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Bardeen-Cooper-Schrieffer Pairing in Antiferromagnetic Superconductors

M. J. Nass and K. Levin
The James Franck Institute and Department of Physics, The University of Chicago, Chicago, Illinois 60637

and

G. S. Grest
Department of Physics, Purdue University, West Lafayette, Indiana 47907

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The mean-field theory of an antiferromagnetic superconductor is solved and some fluctuation effects are discussed. In contrast to claims of other authors, it is found that the pairing is of the usual BCS type, $\Delta = \langle C_{\vec{k},\uparrow}^{\dagger} C_{-\vec{k},\downarrow}^{\dagger} \rangle$. Results for the gap parameter $\Delta(T)$ and $H_c(T)$ are presented. The latter is similar to the measured $H_{c2}(T)$. The ratio $\Delta(0)/T_c$ and the (nonmonotonic) temperature T dependence of H_c and $\Delta(T)$ are shown to deviate markedly from BCS theory.

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The recent discovery of antiferromagnetic (AF) superconductors[1] has revived interest in the problem of coexistent magnetic and superconducting order. In this Letter we present a mean-field theory and discuss some fluctuation effects for a system of superconducting electrons interacting with antiferromagnetically ordered localized spins. While we treat a somewhat idealized three-dimensional system, our qualitative results are relevant to the Chevrel-phase and rare-earth rhodium boride AF superconductors.

One purpose of this paper is to establish the nature of the (most favorable) Cooper pairs: We find, in contrast to a previous claim,[2] that the order parameter is of the usual BCS type, $\langle C_{\vec{k},\uparrow}^{\dagger} C_{-\vec{k},\downarrow}^{\dagger} \rangle = \Delta_0 \equiv \Delta$. Another aim is to calculate the thermodynamic variables Δ, T_c, and H_c. In particular, we find a nonmonotonic temperature T dependence of Δ and H_c. The latter quantity, which is related to the difference of the free energies in the normal and superconducting phases, is found to have a T dependence rather similar to that of the measured upper critical field H_{c2} (Ref. 3) for the Chevrel-phase AF superconductors.

The importance of doing a mean-field calculation should be emphasized. First, it is essential in order to properly characterize the Cooper pairs. Second, it is a necessary first step in any treatment of fluctuation effects. Using mean-field theory as a basis, we can then obtain the Eliashberg-like equations for the renormalized gap function $\tilde{\Delta}$ and effective mass from which we derive the superconducting density of states and an effective spin-flip lifetime τ_s. We will discuss this briefly at the end of this paper and in more detail in a subsequent work.

Our Hamiltonian contains the d-electron kinetic energy, the d-electron–f-electron exchange interaction J^{df} (assumed constant for simplicity), and the d-d interaction arising from the phonons. In our mean-field theory we replace the Fourier transform of the f-electron spin operator S_i by a temperature-dependent molecular field $H_Q \equiv J^{df}\langle S_Q \rangle / 2N$, where $\vec{Q}$ is the wave vector of the antiferromagnetic order. The electron-electron term, which is written as

$$-\sum_{\substack{\vec{k},\vec{k}',\vec{q},\\ \sigma,\sigma'}} V_{\vec{k}\vec{k}',\vec{q}} C_{\vec{k}+\vec{q},\sigma}^{\dagger} C_{\vec{k}',-\vec{q},\sigma'}^{\dagger} C_{\vec{k}',\sigma'} C_{\vec{k},\sigma},$$

allows electron pairing with $q = 0$ and $q = \pm Q$, all of which must be included in order to proceed in the most general way.

