$ and (b) $|I_0|/2D=0.5$.

We notice a behavior which is clearly a sort of superposition of the two limiting cases ($J_0\neq 0, I_0=0$ and $J_0=0, I_0\neq 0$). Upon decreasing Δ_0/D, one first observes a very rapid increase of T_c as one approaches the situation where the local-pair level becomes populated (i.e., for $\Delta_0/D\gtrsim n$). Upon further decreasing Δ_0/D, T_0 first increases and goes through a maximum before it decreases and saturates at a finite value (except for $n=2$) for $\Delta_0/D\ll 0$, where only local pairs are present. The size of this maximum in T_c as a function of Δ_0/D strongly depends on n. It is biggest for $n=2$ and almost disappears, as n is reduced.

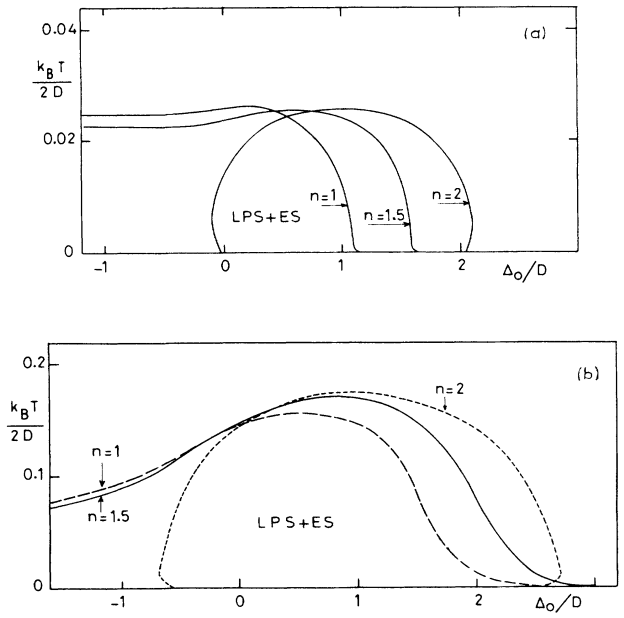

FIG. 10. Finite-temperature phase diagram as a function of Δ_0/D for total number of particles $n=1$, 1.5, and 2, and $J_0/2D=0.05$. (a) $|I_0|/2D=0.025$, (b) $|I_0|/2D=0.5$. LPS+ES denotes the superconducting state involving both local pairs and wide-band electrons.

It is worthwhile to study in detail the two limiting cases $\Delta_0/D\gtrsim n$ and $\Delta_0/D\lesssim 0$ with predominantly wide-band electrons and predominantly local pairs, respectively. This can be done analytically. In the first case, for $\Delta_0\gg nD$ the chemical potential $\mu\simeq nD$. Using the conditions $(2D-\mu)\beta_c\gg 1$ and $\mu\beta_c\gg 1$, which are trivially satisfied, we obtain, after some straightforward calculations,

$$k_BT_c=\frac{2\gamma}{\pi}D\sqrt{n(2-n)}\exp\left[-\frac{\Delta_0-nD-J_0/2}{I_0^2/4D}\right]\ , \tag{4.21}$$

with $\gamma=e^C$, $C=0.577$.

This indicates an exponentially sharp dropoff of T_c as Δ_0/D exceeds the characteristic value of $\Delta_0=nD+J_0/2$, where practically all particles exist in the form of wide-band electrons with only a small number of local pairs present.

As to the second case, $\Delta_0<0$ is the opposite limit of predominantly local pairs and very few wide-band electrons. In this case, for $|\Delta_0|/D\ll 0$, we have $\mu=\Delta_0$ and $n_2\simeq n-(T/D)\exp(-\Delta_0/T)$. Similarly, as before, we now have $(2D-\mu)\beta_c\gg 1$ and $-\mu\beta_c\gg 1$, from which we obtain

$$k_BT_c=\left[J_0+\frac{I_0^2}{4D}\ln\left[\frac{2D+|\Delta_0|}{|\Delta_0|}\right]\right]\frac{n-1}{\ln[n/(2-n)]}\ , \tag{4.22}$$

indicating a slow dropoff of T_c towards a saturation value equal to

$$J_0(n-1)/\{\ln[n/(2-n)]\}$$

upon diminishing Δ_0/D.

Setting $J_0=0$ in Eq. (4.22), we recognize the remaining contribution as one of the two contributions (i.e., $A_{\mathbf{k}=0}$) which we obtained in the more refined treatment using a perturbational approach [see Eq. (4.18)]. From this it is evident that the present mean-field approach largely overestimates the value of T_c in the regime $\Delta_0/D<0$, where all the electrons are in local-pair states.

Let us conclude this section with some remarks on the thermodynamic and magnetic properties of the superconducting state discussed above. A detailed microscopic description of these quantities necessitates a random-phase-approximation (RPA) treatment—a work which is presently in progress. In the following we summarize some preliminary results.

For the case $J_0\neq 0$, $I_0=0$ the situation is very similar to the case of a mixture of local pairs and itinerant electrons with properties which are essentially given by the sum of properties for each of the two subsystems. An essential feature is a linear spectrum of the collective excitations for the phase fluctuations of the order parameter of the local-pair subsystem, giving rise to a T^3 law in the low-temperature specific heat. The wide-band-electron subsystem, in contrast, contributes a linear term to the specific heat in the superconducting phase of the mixture due to the fact that this subsystem remains in the normal state. From the local-pair subsystem we expect,[1] moreover, a large penetration depth in the Meissner effect, large values for the upper critical fields, and a $d^2H_{c2}/dT^2\,|_{T=T_c}>0$ due exclusively to the diamagnetic coupling of the magnetic field to the charge of the local pairs. The paramagnetic coupling of the field to the spins of the wide-band electron will give rise to a Pauli susceptibility.

