Superconductivity in systems with a low particle density

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A regular procedure for going over from the Fermi picture to the Bose picture of elementary excitations is proposed for Fermi systems with a low density of charge carriers. The residual interaction between bosons can be taken into account. The possibility of describing a low-density system in the mean-field approximation is analyzed. Systems which are equivalent from the standpoint of the mean-field approach may differ substantially in the strength of the residual interactions and thus in the nature of the transition to the condensed state. When a system contains localized impurity states, the interaction of the carriers with impurities can be described through renormalization of the binding energy of the two-particle state. This energy is increased by virtual transitions of particles from the band to impurity levels.

1. INTRODUCTION

Among the various unusual properties of the high T_c superconductors, one which is particularly interesting is the behavior of the energy gap near the superconducting transition temperature T_c. In contrast with the "old" superconductors, whose energy gap increases monotonically from zero as the temperature is lowered below T_c, in complete agreement with the standard BCS theory, the high T_c superconductors have a nonzero gap in the superconducting phase even in the immediate vicinity of T_c, according to optical experiments.[1] This behavior of the energy gap agrees better with a picture of the superconducting transition as a Bose condensation of pairs with a finite binding energy (that picture arose with the ideas of Schafroth[2]) than with the ordinary BCS mechanism. The latter mechanism assumes that large-radius Cooper pairs form and condense simultaneously. The optical experiments[1] suggest more of a tendency toward the formation of pairs (there are significant pair correlations) than the actual existence of these pairs above T_c. It thus seems more appropriate to speak of the realization in the high T_c superconductors of a region, between the Cooper and Schafroth limits, in which characteristic features of these two models coexist.

Legget[3] has pointed out that a necessary condition for the realization of the Schafroth picture of the condensation of local pairs is that the system have a two-particle bound state. Otherwise, in the absence of a bound state, the superconducting (or superfluid) transition would always correspond to the picture of Cooper pairing. In band-theory terms, a transition from the Cooper picture to the Schafroth picture occurs because the chemical potential μ goes into the band gap. The energy gap (in the mean-field approximation) is determined in this case not by the amplitude of the superconducting order parameter Δ but by the quantity $\sqrt{\mu^2+\Delta^2}$. In the $2D$ case, in which bound states exist for an arbitrarily weak attractive potential, a continuous transition from the Cooper picture to the Schafroth picture occurs as the density of charge carriers decreases from values $n \gg r_p^{-2}$, where r_p is the radius of the two-particle bound state, to values $n \ll r_p^{-2}$ (Ref. 5). In the $3D$ case, a bound state exists only if the strength of the interaction potential or the energy dependence of the density of states satisfies certain conditions. If these conditions are satisfied, the Schafroth picture is also realized in the limit of low carrier densities.

In this paper we analyze the superconducting order in systems with a low density of charge carriers, in which particular features of the superconducting order associated with the proximity to the Bose limit play an important role. In Sec. 2 we take up the description of the superconducting order in the mean-field approximation for systems of arbitrary dimensionality D with an arbitrary dispersion relation. We show that when there is a two-particle bound state with an energy ε_p and a radius r_p the formal characteristics of the superconducting state in the Schafroth limit (specifically, the position of μ and the functional dependence of the order parameter Δ on the number of particles, n) are identical for systems of any dimensionality. However, the mean-field approximation, used in Sec. 2 (and in Refs. 4–7), leaves out many important aspects of the problem. This deficiency is particularly glaring in a calculation of the transition temperature T_c: The mean-field value has nothing in common with the Bose condensation temperature. This result can be explained quite naturally on the basis that, formally, the mean-field approximation is not valid at low densities. The qualitative agreement of the mean-field description at $T=0$ and the picture of Bose condensation of local pairs can thus serve only as physical justification for the approach taken in those papers. In Sec. 3 we take up a systematic description of a low-density electron liquid with an attraction. Using a functional-integration technique, we show that under the condition $n^{1/D} r_p \ll 1$ the Lagrangian of strongly interacting fermions can be represented as the Lagrangian of a Bose liquid of pairs with a residual interaction. The role of the chemical potential of the bosons is played in this case by the quantity $\mu^* = \varepsilon_p - 2\mu$, and the strength of the interaction between bosons is determined to a large extent by D, the dimensionality of the system. Specifically, systems with large D correspond to a weaker interaction, so the mean-field approximation is better justified (only at $T=0$, of course).