Our mean-field Hamiltonian thus becomes

$$H^{\mathrm{mf}} = \sum_{\vec{k},\sigma} \epsilon_k C_{\vec{k},\sigma}^{\dagger} C_{\vec{k},\sigma} - \sum_{\vec{k},\sigma} H_{Q,\sigma} (C_{\vec{k},\sigma}^{\dagger} C_{\vec{k}+\vec{Q},\sigma} + C_{\vec{k}+\vec{Q},\sigma}^{\dagger} C_{\vec{k},\sigma})$$
$$- \sum_{\vec{k}} \Delta_0(\vec{k}) C_{\vec{k},\uparrow}^{\dagger} C_{-\vec{k},\downarrow}^{\dagger} - \sum_{\vec{k}}{}' \Delta_Q(\vec{k}) C_{\vec{k}+\vec{Q},\uparrow}^{\dagger} C_{-\vec{k},\downarrow}^{\dagger}$$
$$- \sum_{\vec{k}}{}' \Delta_{-Q}(\vec{k}) C_{\vec{k},\uparrow}^{\dagger} C_{-\vec{k}-\vec{Q},\downarrow}^{\dagger} + \text{c.c.} \qquad (1)$$

The prime on the summation indicates that we are dealing with a restricted region of $\vec{k}$ space; namely, that region (called region I) near the Fermi surface (FS) in which both $\epsilon_{|\vec{k}|}$ and $\epsilon_{|\vec{k}+\vec{Q}|}$ are within the BCS cutoff frequency, ω_c, of the Fermi energy, E_F. Here we will ignore the very small additional contribution to the magnetic mean field which comes about from a factorization of the phonon-induced electron-electron interaction. We treat H_Q exactly only in region I, since its effects are most significant there. In the remainder of the FS (called region II), H_Q leads to only weak perturbative corrections, which we ignore here.[4] The order parameters are defined by the self-consistent equations

$$\Delta_0(\vec{k}) = \sum_{\vec{k}'} \langle C_{-\vec{k}',\downarrow} C_{\vec{k}',\uparrow} \rangle V_{\vec{k}',-\vec{k}',\vec{k}-\vec{k}'}, \qquad (2a)$$

$$\Delta_Q(\vec{k}) = 2 \sum_{\vec{k}'}{}' \langle C_{\vec{k}',\uparrow} C_{-\vec{k}'+\vec{Q},\downarrow} \rangle V_{-\vec{k}'+\vec{Q},\vec{k}',\vec{k}'+\vec{k}}, \qquad (2b)$$

$$\Delta_{-Q}(\vec{k}) = 2 \sum_{\vec{k}'}{}' \langle C_{-\vec{k}'-\vec{Q},\downarrow} C_{\vec{k}',\uparrow} \rangle V_{\vec{k}',-\vec{k}'-\vec{Q},\vec{k}-\vec{k}'}. \qquad (2c)$$

The anomalous pairing with $Q \neq 0$ is presumed to take place only in region I. The inclusion of these terms allows us to consider the "new pairing state" proposed in a recent Letter by Machida, Nokora, and Matsubara[2] on the basis of some suggestions by Baltensperger and Strässler.[5] Their pairing may be written as a particular linear combination of the pairings in Eqs. (2). However, we have found that the Machida, Nokora, and Matsubara order parameter leads to inconsistencies, because, as Baltensperger and Strässler state,[5] "only the interactions between the chosen pairs are retained." Since the other discarded interactions are nonzero, this assumption leads to a violation of the self-consistent gap equations given by Eqs. (2).

The solution of Eqs. (2) involves the diagonalization of a 4×4 matrix, as in the case of previous work on the charge-density wave.[6] Simple analytic expressions can be obtained only in the one-dimensional limit. In this case, we take $Q = 2k_F$ so that $\epsilon_{|\vec{k}|} \sim -\epsilon_{|\vec{k}+\vec{Q}|}$ for k near $-k_F$. We have looked for solutions for arbitrary Δ_Q and Δ_{-Q}. In the case $\Delta_Q = -\Delta_{-Q}$, which is the only one which can be easily handled analytically, we have

$$\Delta_Q = \sum_{\vec{k}',\sigma} V\{[1-2f(E_\sigma)]/2E_\sigma\}(\Delta_Q + \sigma\epsilon_k), \qquad (3a)$$

$$\Delta_0 = \sum_{\vec{k}',\sigma} V\{[1-2f(E_0)]/2E_\sigma\}(\Delta_0 + \sigma H_Q), \qquad (3b)$$