The situation for $J_0=0$, $I_0\neq 0$ is quite different from $J_0\neq 0$, $I_0=0$ in both the superconducting and normal phases. Due to the interaction between local pairs and pairs of wide-band electrons, a gap in the single-particle spectrum of the wide-band electrons opens up in the superconducting phase. Inside of this gap lies the level of the localized electrons that are in pair states. The collective excitation spectrum arising from the phase fluctuations of the order parameters now involving both subsystems is again sound-wave-like, provided certain conditions on the range of range of the interparticle Coulomb interactions are being satisfied. The consequence of these excitations is an overall T^3 law for the low-temperature specific heat. The main effect of a magnetic field will now be its paramagnetic coupling to the spins of the wide-band-electron subsystem. H_{c2} will be determined by the field closing the gap in the single-particle spectrum of the wide-band electrons, implying a simultaneous break up of the condensate state of the local pairs. The Meissner effect in this case will be rather like that for standard BCS superconductors.

Finally, the case $J_0\neq 0$, $I_0\neq 0$ is expected to show a specific heat proportional to T^3 at low temperatures. As far as its magnetic behavior is concerned, it ought to show rather interesting properties since now we have two independent mechanisms which can give rise to superconductivity: the direct hopping of local pairs and the contact interaction between local pairs and pairs of wide-band electrons. This should permit us to suppress superconductivity in the wide-band-electron subsystem upon applying a magnetic field. The subsystem of the local pairs at the same time would continue to be superconducting.

V. THE NORMAL STATE

The most striking characteristics of our superconducting system studied in this work is the fact that upon the disappearance of the superconducting order at T_c the bosons (i.e., local pairs of narrow-band electrons which have Bose character) continue to exist in the normal phase up to a certain temperature (comparable to the binding energy for the formation of the local-pair state) where they dissociate into two independent polarons. This picture is obviously in great contrast with a classical BCS superconductor, where the break up of the bosons (Cooper pairs) is tighly linked to the break up of the macroscopic quantum state describing the superconducting order. In the system we study here the superconducting order is established independently of the formation of the local-pair state and is analogous to superfluidity in ^{4}He II.

The fact that bosons of generally very narrow bandwidth exist in the normal phase ought to show up in quite characteristic thermodynamic properties. As shown by Alexandrov *et al.*,[1,23] the specific heat of a Bose gas on a lattice in the normal phase shows a temperature variation quite similar to that of an electron gas with comparable bandwidth. New interesting features show up in the normal phase for systems with very narrow bandwidth since in the experimentally available temperature regime one can easily sweep through the entire band and beyond, thus sensing the upper bound of the fermion and boson band, respectively. The specific heat for both fermions and bosons on a lattice drops off as $1/T^2$ for T much larger than the band width.

The study of the normal phase is considerably more complicated than that of the superconducting phase. A simple mean-field approach as adopted here (fully taking into account the hard-core character of the bosons and, to a lesser extent, the interparticle Coulomb interaction) is unable to treat the motion of hard-core bosons and the off-diagonal coupling between bosons and fermions and reduces effectively to the case $J_0=0$, $I_0=0$. Most of the physics is hence lost in this approximation. A much more sensible approximation to make for the study of the normal-state properties is simply to describe our model by a mixture of free bosons and electrons on a lattice. This permits one to take into account the finite bandwidth of bosons but neglect their hard-core character. For relatively low concentrations of bosons this is a useful and well-defined limit to be studied,[1,23] for which we shall adopt the following Hamiltonian:

$$H=\sum_{i\neq j} t_2^{ij} b_i^\dagger b_j+\sum_{i\neq j,\sigma} t_1^{ij} c_{i\sigma}^\dagger c_{j\sigma} -(\Delta+2\mu)\sum_i b_i^\dagger b_i+(\bar{\varepsilon}_0-\mu)\sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}\ . \tag{5.1}$$

This Hamiltonian follows from our initial one, Eqs. (2.15) and (4.6), used in the preceding sections, upon replacing the pseudospin operators by boson operators and neglecting all interaction effects. The quantities t_1, t_2, and Δ are related to our starting Hamiltonian in the following way:

$$t_1=\sum_{i\neq j} t_I^{ij}\equiv D \ ,$$
$$t_2=\sum_{i\neq j} t_2^{ij}\equiv -J_0 \ , \tag{5.2}$$
$$\Delta=-2(\Delta_0-D) \ .$$

We now calculate the number of bosons per site,

$$n_2^*=\frac{1}{N}\left\langle \sum_i b_i^\dagger b_i \right\rangle = n_2/2 \ ,$$

and the total number of electrons (in wide-band and local-pair states), $n=n_1+2n_2^*$.

In order to study the normal-state properties of the above Hamiltonian, we choose a square density of states for the bosons,

$$D_2(\varepsilon)=\begin{cases} 1/2t_2 & \text{for } 0\leq \varepsilon-\Delta\leq 2t_2 \ , \\ 0 & \text{otherwise} \ , \end{cases} \tag{5.3}$$

and a square density of states for the fermions,

$$D_1(\varepsilon)=\begin{cases} 1/2t_1 & \text{for } 0\leq \varepsilon+\bar{\varepsilon}_0\leq 2t_1 , \\ 0 & \text{otherwise.} \end{cases} \tag{5.4}$$

Having chosen a square density of states for the bosons will present us with a picture where the Bose condensation temperature is zero, but which will give us practically identical results to those we would obtain for a more realistic density of states provided T is above T_c. The reason for this is that condensation is exclusively controlled by the density of states in a narrow regime near the bottom of the band. For temperatures large compared to this regime (i.e., for $T>T_c$), the system is in the normal state described by a large portion of the density of states which is relatively flat and which justifies our model square density for the normal state.