A doped semiconductor can serve as a specific physical realization of a system with a low density of particles. The new high T_c superconductors can also be put in this category. When such systems are doped, localized impurity states usually arise in the band gap. It is particularly important to consider these levels in the case of an elevated density

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of states at the edges of the allowed spectrum. This is just the situation which arises in descriptions of the conversion to an insulating state in the high T_c superconductors by models with a nesting of the Fermi surface.[8] In this situation, a one-dimensional structural feature appears in the density of states and gives rise to discrete levels for an arbitrarily weak impurity potential. In Sec. 4 we use the mean-field approximation to examine superconducting order for the case in which there are localized states in the band gap. We find that the impurity levels increase the energy of the paired state, as a result of virtual transitions from the band to impurity levels, and superconductivity may be promoted by these levels. We should of course remember that, in accordance with Sec. 3 of this paper, these results are valid only for $T=0$, and then only for a limited class of systems in which there is a weak residual interaction between bosons.

2. DESCRIPTION OF THE SUPERCONDUCTING ORDER AT LOW DENSITY IN THE MEAN-FIELD APPROXIMATION

We consider a system of Fermi particles with density n and an attractive interaction. Under the assumption that the s harmonic of the overall interaction potential v_{kk} is the largest one, we restrict the discussion to the s scattering channel. The Hamiltonian of a system of dimensionality D is written in this case as

$$H=\int d^D\mathbf{r}\{\sum_\sigma \Psi^+_\sigma(\mathbf{r})[\varepsilon(\nabla)-\mu]\Psi_\sigma(\mathbf{r})$$

$$-g\Psi^+_\uparrow(\mathbf{r})\Psi^+_\downarrow(\mathbf{r})\Psi_\downarrow(\mathbf{r})\Psi_\uparrow(\mathbf{r})\}. \tag{1}$$

The operator Ψ^+_σ creates a particle with spin σ, $\varepsilon(k)$ is the dispersion relation, and g is an effective interaction constant. The latter can be expressed in terms of the scattering length in the s channel. The self-consistency condition for the mean-field order parameter Δ is written in the standard form,

$$\frac{1}{g}=\frac{1}{2}\int_0^\infty \frac{N(\varepsilon)d\varepsilon}{\sqrt{(\varepsilon-\mu)^2+\Delta^2}}, \tag{2}$$

where $N(\varepsilon)$ is the density of states. This equation must be supplemented with the condition that the number of particles is conserved:

$$n=\int_0^\infty\left(1-\frac{\varepsilon-\mu}{\sqrt{(\varepsilon-\mu)^2+\Delta^2}}\right)N(\varepsilon)d\varepsilon. \tag{3}$$

The system of equations (2), (3) unambiguously determines Δ and μ as a function of the density n and the coupling constant g. In the high-density limit we find the standard expressions of the BCS theory:

$$\Delta=2\omega\exp\{-1/N(\varepsilon_F)g\},\quad \mu=\varepsilon_F;\quad \Delta/\varepsilon_F\ll 1. \tag{4}$$

As the density decreases, the system (2), (3) has different solutions, depending on whether there is a two-particle bound state or, formally, on whether there is a nontrivial solution of an equation for the binding energy of a pair, ε_p:

$$\frac{1}{g}=\int\frac{N(\varepsilon)d\varepsilon}{2\varepsilon+\varepsilon_p}. \tag{5}$$

With $\varepsilon_p=0$ we can find a solution of (4) for arbitrarily small n. If Eq. (5) instead has a nonzero binding energy, then Δ falls off more slowly with decreasing n than in (4). As a result, there is a spreading of the distribution function in (3), which in turn causes a lowering of the chemical potential μ. Ultimately, μ reaches zero and drops into the band gap. If the density is lowered even further, the condition $-\mu/\Delta\gg 1$ becomes satisfied. In this case Eqs. (2) and (3) become, respectively,

$$\frac{1}{g}=\int\frac{N(\varepsilon)d\varepsilon}{2\varepsilon+2|\mu|}, \tag{6}$$

$$n=\frac{1}{2}\int\frac{\Delta^2}{(\varepsilon+|\mu|)^2}N(\varepsilon)d\varepsilon. \tag{7}$$

From (6) and (7) we find the following asymptotic expressions for Δ and μ in the limit $n\to 0$:

$$\Delta=\left[\frac{1}{g^2}\frac{dg}{d\varepsilon_p}\right]^{-1/2}\sqrt{\frac{n}{2}};\quad \mu=-\frac{\varepsilon_p}{2}. \tag{8}$$

In deriving (8) we used expression (5) for g in terms of ε_p. The general expression (8) depends on neither the dimensionality D of the system nor the particular dispersion relation $\varepsilon(k)$. In the case $D=2$ and $\varepsilon(k)=k^2/2m$, this expression easily leads to the results of Refs. 4 and 5. The $\Delta\sim\sqrt{n}$ dependence in (8) is analogous to the dependence of the condensate density in an ideal Bose gas and justifies our use of the mean-field equations (2) and (3) to describe the continuous transition to a BCS state to a Bose condensate of local pairs. Formally, of course, this assumption is groundless. That the mean-field approximation is not valid for small n is especially clear at $T=0$. In particular, the transition temperature calculated in this approximation is wildly different from the Bose condensation temperature. In the following section of this paper we take a rigorous approach using a functional-integration method. We will see that there nevertheless are cases in which the mean-field approximation can still be used at $T=0$.