where

$$E_\sigma = [(\Delta_0 + \sigma H_Q)^2 + (\Delta_Q + \sigma\epsilon_k)^2]^{1/2}$$

and $f(E)$ is the usual Fermi function. Here we have adopted the BCS step function potential (of amplitude V) for $V_{\vec{k}\vec{k}'\vec{q}}$, so that the summations in Eqs. (3) are restricted to within ω_c of E_F. When $\Delta_Q = 0$, one can derive the same equation for T_c either by using Eq. (3b) or by considering the instability of the particle-particle vertex function. This latter approach was incorrectly applied in Ref. 2. A general detailed numerical study suggests that the case $\Delta_0 \neq 0$, with $\Delta_Q = \Delta_{-Q} = 0$, $Q \neq 0$, is the only allowed nontrivial solution of Eqs. (2), so that in one dimension the usual BCS pairing is preferred. Physically, this is a consequence of the fact that $Q = 2k_F$ is large compared to the inverse coherence length ξ_0^{-1}, so that Cooper pairing of this large momentum Q is highly unfavorable. Mathematically, for Eq. (3a) this arises because the $d\epsilon_k$ integration can be transformed to a new variable $d(\epsilon_k \pm \Delta_Q)$ without significantly changing the limits of integration, $\pm\omega_c$. Then the right-hand side of Eq. (3a) vanishes. More generally, this can be seen with use of the Green's function analysis discussed below.

Based on these observations, in the three-dimensional case we have numerically solved our equations with $\Delta_Q = \Delta_{-Q} = 0$. The equation for $\Delta_0 \equiv \Delta$ is

$$\Delta = \sum_{\mathrm{I},i} V\Delta\{(x_i y_i + z_i t_i)[1-2f(E_i)]\} + \sum_{\mathrm{II}} V(\Delta/2E)[1-2f(E)], \qquad (4)$$

where $E=(\epsilon_k^2+\Delta^2)^{1/2}$ and the index $i=+$ or $-$, corresponding to the eigenvalues

$$E_\pm=(\tfrac{1}{2}(\epsilon_k^2+\epsilon_{|\vec{k}+\vec{Q}|}^2)+\Delta^2+H_Q^2\pm\tfrac{1}{2}\{(\epsilon_k^2-\epsilon_{|\vec{k}+\vec{Q}|}^2)^2+4H_Q^2[(\epsilon_k+\epsilon_{|\vec{k}+\vec{Q}|})^2+4\Delta^2]\}^{1/2})^{1/2}, \tag{5}$$

with

$$x_i=(N_i)^{-1}H_Q(\epsilon_{|\vec{k}+\vec{Q}|}-\epsilon_k+2E_i),\quad y_i=(N_i)^{-1}H_Q[\Delta^2-H_Q^2+(\epsilon_k+E_i)(\epsilon_{|\vec{k}+\vec{Q}|}+E_i)],$$
$$z_i=(N_i)^{-1}[H_Q^2-\Delta^2-\epsilon_k^2+E_i^2],\quad t_i=(N_i)^{-1}[H_Q^2(\epsilon_k-E_i)-\Delta^2(\epsilon_{|\vec{k}+\vec{Q}|}+E_i)-(\epsilon_{|\vec{k}+\vec{Q}|}+E_i)(\epsilon_k^2-E_i^2)], \tag{6}$$