We are interested here mainly in the temperature behavior of the specific heat and entropy. In order to evaluate these quantities we must first determine the chemical potential for this two-fluid system as a function of temperature. In order to do this we first evaluate n_2^* and n_1, for which we obtain

$$n_1=2\left[\frac{1}{2t_1}\right]\int_0^{2t_1} d\varepsilon\{\exp[\beta(\varepsilon+\varepsilon_0-t_1-\mu)]+1\}^{-1}=(\beta t_1)^{-1}\left[2\beta t_1-\ln\left[\frac{\exp[\beta(t_1+\bar{\varepsilon}_0-\mu)]+1}{\exp[-\beta(t_1-\bar{\varepsilon}_0+\mu)]+1}\right]\right] ,$$

$$n_2^*=\frac{1}{2t_2}\int_0^{2t_2} d\varepsilon\{\exp[\beta(\varepsilon-\Delta-t_2-2\mu)]-1\}^{-1}=(2\beta t_2)^{-1}\left[-2\beta t_2+\ln\left[\frac{\exp[\beta(-\Delta+t_2-2\mu)]-1}{\exp[\beta(-\Delta-t_2-2\mu)]-1}\right]\right] . \tag{5.5}$$

Eliminating $\beta\mu$ in the two expressions (5.5), we obtain, with $n_2^*=(n-n_1)/2$, the following equation,

$$\frac{n-n_1}{2}=-1+(2\beta t_2)^{-1}\ln\left[\frac{(e^{\beta t_1}-e^{\beta(n_1-1)t_1})^2 e^{-\beta(\Delta-t_2)}-(1-e^{\beta n_1 t_1})^2}{(e^{\beta t_1}-e^{\beta(n_1-1)t_1})^2 e^{-\beta(\Delta+t_2)}-(1-e^{\beta n_1 t_1})^2}\right] , \tag{5.6}$$

which determines the variation of the density of wide-band electrons, n_1, as a function of temperature. $n_2^*(T)$ is then easily determined as $n_2^*(T)=[n-n_1(T)]/2$. Equation (5.6) has been solved numerically for a choice of values of the parameters $t_1=500$ K, $t_2=10$ K, $n=1$, and three values of Δ (1040, 500, and -40 K) which describe three characteristically different physical situations: predominantly local pairs, a mixture of local pairs and electrons of comparable concentration, and, finally, the situation of predominantly electrons. The solutions are given in Fig. 11, where we have plotted the temperature variation of n_1 and n_2^*. The temperature dependence of μ is then determined by inverting Eqs. (5.5). With the knowledge of $\mu(T)$ we are then able to evaluate the specific heat and entropy of our system.

The specific heat is a sum of two contributions C_1 and C_2 (coming from the wide-band electrons and bosons) given by

$$C_1=(4\beta t_1)^{-1}\int_{\beta(-t_1+\bar{\varepsilon}_0-\mu)}^{\beta(t_1+\bar{\varepsilon}_0-\mu)} dx(x+\beta\mu)\left[x+\left[\beta\mu-\frac{\beta\partial(\beta\mu)}{\partial\beta}\right]\right]\cosh^{-2}\left[\frac{x}{2}\right] ,$$

$$C_2=(8\beta t_2)^{-1}\int_{\beta(-\Delta-t_2-2\mu)}^{\beta(-\Delta+t_2-2\mu)} dx(x+2\beta\mu)\left[x+2\left[\beta\mu-\beta\frac{\partial(\beta\mu)}{\partial\beta}\right]\right]\sinh^{-2}\left[\frac{x}{2}\right] . \tag{5.7}$$

Similarly, the entropy is the sum of two contributions S_1 and S_2 given by

$$S_1=-(\beta t_1)^{-1}\int_{\beta(-t_1+\bar{\varepsilon}_0-\mu)}^{\beta(t_1+\bar{\varepsilon}_0-\mu)} dx\{f(x)\ln[f(x)]+[1-f(x)]\ln[1-f(x)]\} ,$$
$$S_2=-(2\beta t_2)^{-1}\int_{\beta(-\Delta-t_2-2\mu)}^{\beta(-\Delta+t_2-2\mu)} dx\{n(x)\ln[n(x)]-[1+n(x)]\ln[1+n(x)]\} , \tag{5.8}$$

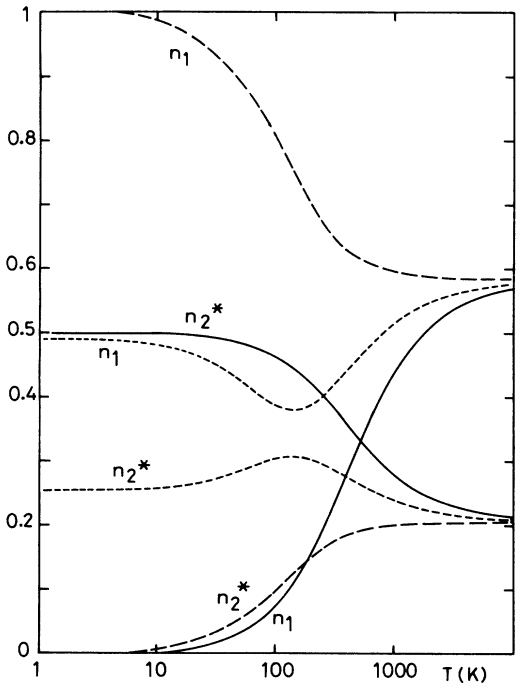

FIG. 11. The temperature variation of the number of local pairs per site ($n_2^* = n_2/2$) and the number of wide-band electrons per site (n_1) for $n \equiv n_2^* + n_1 = 1$, $t_1 = 500$ K, and $t_2 = 10$ K. The solid lines correspond to $\Delta = 1040$ K, the dotted to $\Delta = 500$ K, and the dashed to $\Delta = -40$ K.

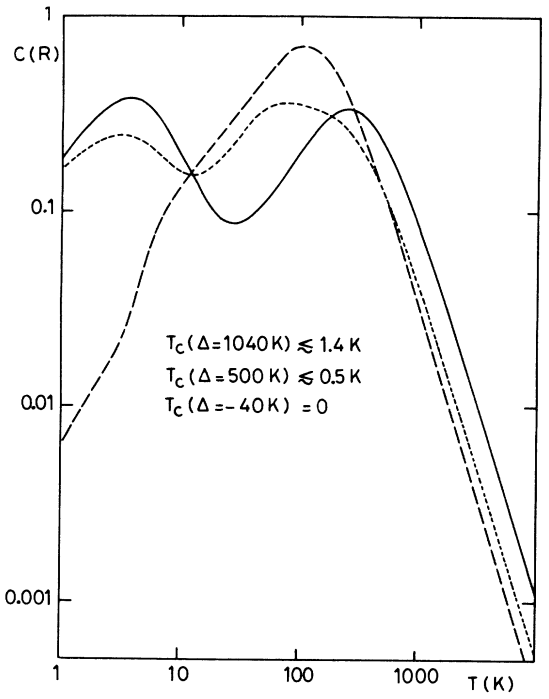

FIG. 12. The temperature variation of the specific heat (in units of R) in the normal phase for $n = 1$, $t_1 = 500$ K, and $t_2 = 10$ K. The solid lines correspond to $\Delta = 1040$ K, the dotted to $\Delta = 500$ K, and the dashed to $\Delta = -40$ K. The estimated critical temperature T_c for the Bose condensation is indicated for the various cases. The extension of the normal specific heat below these values of T_c project the specific heat that would be observed if the superconducting order were suppressed.

where $f(x)$ and $n(x)$ denote the Fermi and Bose distribution function, respectively.