3. REPRESENTATION OF A LOW-DENSITY FERMI SYSTEM WITH AN ATTRACTION AS AN INTERACTING BOSE LIQUID

We start by writing the partition function Z in terms of a functional integral in terms of the Grassmann variables $\Psi_\sigma(\mathbf{r},\tau)$ describing fermion degrees of freedom:

$$Z=\int D\Psi^*_\sigma D\Psi_\sigma e^{-S}, \tag{9}$$

where the action S is

$$S=\int_0^{1/T}d\tau\int d^D\mathbf{r}\left\{\sum_\sigma\Psi^*_\sigma\left[\frac{\partial}{\partial\tau}+\varepsilon(\nabla)+\mu\right]\Psi_\sigma\right.$$

$$\left.-g\Psi^*_\uparrow\Psi^*_\downarrow\Psi_\downarrow\Psi_\uparrow\right\}. \tag{10}$$

Here we have used the condition $\mu < 0$, which holds at small n, and we have changed notation: $\mu \rightarrow -|\mu|$. The number of particles is expressed in terms of the derivative of the logarithm of Z with respect to the chemical potential:

$$n = \frac{\partial}{\partial \mu} \ln Z. \tag{11}$$

In (9) we introduce a Gaussian integral over the auxiliary Bose field $\Delta(\mathbf{r},\tau)$, and we use the Hubbard–Stratonovich transformation to eliminate the four-fermion term in action (9). As a result, the action becomes

$$S' = \int d\tau\, dr \left\{ \Phi^+(\mathrm{r}, \tau)\hat{M}\Phi(\mathrm{r}, \tau) + \frac{|\Delta(\mathrm{r}, \tau)|^2}{g} \right\}, \tag{12}$$

where

$$\hat{M} = \begin{bmatrix} \frac{\partial}{\partial \tau} + \varepsilon(\nabla) + \mu & \Delta \\ \Delta^* & \frac{\partial}{\partial \tau} - \varepsilon(\nabla) - \mu \end{bmatrix}; \quad \Phi = \begin{bmatrix} \Psi_\uparrow \\ \Psi^*_\downarrow \end{bmatrix}. \tag{13}$$

The integral with action S' in (12) is Gaussian in the Fermi fields. The integration over Ψ can thus be carried out exactly. As a result we find an effective action which depends only on the boson variables $\Delta(r,\tau)$. Specifically, the partition function is given by the integral

$$Z = c \int D\Delta D\Delta^* \exp\{-S_{eff}\{\Delta, \Delta^*\}\}, \tag{14}$$

and the effective action S_{eff} becomes

$$S_{eff}\{\Delta, \Delta^*\} = -\ln \det \hat{M} - \int \frac{|\Delta|^2}{g} d\tau dr - S_{eff}(\Delta = 0). \tag{15}$$

For convenience below, we have added and subtracted the value of S_{eff} at $\Delta = 0$ in the argument of the exponential function in (14) and (15). This procedure makes it possible to rewrite (15) as

$$S_{eff} = -\mathrm{Sp} \ln(1 - \hat{G}\hat{\Delta}) - \int d\tau dr \frac{|\Delta|^2}{g}, \tag{16}$$

where

$$\hat{\Delta} = \begin{bmatrix} 0 & \Delta \\ \Delta^* & 0 \end{bmatrix}; \quad \hat{G} = \begin{bmatrix} G_- & 0 \\ 0 & G_+ \end{bmatrix},$$

$$G_\pm = \left[-\frac{\partial}{\partial \tau} \pm (\varepsilon(\nabla) + \mu) \right]^{-1}. \tag{17}$$

Expanding the logarithm in (16) in powers of Δ, and noting that only even powers are present in this expansion, we write S_{eff} in series form:

$$S_{eff} = \sum_{l=1}^{\infty} S^{(2l)}_{eff}, \tag{18}$$

where

$$l = 1, \quad S^{(2)}_{eff} = \int dr d\tau \frac{|\Delta|^2}{g} + \frac{1}{2} \mathrm{Sp}(\hat{G}\hat{\Delta})^2, \tag{19a}$$

$$l > 1, \quad S^{(2l)}_{eff} = \frac{1}{2l} \mathrm{Sp}(\hat{G}\hat{\Delta})^{2l}. \tag{19b}$$