where N_i is chosen so that $x_i^2\Delta^2+y_i^2+z_i^2\Delta^2+t_i^2=1$. In order to perform the indicated integrations over regions I and II, we assume that when $H_Q=0$, the FS is spherical: $\epsilon_k=k^2-E_F$. The factor ω_c/k_FQ for $Q<2k_F$ thus denotes the relative "size" of region I. However, it is difficult to estimate this parameter. The other parameter which determines the importance of the contribution from region I is H_Q/ω_c. The quantity H_Q, which is determined by J^{df}, is believed to be of the order of ~ 100 K at low temperatures.[7] Note that the Néel temperature (which is not determined by J^{df} alone) is of the order of 1–10 K. For definiteness, we assume a temperature-dependent H_Q given by $H_Q(T)=H_Q(0)(1-T/T_N)^{1/2}$ for T less than the Néel temperature T_N and 0 otherwise. We also take the phonon-coupling constant $N(0)V=0.2$ throughout this work. From the experimental findings,[7] we have $0.1\lesssim H_Q(0)/\omega_c\lesssim 1.0$. One would expect that in a strictly one-dimensional system, pairing can only take place for H_Q somewhat less than $\sim\omega_c$, since the antiferromagnetic "gap" must be small compared to the cutoff frequency. In this way both the upper and lower magnetic bands participate in the pairing. The situation is more complicated in three dimensions. As may be expected, as H_Q increases, the contribution of the anomalous region to the superconductivity decreases. When the entire FS is in I, we find a critical $H_Q=0.15\omega_c$ above which T_c vanishes. For $\omega_c/k_FQ=0.2$, the contribution of I is very small only for $H_Q\gtrsim 5\omega_c$. Thus it takes a surprisingly large H_Q to significantly suppress the pairing in region I. This is a consequence of the coupling between the two regions. Because region II does not experience the magnetic field, it helps to "maintain" the pairing in region I.

In Fig. 1 we plot $\Delta(T)/\Delta(0)$ and $H_c(T)/H_c(0)$ as a function of temperature T. The square of $H_c(T)$ is proportional to the free-energy difference between the normal and superconducting phases. We choose $H_Q(0)/\omega_c=0.3$ and $T_N=T_c/2$. The curves a and b for $H_c(T)$ correspond to $\omega_c/k_FQ=0.08$ and 0.2, respectively. The $\Delta(T)$ plotted (curve c) corresponds to $\omega_c/k_FQ=0.08$. All curves are nonmonotonic in contrast to the nonmagnetically ordered case. The decrease in Δ with decreasing T near T_N arises because the "turning on" of H_Q suppresses the pairing. This effect was also found by Machida, Nokora, and Matsubara,[2] although incorrect equations for $\Delta(T)$ were used. In the case of a larger region I (curve b) the H_c curve deviates more dramatically from BCS theory than in curve a. This characteristic behavior has been observed in H_{c2} measurements[3] in XMo_6S_8 (with X a rare-earth element), which look very similar to our H_c curves. Thus the quantitative behavior of the H_{c2} data can be explained if one assumes, as in the usual type-II superconductors,[8] that $H_{c2}=\sqrt{2}\kappa H_c$, where κ varies slowly with T. However, this relation must be established within a more detailed theory. It is of interest to note that the value of the quantity $\Delta(0)/T_c$ is 40% smaller than the BCS value

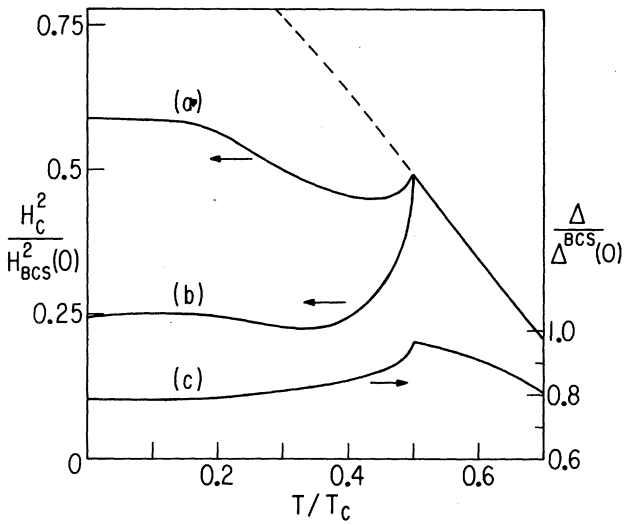

FIG. 1. Temperature dependence of the normalized free-energy difference H_c^2 and gap parameter Δ for ω_c/k_FQ given by 0.08 (a and c) and 0.2 (b). The parameter $H_Q(0)/\omega_c=0.3$ in all three curves. The dashed line is the BCS result.