Evaluating the expressions for the specific heat [Eqs. (5.7)] numerically after having determined the temperature variation of $\mu(T)$, we find the following results for the three cases of Δ (1040, 500, and -40 K) which we plot in Fig. 12. We clearly notice the two distinct contributions coming from the specific heat of the local pairs and of the electrons with, in general, two separated peaks and a drop off of C for temperature exceding the bandwidth of local pairs and wide-band electrons, respectively. This drop off of the specific heat at high temperature is a characteristic feature of systems with small enough bandwidth such that the temperature regime can be attained where $k_B T$ is much larger than the bandwidth.

Apart from the anomalous specific-heat behavior for our two-fluid boson-fermion model, we can easily evaluate the variation of the entropy with temperature (Fig. 13). This entropy is predominantly related to the translational degrees of freedom, which are more and more frozen out as the temperature is lowered and the quantum nature of the Fermi and Bose particles, respectively, becomes more and more manifest. This is quite different from the usually considered case of the entropy interpreted in terms of spin degrees of freedom. We want to mention that we have successfully applied[22] the above two-fluid boson-fermion model [Eq. (5.1)] in interpreting the specific heat and magnetic susceptibility of several heavy-fermion systems and ^{3}He, for the latter of which we assumed triplet rather than singlet bosons.

To close this section, let us point out that the transition temperature of the Bose condensation can easily be estimated on the basis of a free Bose gas on a lattice,

$$T_c \simeq 0.4 t_2 (n_2^*)^{2/3} , \tag{5.9}$$

which is valid in the low-density limit and assuming cubic structure.[1] For an arbitrary density of local pairs the transition temperature of the superconducting state for the case $J_0 \neq 0$, $I_0 = 0$ and no density-density interactions present can be deduced within the RPA treatment of our Hamiltonian (2.15). The analysis is a generalization of our previous results[1] for the pure local-pair superconductor when determining the number of local pairs and wide-band electrons self-consistently.

VI. COMMENTS ON THE COULOMB INTERACTIONS

Let us now briefly comment on the effects of Coulomb (density-density) interactions which we neglected during the analysis of superconducting and normal-state properties. The density-density interactions are quite essential as far as the stability of superconducting state and its competition with the charge-density waves is concerned.

We merely give here the results that follow from the

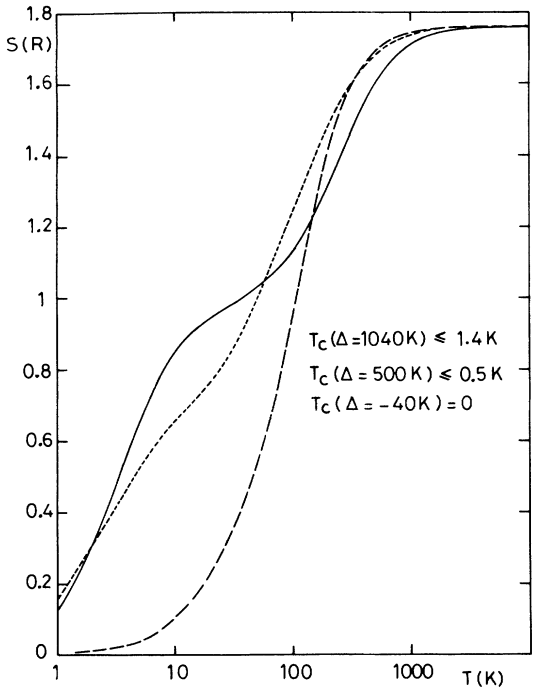

FIG. 13. The temperature of the entropy (in units of R) in the normal phase for $n=1$, $t_1=500$ K, and $t_2=10$ K. The solid line corresponds to $\Delta=1040$ K, the dotted to $\Delta=500$ K, and the dashed to $\Delta=-40$ K. The estimated critical temperature T_c for the various cases is indicated. The extension of the entropy curves below these values project the entropy which would be obtained if the superconducting order were suppressed.

mean-field- (or Hartree-) type treatment of the Coulomb interactions as related to superconducting and normal-state properties, leaving a full analysis of that problem to a separate paper.

In general, three types of the density-density interactions have to be considered (cf. Sec. II). Retaining only the effective density-density interaction parameters of the form $V_0=\sum_j V_{ij}$, $K_0=\sum_{j(\neq i)} K_{ij}$, and $V_0^{cc}=\sum_j V_{ij}^{cc}$, we obtain the following results.

In the normal state, the main effect of K_0 and V_0^{cc} is to enlarge the coexistence region of local pairs and wide-band electrons, and the densities of two types of particles change smoothly with varying Δ_0. In contrast, the influence of the intersubsystem Coulomb interaction V_0 is more drastic as it tends to reduce the coexistence region and may induce discontinuous changes in the concentrations of the two types of carriers, n_1 and n_2, versus Δ_0. For $V_0<D$, D being the half-bandwidth, changes in n_1 and n_2 are always smooth, but for $V_0>D$ discontinuous changes in n_1 and n_2 with variation of temperature and Δ_0 can take place.

Let us stress that for $V_0>D$ the treatment of the normal phase within the framework of Hartree approximation encounters the same problems as in the Falicov-Kimball model of mixed valence,[37–39] i.e., it is not yet established whether the discontinuous changes in electron occupancies are an inherent property of the model or if they are due to the approximation used.[40,41]

The effects of the short-range Coulomb interactions on the superconducting state are the following. If $I_0\neq 0$, $J_0=0$, the main influence of K_0 is to enhance T_c in the local-pair limit and shift the maximum of T_c towards lower values of Δ_0. V_0^{cc} enhances T_c in the predominantly wide-band-electron regime and also shifts the maximum of T_c, but towards the higher values of Δ_0. These are simply the consequences of enlarging the coexistence region of local pairs and width-band electrons by either K_0 or V_0^{cc}. The effect of V_0 is just the opposite; it tends to reduce T_c in both limits without any essential shift of the maximum T_c versus Δ_0.