In (18) and (19) we go over to Fourier components of Δ in terms of both the spatial coordinate and the temporal coordinate, and we find the quadratic term in the action $S^{(2)}_{\mathrm{eff}}$ in (19a). Taking the trace in (19a), we then find

$$S^{(2)}_{eff} = T \sum_{\varepsilon} \int d^D q \Delta^* \left(\frac{1}{g} + \Pi_2(\mathrm{q}, \varepsilon) \right) \Delta, \tag{20}$$

where ε represents the even Matsubara frequencies, and $\Pi_2(\mathbf{q},\varepsilon)$ is the polarization operator in the Cooper channel, given by

$$\Pi_2(\mathrm{q}, \varepsilon) = T \sum_{\omega} \int \frac{d^D \mathrm{k}/(2\pi)^D}{(i\omega - \varepsilon(\mathrm{k}) - \mu)(i\omega - i\varepsilon + \varepsilon(\mathrm{k} + \mathrm{q}) + \mu)},$$

$$\omega = \pi T(2n + 1). \tag{21}$$

We assume that there is a two-particle bound state in the system. Accordingly there is a nontrivial solution of Eq. (5) for the binding energy ε_p. In accordance with the results of the mean-field approximation, we then assume that μ lies near $1/2\varepsilon_p$. We also restrict the discussion to temperatures T which are below the ionization potential ε_p of the two-particle state. As a result we find

$$\Pi_2(\mathrm{q}, \varepsilon) = -\int \frac{d^D \mathrm{k}/(2\pi)^D}{\varepsilon_{\mathrm{k}} + \varepsilon_{\mathrm{k+q}} + \varepsilon_p - i\varepsilon + (2\mu - \varepsilon_p)}. \tag{22}$$

Since the typical ranges of ε and q are determined by the temperature $T \ll \varepsilon_p$, and since the condition $(2\mu - \varepsilon_p)/(\varepsilon_p \ll 1)$ also holds, we can expand $\Pi_{2,}(\mathbf{q},\varepsilon)$ in ε and q near the origin and in μ near $\varepsilon_p/2$. As a result we find from (22)

$$\Pi_2(\mathrm{q}, \varepsilon) = -\int \frac{d^D \mathrm{k}/(2\pi)^D}{2\varepsilon(\mathrm{k}) + \varepsilon_p} + \frac{\partial \Pi_2}{\partial 2\mu} \{-i\varepsilon + \frac{q^2}{2m^*} - (\varepsilon_p - 2\mu)\}, \tag{23}$$

where

$$\frac{1}{m^*} = \left(\frac{\partial \Pi_2}{\partial 2\mu} \right)^{-1} \frac{\partial^2 \Pi_2}{\partial \mathrm{q}^2}. \tag{24}$$

Substituting (23) into (20), and using Eq. (5) for ε_p, we find the following expression for the quadratic part of the action, $S^{(2)}_{\mathrm{eff}}$:

$$S^{(2)}_{eff} = T \sum_{\varepsilon} \int d^D q \varphi^* \left\{ -i\varepsilon + \frac{\mathrm{q}^2}{2m^*} - \mu^* \right\} \varphi,$$

$$\mu^* = \varepsilon_p - 2\mu. \tag{25}$$

The Bose fields have been renormalized in (25):

$$\Delta(\mathrm{q}, \varepsilon) = \left(\frac{\partial \Pi_2}{\partial 2\mu}\right)^{-1/2} \varphi(\mathrm{q}, \varepsilon). \tag{26}$$

The quantity $S_{\text{eff}}^{(2)}$ in (25) is evidently the action for an ideal gas of Bose particles with a mass m^* and a chemical potential $\mu^* = \varepsilon_p - 2\mu$. The other contributions to the total action (19b) determine the residual interaction between bosons. If we retain only the quadratic part of the action S_{eff} in (18), we find the following result for the number of particles n from (11), using (14) and (25):

$$n = 2\langle\varphi^*\varphi\rangle = \int \left[\exp\left(\frac{-\mathrm{q}^2/2m^* + \mu^*}{T}\right) - 1\right]^{-1} d^D\mathrm{q}/(2\pi)^D. \tag{27}$$

For the condensate density and the chemical potential at $T=0$ we then find

$$\langle\varphi\rangle = \sqrt{n/2}, \quad \mu^* = \varepsilon_p - 2\mu = 0. \tag{28}$$

The transition temperature T_0 is given by the usual expression of Bose-gas theory. It is determined by the vanishing of the chemical potential μ^*:

$$T_0 \sim \frac{(n/2)^{2/D}}{m^*}. \tag{29}$$

With the renormalization (26), expression (28) is exactly the same as the mean-field result, (8). Expression (25) for the action can thus be thought of as a sort of improved mean-field approximation, whose validity is not restricted to $T=0$.