(1.77) for the parameters in curve b.

We have derived the Green's functions for the present theory G_0, and in the presence of spin and density fluctuations $\tilde{G}$. We take as our *Ansatz* in one dimension for the renormalized 4×4 matrix Green's function in the basis $(C_{\vec{k},\uparrow} C_{-\vec{k},\downarrow}{}^{\dagger} C_{\vec{k}+\vec{Q},\uparrow} C_{-\vec{k}-\vec{Q},\downarrow}{}^{\dagger})$,

$$\underline{\tilde{G}}^{-1} = \tilde{\omega}\underline{1} - \epsilon_k \underline{\rho_3}\underline{\sigma_3} + \tilde{H}_Q \underline{\rho_1} + \tilde{\Delta}_0 \underline{\sigma_1} + \tilde{\Delta}_Q{}^{+} \underline{\rho_1}\underline{\sigma_1} - \tilde{\Delta}_Q{}^{-} \underline{\rho_2}\underline{\sigma_2}, \tag{7}$$

where $\Delta_Q{}^{\pm} \equiv \frac{1}{2}(\Delta_{-Q} \pm \Delta_Q)$ and $\underline{\rho_i}$ and $\underline{\sigma_j}$ are the Pauli matrices in the electron-hole and spin spaces, respectively.[9] Here $\tilde{\omega}$, $\tilde{H}_Q$, $\tilde{\Delta}_0$, and $\tilde{\Delta}_Q{}^{\pm}$ are the renormalized frequency (or mass), magnetic field, and gap parameters. We find for elastic scattering that $\tilde{\Delta}_Q{}^{-} = 0$ and

$$(\tilde{\Delta}_0 \pm \tilde{H}_Q) - (\Delta_0 \pm H_Q) = \frac{1}{2\tau_1} \int \frac{\tilde{\Delta}_0 \mp \tilde{H}_Q}{D_{\mp}}\, d\epsilon, \tag{8a}$$

$$(\tilde{\omega} \pm \tilde{\Delta}_Q{}^{+}) - (\omega \pm \Delta_Q{}^{+}) = \frac{1}{2\tau_1} \int \frac{\tilde{\omega} \mp \tilde{\Delta}_Q{}^{+}}{D_{\mp}}\, d\epsilon, \tag{8b}$$

where $D_{\pm} = [\epsilon_k{}^2 - (\tilde{\omega} \pm \tilde{\Delta}_Q{}^{+})^2 + (\tilde{\Delta}_0 \pm \tilde{H}_Q)^2]$, and τ_1 is the appropriate golden-rule lifetime associated with charge fluctuations. Analogous equations hold for inelastic processes, except that then the right-hand sides of Eq. (8) each involve a summation over the Matsubara frequency ω_n, a variable which appears as an argument in all the renormalized parameters $\tilde{\omega}_n(\omega_n)$, etc. One can use Eqs. (8) to rederive the weak-coupling results obtained earlier. In this case we obtain $\underline{G}_0$ from $\underline{\tilde{G}}$ by replacing renormalized quantities by bare ones and replace $1/\tau_1$ by the BCS step-function potential (which depends only on ϵ) and then integrate over ϵ and sum over ω_n. The latter summation leads to the immediate conclusion that $\Delta_Q{}^{\pm} = 0$ in weak-coupling theory. It is important to note, following Ref. 9, that Eqs. (8) show that in the one-dimensional limit the Anderson theorem (for spin-independent impurities) is violated in antiferromagnetic superconductors. For spin-dependent impurities, spin fluctuations, and spin-orbit scattering, equations analogous to (8) have been obtained by generalizing Eq. (7) to an eight-dimensional vector space. Furthermore, there will generally be additional terms in Eqs. (8) deriving from "umklapp" processes; these lead to terms in $\tilde{\omega}$, etc., which couple to the "mixed" susceptibility χ_{NM}. In three dimensions the analogous equations are more complicated since $\tilde{\omega}$, etc., are functions of the direction of the momentum of the Fermi surface. All of these interesting effects will be discussed in a future paper.

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