If $I_0=0$, but $J_0\neq 0$, K_0 enhances T_c in the local-pair limit for $n>1$ and lowers it for $n<1$. The effect of V_0^{cc} is to enhance T_c in the wide-band-electron limit and to extend the superconducting state towards higher values of Δ_0. The intersubsystem Coulomb interaction V_0 acts differently in this case, lowering T_c only $n>1$, in both the local-pair or wide-band-electron–dominated regimes. For $n<1$, V_0 reduces T_c only in the wide-band-dominated regime, whereas an enhancement of T_c by V_0 is observed in the local-pair regime.

One should stress that all the above conjectures concerning the influence of Coulomb interactions on the superconducting phase diagrams have a restricted range of validity, first because they are based on a Hartree approximation and second because they are due to the nonconsideration of the charge-density waves (CDW's). For these reasons we summarized here only some of the most direct evidence that follows from the Hartree-type analysis.

As far as the charge ordering is concerned, we know from previous studies of purely local-pair systems that the Coulomb interaction K_{ij} tends to stabilize the mixed CDW-superconducting ground state of local pairs, for high enough local-pair density. The superconducting transition temperature is maximal where the superconducting phase becomes unstable versus a charge ordered phase.[1,4] Accordingly, in the model considered here, the mixed CDW-superconducting state is likely to occur in a regime dominated by local pairs. For $I_0\neq 0$, $J=0$, the intersubsystem Coulomb repulsion (V_Q) is able to stabilize the mixed CDW-superconducting state with the spatial modulation of charge density in both narrow-band- and wide-band-electron subsystems.

A more extended analysis of these questions will be the subject of future work.

VII. DISCUSSION AND OUTLOOK

Systems in which electrons exist in form of locally bound pairs are now known for a great variety of different materials ranging from amorphous semiconductors, bipolaronic metals, and insulators to polymers.

These local pairs of electrons having Bose character are thought to be capable of giving rise to a superconducting ground state. In real physical systems one can expect that besides those local pairs of electrons there exist fermions in the form of wide-band electrons. The question we dealt with in this paper was to show to what extent the Bose character of the local pairs of one type of (narrow-

band) electron can induce superconductivity in the other type of (wide-band) electron. We have studied this question on the basis of a generalized periodic Anderson model with strong local attraction and determined the phase diagrams as a function of the relative concentration of the narrow- and wide-band electrons.

We should like to stress that, apart from the hybridization mechanism considered here, we can also have a contribution coming from direct charge exchange coupling between the two types of electrons (in analogy to the direct spin exchange coupling in the s-d model).

In the present paper the attractive on-site interaction has been derived from the coupling between the narrow-band electrons and the local phonon modes. Such a derivation is in the spirit of other approaches starting with Anderson[10] and developed by many others (see, e.g., Refs. 1, 3, and 42–44).

Other mechanisms that can also lead to local attraction in a definite electronic subsystem have been proposed for example, (i) excitonic mechanisms,[45–48] (ii) the coupling of electrons to other electronic subsystems in a solid or chemical complex,[12,15,49] and (iii) the existence of "internal coordinates" such as dangling bonds or abnormal bond configurations in nonsimple metals.[50]

Indeed, the structure of the effective Hamiltonian (2.15) is independent of the possible microscopic origins of the local attraction, provided the starting Hamiltonian is of the form (2.8) and $\tilde{U}<0$, $|\tilde{U}| \gg \tilde{T}_{ij}, |I_0|$.

Consequently, our findings concerning the limit of strong attraction remain equally valid for systems with other mechanisms of local attraction.

Let us now turn to the discussion of predictions concerning the thermodynamic and magnetic properties of the model studied in this paper, some of which were already summarized in Sec. IV. First of all, the study of quantities such as specific heat, the Meissner effect, the critical fields, and transport coefficients requires detailed knowledge of the excitation spectrum of our model. Within the framework of the random-phase approximation (a work in progress) we can make qualitative assessments on the nature of collective excitations. For simplicity we consider the limit $J_0 \gg |I_0|$.

If the density of the wide-band electrons is large enough ($\Delta_0>0$), they can effectively screen the long-range Coulomb interaction between the charged pairs of narrow-band electrons. In the superconducting state, the phase fluctuations of the order parameter lead to a sound-like collective mode. There will also be a second branch of collective excitations of plasma type because the wide-band electrons "sense" the long-range Coulomb interaction.

The single-particle spectrum of localized electrons has a gap of the order of the binding energy of the pair of localized electrons. This binding energy is considered to be very large and, consequently, the single-particle spectrum of narrow-band electrons will lie well above the two lowest collective modes of our system. Such a picture of excitations has immediate consequences as regards the specific-heat behavior in the superconducting phase. At low temperatures one has a T^3 contribution resulting from the sound-wave-like collective mode and an exponential contribution due to the gap in the single-particle spectrum of wide-band electrons.

In the regime of predominantly local pairs, the long-range Coulomb interactions are practically unscreened and lead to a plasmon mode in the collective excitation spectrum (as in the charged Bose gas). Due to this, the low-temperature specific heat will show an exponential behavior.

There will be essential differences in the magnitude and temperature dependence of the upper critical field between the pure local-pair superconductivity ($I_0=0$) and the superconductivity of the mixture ($I_0\neq 0$). For pure local-pair superconductors the upper critical field at zero temperature is expected to be rather large. However, at present no reliable theory on this matter exists. In contrast, in the superconducting state of the mixture of local pairs and wide-band electrons, paramagnetic coupling of the magnetic fields can be easily realized and lead to a H_{c2} which is of the order of the gap in the single-particle spectrum of the wide-band electrons.

Furthermore, the critical behavior of the system should depend whether we are in the predominantly local-pair regime or in the opposite regime dominated by wide-band electrons. In the first case, as for pure bipolaronic superconductors, we have a strong analogy with the λ transition in ^{4}He II with a large fluctuation region, while in the second case the critical behavior should approach the classical Ginzburg-Landau type.