The terms of higher order in the Bose fields in S_{eff} characterize the strength of the residual interaction between bosons, so these are the terms which determine whether the mean-field description is valid even at $T=0$. Let us examine these terms in detail.

In the calculation of $S_{\text{eff}}^{(2l)}$ at $l>1$ we can ignore the ε and q dependence of the coefficients of $(\Delta)^{2l}$, since each power of the Bose field appears with an additional small factor $\sim\sqrt{n}$. Using renormalization (26), we then find the following expression for $S_{\text{eff}}^{(2l)}$ from (19b):

$$S_{eff}^{(2l)} = \frac{1}{l}\left(\frac{\partial \Pi_2}{\partial 2\mu}\right)^{-l} \Pi_{2l}(\varphi^*\varphi)^l, \tag{30}$$

where

$$\Pi_{2l} = T\sum_{\omega} \int \frac{d^D\mathrm{k}/(2\pi)^D}{(i\omega - \varepsilon(\mathrm{k}) - \mu)^l (i\omega + \varepsilon(\mathrm{k}) + \mu)^l}. \tag{31}$$

Carrying out the summation in (31), we find our final expression S_{eff} for a Bose liquid of local pairs:

$$S_{eff} = T\sum_{\varepsilon} \int d^D\mathrm{q} \left\{\varphi^*\left[-i\varepsilon + \frac{q^2}{2m^*} - (\varepsilon_p - 2\mu)\right]\varphi + \sum_{l=2}^{\infty} v_l(\varphi^*\varphi)^l\right\}. \tag{32}$$

The constants v_l, which determine the potentials of the l-particle interaction, are given by

$$v_l = (-1)^l \frac{(2l-2)!}{l[(l-1)!]^2}\left(\frac{\partial \Pi_2}{\partial 2\mu}\right)^{-l} \int \frac{d^D\mathrm{k}/(2\pi)^D}{(2\varepsilon(\mathrm{k}) + \varepsilon_p)^{2l-1}}. \tag{33}$$

For a D-dimensional system with a parabolic dispersion relation in the band we find the following estimate of v_l:

$$v_l \sim \varepsilon_p r_p^{D(l-1)}, \quad r_p \sim (m^*\varepsilon_p)^{1/2}. \tag{34}$$

To find the relative strength of the interaction, we rewrite S_{eff} in dimensionless variables. For this purpose, we normalize the density of the Bose fields to $\sqrt{n}$, and we scale all quantities with units of energy by the condensation temperature T_0. For the dimensionless constant of the l-particle interaction we then find

$$v_l \sim \frac{v_l}{T_0} n^{l-1} \sim (r_p n^{1/D})^{D(l-1)-2}. \tag{35}$$

It follows from (35) that representation (32) for the action of the original Fermi system is an asymptotic expansion in terms of the "gaseousness" parameter $r_p n^{1/D}$ and is valid to the extent that this parameter is small ($r_p n^{1/D} \ll 1$), as we might expect on physical grounds. Furthermore, (35) shows that the binary interaction, $v_2(l=2)$, is the governing interaction for any dimensionality. According to general expression (33), this interaction corresponds to a repulsion, determining the stability of the Bose liquid of pairs and properties analogous to those of He^4. For v_2 we find the estimate

$$v_2 \sim (r_p n^{1/D})^{D-2}. \tag{36}$$

For 3D systems ($D=3$) under the condition $n^{1/3} r_p \ll 1$, we thus have a Bose liquid with a weak interaction; for $D=2$ we have a liquid with an intermediate interaction strength $v_2 \sim 1$; and for $D=1$ we have a strongly interacting Bose system ($v_2 \gg 1$). In the case of a quadratic dispersion relation, the picture of a Bose condensation of an ideal gas of local pairs (which corresponds in the case $T=0$ to the mean-field approximation) with a condensate density $\langle\varphi\rangle \sim \sqrt{n}$ is really accurate only for 3D systems. For systems of lower dimensionality, the corrections to the mean-field approximation for the residual interaction are large even at $T=0$.