For many physical properties the two-fluid picture developed in this paper shows features which are intermediate between those of pure local-pair superconductors and those of classical BCS systems. This concerns, among others, the gap in the single-particle excitation spectrum, the ratio $k_B T_c/E_g(0)$, and the coherence length, as well as the properties of the normal state. Contrary to the standard BCS superconductivity, the effects of structural disorder (nonmagnetic impurities) are expected to be strong, as in the pure local-pair systems.[51–53] Magnetic disorder has only a weak effect on the superconducting state in the local-pair-dominated regime.

Taking into account the findings of this paper as well as some of our previous results concerning the case of pure local-pair systems, one is tempted to classify existing experimental materials into three classes. This division of compounds for which the existence of local-pair states has been established, corresponds to the three different regimes, as regards the relative position of the local-pair level Δ_0 with respect to the wide-electron band (compare Fig. 1).

(i) $\Delta_0<0$, i.e., the case where the local-pair level lies below the bottom of the wide band and all the electrons remain in the local-pair states at $T=0$ K.

An effective superconducting coupling between the local pairs (J_{ij}^{eff}) will consist of the direct hopping and the indirect coupling via the wide-band-electron states.

The density-density interactions (K_{ij}^{eff}) are practically unscreened and the case $K_{ij}^{\text{eff}} \gg J_{ij}^{\text{eff}}$ (J_{ij}^{eff} denoting the off-diagonal coupling of the charge operators) is most probable. Under such conditions the system can exhibit either a charge-order, or a mixed, charge-order–superconducting state (for low enough tempera-

tures),[1,3,4] or it will stay in the normal phase due to disorder or lower dimensionality.[51-52]

Possible candidates for this class are Ti_4O_7 and $Ti_{4-x}V_xO_7$ with $[(Ti^4\text{-}Ti^{4+})\ (Ti^{3+}\text{-}Ti^{3+})]$,[2] $Na_xV_2O_5$ $[(V^{4+}\text{-}V^{4+})\ (V^{5+}\text{-}V^{5+})]$,[2] $Pb_{1-x}In_xTe[In^{1+},In^{3+}]$ (Refs. 12 and 44) and $Pb_{1-x}Sn_xSe$,[27] $BaBiO_3$ $[Bi^{3+},Bi^{5+}]$,[18] and a large group of materials cited in the Introduction, such as $Cs_2SbCl_6[Sb^{3+},Sb^{5+}]$,[5,6] etc. All of these compounds exhibit either a charge-ordered state or they remain in the normal phase. To this group we can also add amorphous semiconductors and chalcogenide glasses with the impurity levels situated in the forbidden gap between the valence and conduction band,[10,12,44] and $SrTiO_3$.[20]

The local-pair superconductivity for $\Delta_0 < 0$ can be a real possibility in the low-electron-density limit. Due to an absence of screening of the Coulomb interactions, the collective excitations in this case will show up in the plasmon gap and the superconducting properties will be reminescent of those of a charged Bose gas. Let us also stress that little is known in this case as far as the competition between superconductivity and the Wigner cristallization is concerned.

(ii) $0 < \Delta_0 < nD$, i.e., the systems where the local-pair level falls into the wide-electron band and both types of states are partially occupied at $T = 0$ K.

The facts of nonintegral occupation of the local-pair states, enhancement of J_{ij}^{eff} due to the contact interaction between subsystems, and the screening of the Coulomb interaction by wide-band electrons make the appearance of local-pair superconductivity much more favorable than in case (i).

The following compounds can be classified in this group: the superconducting materials $BaPb_{1-x}Bi_xO_3(0.2 < x < 0.35)[Bi^{3+},Bi^{5+}]$,[12,18] $PbTl_xTe[Tl^{1+},Tl^{3+}]$,[19] and $Li_{1+x}Ti_{2-x}O_4[(Ti^{3+}\text{-}Ti^{3+})(Ti^{4+}\text{-}Ti^{4+})]$;[12,21] the compounds WO_{3-x},[9] $Na_xV_2O_5$ $(x \neq 0.33)$,[2] and some of the chalcogenide glasses such as As_2Te_3, α-$Ge_{33}As_{12}Se_{55}$.[54,55]

Moreover, if the existence of local pairs is ever confirmed in other nonstandard superconductors mentioned in the Introduction, they should also fall into this class. This concerns some of the Chevrel phases $M_xMo_6S_8$, and other clusterlike systems, e.g., MRh_4B_4, as well as $A15$ (V_3Si, Nb_3Ge), $C15$ $[(Hf_{0.5}Zr_{0.5})V_2]$, the carbides and nitrides (NbC),[13-17] and the recently discovered Ba-La-Cu-O (Ref. 56) system. Let us emphasize that for this case the standard BCS coupling V^{BCS} for wide-band electrons is always a possibility, and all three mechanisms, J_{ij}, I_0, and V^{BCS}, might contribute to the superconducting state.

(iii) $\Delta_0 > Dn$ $(=\varepsilon_F)$, i.e., the systems where the local-pair states lie above the Fermi energy and only a virtual occupation of such states is possible. In such a case superconductivity can be established by the BCS mechanism for wide-band electrons. An additional superconducting coupling due to virtual excitations into local-pair states will be usually much smaller, except for the case $\Delta_0 \sim \varepsilon_F$, where it can yield strong enhancement of T_c and become an essential factor determining superconducting properties. As possible candidates to this group we can consider the following compounds: Na_xWO_3,[12] PdH_x, $Pd_{1-x}Ag_xH$, PdD_x,[12,57] and $BaPb_{1-x}Bi_xO_3$ $(x < 0.2)$.[12,18]

We should like to mention that our preliminary phenomenological classification does not include such essential factors as disorder or restricted dimensionality effects which certainly need further studies.