It follows from the results found by the mean-field approach (Sec. 2) that the dimensionality D of the system enters the problem only through the density of states, so systems which have different dimensionalities but identical densities of states $N(\varepsilon)$ behave identically. We can demonstrate that it is the dimensionality D which has the governing effect on the strength of the residual interaction. As an illustration of this assertion, we might compare a 1D system with systems which have a higher dimensionality but the same energy dependence of the density of states. We know that a 1D behavior of the density of states, $N(\varepsilon) \sim 1/\sqrt{\varepsilon}$, arises at $D>1$ at the edges of the allowed bands which form as the result of an exciton instability in metals with a Fermi surface with flat regions or in a semimetal whose electron and hole Fermi surfaces are congruent (an exciton insulator[9]). An example of a system with a Fermi surface which has this property is a half-filled square lattice in the strong-coupling approximation. The $1D$ structural feature in the density of states arises in this case as the result of the opening of a gap over the entire Fermi surface. For definiteness we consider the $3D$ spectrum which is formed at the insulating transition in an isotropic semimetal. Near the bottom of the band we have the quadratic dispersion relation

$$\varepsilon(\mathbf{k}) = \frac{(|k| - k_0)^2}{2\Delta}, \tag{37}$$

where k_0 is the Fermi momentum of the original semimetal phase. The density of states in a system with $\varepsilon(\mathbf{k})$ as in (37)

$$N(\varepsilon) = \frac{k_0^2}{2\pi^2}\sqrt{\frac{\Delta}{2\varepsilon}}. \tag{38}$$

Calculating the parameters of the effective boson action in (32), we find

$$\varepsilon_p = \Delta\left(\frac{2\pi}{k_0^2}\right)^2; \quad m^* = 6\Delta;$$

$$v_2 = \frac{3\pi}{2}k_0^{-2}\sqrt{\frac{\varepsilon_p}{\Delta}} \equiv 3\sqrt{2}\,\varepsilon_p(r_p k_0^{-2}). \tag{39}$$

For the dimensionless binary-interaction constant we find the estimate

$$v_2 \sim (k_0^{-2} r_p n^{1/2})^{-1} \ll 1.$$

Consequently, despite the $1D$ behavior of the density of states, (38), we have obtained for this $3D$ system a nearly ideal Bose gas which is very different from the $1D$ case, in which we have $v_2 \gg 1$ according to (36), and the mean-field approximation is not valid even at $T = 0$.

4. SUPERCONDUCTING ORDER IN SYSTEMS WITH LOCALIZED IMPURITY STATES

In real systems with only a few particles, e.g., doped semiconductors, charge carriers usually appear because of the introduction of impurity atoms which create a randomly distributed nonuniform potential. Such a potential usually leads to the formation of local impurity states in the band gap. Let us examine the effect of these states on the superconducting ordering in the mean-field approximation. We should of course recall that this approximation is justified for only a limited case of systems, according to the results of the preceding section of this paper.

The introduction of M impurity atoms with a potential $u(\mathbf{r})$ is described by adding a term

$$H_{imp} = \int dr \sum_{\sigma} \sum_{j-1}^{M} u(r - R_j)\Psi_\sigma^+(r)\Psi_\sigma(r) \tag{40}$$

to the Hamiltonian (1), where $\mathbf{R}_j$ is the coordinate of the jth impurity atom. We assume that, as the result of the appearance of inhomogeneities, localized states with energies ε_0 arise. When there is an attraction in the system, these states participate in forming a superconducting condensate.

We assume that the order parameter Δ is a self-averaging quantity. In the case at hand, this assumption can be justified if the binding energy of a pair in the band satisfies $\varepsilon_p > 2\varepsilon_0$. Under this condition, the spatial variations in $\Delta(\mathbf{r})$ are slight. The self-consistency equation, averaged over the positions of the impurity atoms, is

$$\frac{1}{g} = \frac{1}{2}\int \frac{\widetilde{N}(\varepsilon)d\varepsilon}{\sqrt{(\varepsilon + \mu)^2 + \Delta^2}} + \frac{1}{2}\frac{n_{im}}{\sqrt{(\varepsilon_0 - \mu)^2 + \Delta^2}}. \tag{41}$$

The quantity $\widetilde{N}(\varepsilon)$ in (41) is the band density of states, renormalized because of scattering by impurities, and $n_{\rm im}$ is the impurity concentration. In addition, we have allowed for the circumstance that the chemical potential is negative (as we have done everywhere else in this paper). If one particle is introduced along with each impurity atom, the equation for the number of particles becomes

$$n_{im} = \int_0^\infty \left(1 - \frac{\varepsilon + \mu}{\sqrt{(\varepsilon + \mu)^2 + \Delta^2}}\right)N(\varepsilon)d\varepsilon$$

$$+ n_{im}\left(1 - \frac{\mu - \varepsilon_0}{\sqrt{(\mu - \varepsilon_0)^2 + \Delta^2}}\right). \tag{42}$$

We consider the case of light doping ($n_{\rm im} \to 0$). We then have $\Delta/\mu \ll 1$, as in Sec. 2. Furthermore, since the contribution from the change in the band density is on the order of $n_{\rm im}/\mu$ in this case, we can ignore the change in the continuous spectrum under the condition $(\mu - \varepsilon_0)/\mu \ll 1$. From Eqs. (41) and (42), we then find, respectively,

$$\frac{1}{g} = \int_0^\infty \frac{N(\varepsilon)d\varepsilon}{2\varepsilon + \tilde{\varepsilon}_p} + \frac{n_{im}}{\sqrt{(\tilde{\varepsilon}_p - 2\varepsilon_0)^2 + 4\Delta^2}}, \tag{43}$$

$$n_{im}\frac{\tilde{\varepsilon}_p - 2\varepsilon_0}{\sqrt{(\tilde{\varepsilon}_p - 2\varepsilon_0)^2 + 4\Delta^2}} = 2\Delta^2\int_0^\infty \frac{N(\varepsilon)d\varepsilon}{(2\varepsilon + \varepsilon_p)}. \tag{44}$$

These equations determine the superconducting order parameter Δ and the binding energy of the two-particle state as renormalized by the impurity, $\tilde{\varepsilon}_p \equiv 2\mu$. Equation (44) demonstrates the (physically understandable) fact that superconducting ordering is possible in a system in which all the charge carriers are localized only if the pair binding energy $\tilde{\varepsilon}_p$ is larger than twice the ionization potential ε_0.

Using the expression (5) for the coupling constant q in terms of the seed energy of the two-particle state, we can rewrite (43) and (44) as

$$\tilde{\varepsilon}_p - \varepsilon_p = \frac{n_{im}g^2 d\varepsilon_p/dg}{\sqrt{(\tilde{\varepsilon}_p - 2\varepsilon_0)^2 + 4\Delta^2}}, \tag{45}$$

$$2n_{im}g^2\frac{d\varepsilon_p}{dg}\frac{\tilde{\varepsilon}_p - 2\varepsilon_0}{\sqrt{(\tilde{\varepsilon}_p - 2\varepsilon_0)^2 + 4\Delta^2}} = 4\Delta^2. \tag{46}$$

From (45) we find an unambiguous increase in the binding energy of the pair in the presence of localized states. As we will see below, this fact is related to an increase in the interaction constant due to virtual transitions of particles from the band to impurity levels.

We introduce some new variables in (45) and (46):

$$t=\frac{\tilde{\varepsilon}_p-2\varepsilon_0}{|\varepsilon_p-2\varepsilon_0|},\quad x=\frac{4\Delta^2}{(\varepsilon_p-2\varepsilon_0)}. \tag{47}$$

We then find the system of equations

$$t\pm 1=\frac{\alpha}{2\sqrt{t^2+x}}, \qquad \frac{dt}{\sqrt{t^2+x}}=x, \tag{48}$$

in which the plus sign corresponds to the case $2\varepsilon_0-\varepsilon_p>0$, and the minus sign to $2\varepsilon_0-\varepsilon_p<0$. The parameter α in (48) is given by

$$\alpha=\frac{2n_{im}g^2d\varepsilon_p/dg}{(\varepsilon_p-2\varepsilon_0)^2}. \tag{49}$$

Eliminating the variable t from (48), we finally find

$$\alpha=x\left\{1+\frac{4x}{(\sqrt{1+2x}\mp 1)^2}\right\}^{1/2}, \tag{50}$$

$$t=\frac{1}{2}(\mp 1+\sqrt{1+2x}).$$

Equations (50) can easily be solved in the asymptotic regions in the parameter α. For $\alpha\ll 1$ we find, for (a) $\varepsilon_p<2\varepsilon_0$,

$$\Delta=\frac{1}{2}\frac{n_{im}g^2d\varepsilon_p/dg}{2\varepsilon_0-\varepsilon_p},\quad \tilde{\varepsilon}_p-2\varepsilon_0=\frac{1}{2}\frac{n_{im}^2g^4(d\varepsilon_p/dg)^2}{(2\varepsilon_0-\varepsilon_p)^3}, \tag{51a}$$

and for (b) $\varepsilon_p>2\varepsilon_0$,

$$\Delta=(g^2d\varepsilon_p/dg)^{1/2}\sqrt{n_{im}},\quad \tilde{\varepsilon}_p=\varepsilon_p. \tag{51b}$$

For $\alpha\gg 1$ we find

$$\Delta=\left[g^2\frac{d\varepsilon_p}{dg}\frac{n_{im}}{\sqrt{6}}\right]^{1/2},\quad \tilde{\varepsilon}_p-2\varepsilon_0=\left[\frac{2}{3}n_{im}g^2\frac{d\varepsilon_p}{dg}\right]^{1/2}. \tag{51c}$$

Figure 1 shows the superconducting order parameter Δ and the binding energy $\tilde{\varepsilon}_p$ versus the impurity concentration $n_{\rm im}$ and the depth of the impurity level, ε_0.