As suggested previously,[25,36] the two-fluid model, Eq. (4.13), studied in this work could possibly apply to the problem of the intermediary electron-phonon coupling involving only one type of electrons. Retardation effects, which are expected to be important here, can approximately be taken care of by assuming that the electrons can exist in two extreme states: electrons moving in a rigid lattice [denoted by the operators c in Eq. (4.13)] and electrons fully renormalized into small polarons [denoted by the operators d in Eq. (4.13)]. The resulting picture is one of a band of electrons with a resonant bound state of two polarons at the Fermi level and a contact interaction between pairs of polarons (bipolarons) and pairs of electrons (Cooper pairs). Such a picture is capable of producing high values for T_c and could possibly apply to the recently discovered high-temperature superconductors.[56]

ACKNOWLEDGMENTS

We would like to than M. Bartkowiak and A. Sulpice for help in the numerical analysis.

*On leave of absence from Institute of Physics, A. Mickiewicz University, Poznani, Poland.

[1] A. S. Alexandrov, J. Ranninger, and S. Robaszkiewicz, Phys. Rev. B **33**, 4526 (1986).

[2] S. Lakkis, C. Schlenker, B. K. Charkraverty, R. Buder, and M. Marezio, Phys. Rev. B **14**, 1429 (1976); B. K. Chakraverty, M. T. Sienko, and J. Bonnerot, *ibid.* **17**, 3781 (1978); M. Onoda, T. Takahashi, and H. Nagasawa, J. Phys. Soc. Jpn. **51**, 3868 (1982); M. Onoda and H. Nagasawa, *ibid.* **52**, 2231 (1983).

[3] A. S. Alexandrov and J. Ranninger, Phys. Rev. B **23**, 1796 (1981); **24**, 1164 (1981).

[4] S. Robaszkiewicz, R. Micnas, and K. A. Chao, Phys. Rev. B **23**, 1447 (1981); **24**, 1579 (1981); **24**, 4018 (1981); **26**, 3915 (1982).

[5] S. P. Ionov, G. V. Ionova, V. S. Lubimov, and E. F. Makarov, Phys. Status Solidi B **71**, 11 (1975); S. P. Ionov, G. V. Ionova, A. I. Maiybaev, L. A. Manakova, and G. K. Semin, Izv. Akad, Nauk. SSSR **45**, 589 (1981); S. P. Ionov, *ibid.* **49**, 310 (1985).

[6] P. Day, in *Chemistry and Physics of One-Dimensional Metals,* edited by H. J. Keller (Plenum, New York, 1977), p. 197; in *The Physics and Chemistry of Low Dimensional Solids,* edited by L. Alcacer (Reidel, Dordrecht, 1980), p. 305; J. S. Miller and A. J. Epstein, Prog. Inorg. Chem. **20**, 2 (1976); H. J. Keller, *Extended Linear Chain Compounds,* (Plenum, New York, 1982), Vol. 1, p. 357.

[7] H. Nagasawa, Phys. Status Solidi B **109**, 749 (1982).

[8] J. C. Scott, P. Pfluger, M. T. Krounbi, and G. P. Street, Phys.

Rev. B **28**, 2140 (1983); T. C. Chung, J. H. Kaufman, A. J. Heeger, and F. Wudl, *ibid.* **30**, 702 (1984).

[9]O. F. Schirmer and E. Salje, J. Phys. C **13**, L1067 (1980); E. Salje and B. Güttler, Philos. Mag. B **50**, 607 (1984).

[10]P. W. Anderson, Phys. Rev. Lett. **34**, 953 (1975); in *Lectures on Amorphous Systems,* edited by R. Balian *et al.* (North-Holland, Amsterdam, 1979), p. 161; N. F. Mott and E. A. Davis, *Electron Processes in Non-Crystalline Materials* (Clarendon, Oxford, 1979); G. D. Watkins, in *Festkörperprobleme XXIV,* edited by H. J. Queisser (Pergamon Vieweg, Braunschweig, 1984), p. 163.

[11]P. W. Anderson and C. C. Yu, in *Proceedings of the International School of Physics, "Enrico Fermi",* Course No. LXXXIX, edited by F. Bassini and M. P. Tosi (North-Holland, Amsterdam, 1985), p. 767.

[12]B. Ya. Moizhes and I. A. Drabkin, Fiz. Tverd. Tela (Leningrad) **25**, 1974 (1983) [Sov. Phys.—Solid State **25**, 1139 (1983)].

[13]S. V. Vonsovskii, Yu. A. Izyumov, and E. Z. Kurmaev, *Superconductivity of the Transition Metals,* Nauka, Moscow (1977), No. 27 of *Springer Series in Solid State Sciences,* edited by P. Fulde (Springer-Verlag, Berlin, 1982); Ø. Fisher, Appl. Phys. **16**, 1 (1978).

[14]A. S. Alexandrov, Zh. Fiz. Khim. **57**, 273 (1983) [Russ. J. Phys. Chem. **57**, 167 (1985)]; A. S. Alexandrov, and V. F. Elesin, Izv. Akad. Nauk. SSSR **49**, 326 (1985); A. S. Alexandrov, V. F. Elesin, and V. V. Kabanov, Zh. Eksp. Teor. Fiz. **86**, 1937 (1984) [Sov. Phys.—JETP **59**, 1125 (1984)].

[15]S. P. Ionov *et al.*, in Ref. 5.

[16]C. S. Ting, K. L. Ngai, and C. T. White, Phys. Rev. B **22**, 2318 (1980); R. Sooryakumar and M. V. Klein, *ibid.* **23**, 3213 (1981); **23**, 3222 (1981).

[17]A. D. Shevchenko, Fiz. Tverd. Tela (Leningrad) **25**, 1864 (1983) [Sov. Phys.—Solid State **25**, 1075 (1983)].

[18]A. W. Sleight, J. L. Gillson, and P. E. Bierstedt, Solid State Commun. **17**, 27 (1975); T. D. Thanh, A. Koma, and S. Tanaka, Appl. Phys. **22**, 205 (1980); I. N. Groznov, S. P. Ionov, I. B. Kevdina, V. S. Lubimov, E. F. Makarov, O. V. Marchenko, N. N. Mikhailov, V. A. Onishchuk, and V. P. Shantarovich, Phys. Status Solidi B **123**, 183 (1984); K. Kitazawa, M. Naito, T. Itoh, and S. Tanaka, J. Phys. Soc. Jpn. **54**, 2682 (1985); K. Kitazawa, S. Uchida, and S. Tanaka (unpublished).

[19]I. A. Chernik, S. N. Likhov, and N. I. Grechko, Fiz. Tverd. Tela (Leningrad) **24**, 2931 (1982) [Sov. Phys.—Solid State **24**, 2931 (1982)].

[20]D. M. Eagles, Phys. Rev. **178**, 668 (1969); **186**, 456 (1969); Solid State Commun. **60**, 521 (1986).

[21]M. R. Harrison, P. P. Edwards, and J. B. Goodenough, Philos. Mag. B **52**, 679 (1985).

[22]J. Ranninger, S. Robaszkiewicz, A. Sulpice, and R. Tournier, Europhys. Lett. **3**, 347 (1987).

[23]A. S. Alexandrov, J. Ranninger, and S. Robaszkiewicz, Phys. Rev. Lett. **56**, 949 (1986).

[24]See Ref. 1 and references therein; also see I. O. Kulik, Physica **126B**, 280 (1984).

[25]J. Ranninger and S. Robaszkiewicz, Physica **135B**, 468 (1985).

[26]For the single-Anderson-impurity case, this problem was considered previously by F. D. M. Haldane, Phys. Rev. B **15**, 281 (1977).

[27]F. S. Nasredinov, L. V. Prokor'eva, A. N. Kurmantaev, and P. P. Seregin, Fiz. Tverd. Tela (Leningrad) **26**, 862 (1984) [Sov. Phys.—Solid State **26**, 522 (1984)].

[28]I. G. Lang and Yu. A. Firsov, Zh. Eksp. Teor. Fiz. **43**, 1843 (1962) [Sov. Phys.—JETP **16**, 1301 (1963)]; T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959); **8**, 343 (1959); Yu. A. Firsov, *Polarons* (Nauka, Moscow, 1975).

[29]J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966); J. R. Schrieffer, J. Appl. Phys. **38**, 1143 (1967).

[30]L. C. Lopes, R. Jullien, A. K. Bhattacharjee, and B. Coqblin, Phys. Rev. B **26**, 2640 (1982).

[31]D. Adler and E. J. Yoffa, Phys. Rev. Lett. **36**, 1197 (1976).

[32]V. J. Emery, Phys. Rev. B **14**, 2989 (1976); in *Highly Conducting One-Dimensional Solids,* edited by J. Devreese, R. Evrard, and V. van Doren (Plenum, New York, 1979), p. 247.

[33]C. Lacroix and M. Cyrot, Phys. Rev. B **20**, 1969 (1979); C. Proetto and A. Lopez, *ibid.* **24**, 3031 (1981).

[34]S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).

[35]For the earliest studies of this case, see V. L. Vinetskii, Zh. Eksp. Teor. Fiz. **40**, 1459 (1961); V. L. Vinetskii and I. I. Semenets, Ukrain. Fiz. Zh. **20**, 353 (1975).

[36]R. Micnas, J. Ranninger, and S. Robaszkiewicz, J. Magn. Magn. Mater. **63-64**, 420 (1987).

[37]L. M. Falicov and J. C. Kimball, Phys. Rev. Lett. **22**, 997 (1969).

[38]R. Ramirez, L. M. Falicov, and J. C. Kimball, Phys. Rev. B **2**, 3583 (1970).

[39]R. Ramirez and L. M. Falicov, Phys. Rev. B **3**, 2425 (1971).

[40]D. I. Khomskii, in *Quantum Theory of Solids,* edited by (I. M. Lifshits Mir, Moscow, 1982), p. 70.

[41]M. D. Nunez-Regueiro and M. Avignon, J. Phys. F **15**, 1661 (1985); **16**, 1181 (1986).

[42]E. Simanek, Solid State Commun. **32**, 731 (1979).

[43]E. Fradkin and J. E. Hirsch, Phys. Rev. B **27**, 1680 (1983).

[44]M. I. Klinger, Usp. Fiz. Nauk **146**, 105 (1985) [Sov. Phys.—Usp. **28**, 391 (1985)]; M. I. Klinger and V. G. Karpov, Zh. Eksp. Teor. Fiz. **82**, 1687 (1982) [Sov. Phys.—JETP **55**, 976 (1982)].

[45]W. A. Little, Phys. Rev. **134**, A1416 (1964); Int. J. Quantum Chem. **15**, 545 (1981).

[46]V. L. Ginzburg, Zh. Eksp. Teor. Fiz. **47**, 2318 (1964) [Sov. Phys.—-JETP **20**, 1549 (1965)]; Usp. Fiz. Nauk **118**, 315 (1976) [Sov. Phys.—Usp. **19**, 174 (1976)].

[47]G. Beni, P. Pincus, and J. Kanamori, Phys. Rev. B **10**, 1896 (1974).

[48]J. E. Hirsch and D. J. Scalapino, Phys. Rev. B **32**, 117 (1985); Phys. Rev. Lett. **56**, 2732 (1986).

[49]E. F. Makarov, I. I. Amelin, and S. P. Ionov, Phys. Status Solidi B **71**, 135 (1975); G. V. Ionova, E. F. Makarov, and S. P. Ionov, Phys. Status Solidi **81**, 671 (1977).

[50]C. S. Ting *et al.*, in Ref. 16.

[51]A. G. Pedan and I. O. Kulik, Fiz. Nizk, Temp. **8**, 236 (1982) [Sov. J. Low Temp. Phys. **8**, 118 (1982)].

[52]R. Micnas, S. Robaszkiewicz, and K. A. Chao, Physica **131A**, 393 (1985).

[53]M. Ma and P. A. Lee, Phys. Rev. B **32**, 5658 (1985).

[54]S. D. Savransky, J. Non-Cryst. Solids **83**, 235 (1986); I. V. Berman, N. B. Brandt, V. A. Alekseev, I. E. Kostyleva, V. I. Sidorov, and O. P. Pyatkina, Pisma Zh. Eksp. Teor. Fiz. **40**, 472 (1984) [JETP Lett. **40**, 1303 (1984)].

[55]N. Sakai and J. Fritzshe, Phys. Rev. B **15**, 973 (1977).

[56]J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).

[57]G. D. Watkins in *Festkörperprobleme XXIV,* Ref. 10.