By changing variables as in (47) we find that the three independent parameters $n_{\rm im}$, ε_p, and ε_0 appear in the self-consistency equations only in the form of the parameter α [see Eq. (49)]. To see the physical meaning of this parameter, we calculate the correction to the interaction constant for virtual transition from the band to impurity levels. Figure 2 shows a diagram corresponding to this process. In the case at hand we find

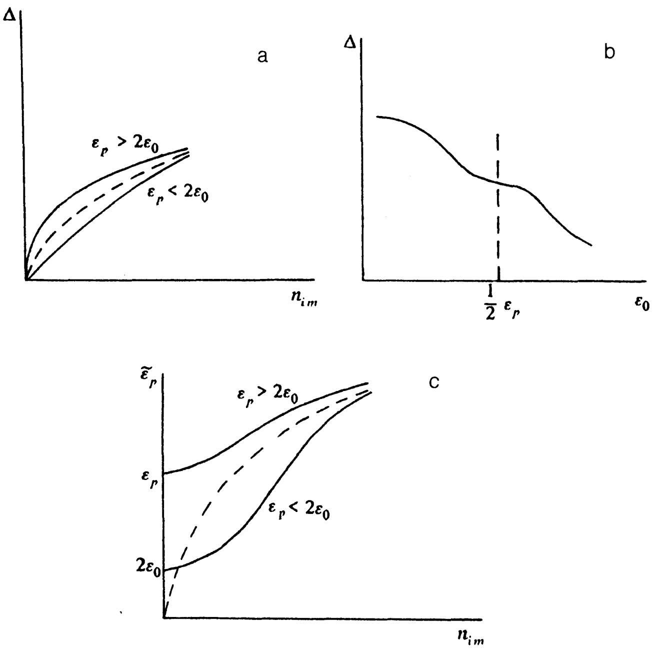

FIG. 1. a—Δ versus the impurity concentration $n_{\rm im}$; b—Δ versus the energy of the impurity level; c—the binding energy $\tilde{\varepsilon}_p$ versus the impurity concentration $n_{\rm im}$.

$$\delta g\sim\frac{g^2}{\varepsilon_p-2\varepsilon_0}.$$

For the relative change in $\varepsilon_p-2\varepsilon_0$, on the other hand, we have

$$\frac{\delta(\varepsilon_p-2\varepsilon_0)}{\varepsilon_p-2\varepsilon_0}=\frac{(d\varepsilon_p/dg)\delta g}{\varepsilon_p-2\varepsilon_0}\sim n_{im}\frac{g^2(d\varepsilon_p/dg)}{(\varepsilon_p-2\varepsilon_0)^2}\sim\alpha.$$

We can thus indeed assert that the increase in the binding energy $\tilde{\varepsilon}_p$ and the appearance of a superconductivity (even if the seed binding energy ε_p is smaller than the energy for excitation of two particles in the band) are consequences of an increase in the interaction constant due to virtual transition from the band to impurity levels.

5. CONCLUSION

There is the widespread belief that an explanation for the unusual properties of the high T_c superconductors should be sought in a common model which interpolates between the limits of strong and weak interactions.[10] The choice of an initial approximation is in many regards just a

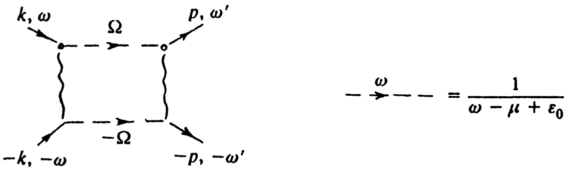

FIG. 2. Diagram for the correction to the interaction constant.

matter of taste. However, the procedure described above for going over to the Bose limit with decreasing carrier density—a procedure which incorporates the strong-interaction region—demonstrates that the band-theory approach has definite advantages. For the case in which the largest energy parameter in the system is the energy of the two-particle bound state, we have proposed a regular procedure not only for describing the transition to the Fermi picture of the excitations to the Bose picture but also for dealing with the residual interactions in the Bose limit. While equivalent from the standpoint of a mean-field description, these pictures may differ substantially in the strength of the residual interactions and thus in the nature of the transition to the condensed state. It has been established here that the interaction of charge carriers with impurities (or other defects) can be described through a renormalization of the bound-state energy. This energy thus does indeed serve as a universal parameter in the low-density limit. Bose degrees of freedom also arise in a fairly natural way in models of nearly localized, strongly interacting charge carriers. However, strong quantum phase fluctuations make it difficult to describe the properties of the system over any appreciable range of densities in this model.

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