Effect of nonmagnetic impurities on antiferromagnetic superconductors

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By the treatment of the electron-impurity scattering exactly by means of a t matrix, the effect of nonmagnetic impurities on antiferromagnetic superconductors has been investigated in detail. Our study is an extension of the recent work of Nass, Levin, and Grest to the strong-scattering case. The appearance of bound states due to impurities for $H_Q > \Delta$ is discussed (here H_Q is the antiferromagnetic molecular field and Δ is the superconducting order parameter). Investigating the density of states $[N(\omega)]$, we show the growth of the "impurity band" with the increase in impurity concentration. The "dirty"-limit behavior of the system and the condition for the appearance of the gaplessness are discussed analytically.

I. INTRODUCTION

Recently, there has been considerable interest in the problem of coexistence of antiferromagnetism and superconductivity.[1] The mean-field theory of antiferromagnetic superconductors (AFS) has been developed by introducing the antiferromagnetic (AF) molecular field into the Bardeen-Cooper-Schrieffer (BCS) model.[2–5] The effect of impurities on AFS has been studied by Nass, Levin, and Grest (NLG).[5]

In Ref. 5, the electron-impurity scattering is considered by using the lowest-order Born-approximation theory of Abrikosov and Gor'kov[6] (AG), and NLG have pointed out some similarities in the behavior of nonmagnetic impurities in AFS with that of magnetic impurities in the usual superconductors. For the latter case, the works of Shiba[7] and Rusinov[8] have shown that an exact treatment of the electron-impurity scattering brings about remarkable changes in the properties of the BCS superconductors.[9] Thus it is important to investigate the influence of nonmagnetic impurities on AFS by considering the scattering of the conduction electrons from the impurities exactly. Such a study has been carried out in the present paper. For the single-impurity problem, we discuss the appearance of the impurity bound states for $H_Q > \Delta$ (where H_Q is an AF molecular field and Δ is a superconducting order parameter). Such bound states in the coexistence region of spin-density wave and superconductivity in highly anisotropic organic conductors were considered by Machida.[10] For the finite-concentration problem, we show the growth of the "impurity band" with the increase in impurity concentration. The appearance and the disappearance of the gaplessness are also discussed. We give an analytical investigation of the interesting behavior of the impurity-concentration dependence which was demonstrated numerically by NLG.[5]

The plan of the paper is as follows. In Sec. II we outline the general formalism. The single-impurity problem is discussed in Sec. III. We consider the problem of the finite impurity concentration in Sec. IV, and obtain the so-called u_n equation. In Sec. V we calculate the density of states as a function of the impurity concentration. Section VI is devoted to summary and discussion. Some of the detailed calculations are given in Appendixes A and B.

II. FORMALISM

The mean-field Hamiltonian for an AFS is

$$\mathcal{H}_0 = \sum_{\vec{k},\alpha} \epsilon_{\vec{k}} C^{\dagger}_{\vec{k},\alpha} C_{\vec{k},\alpha} - \Delta \sum_{\vec{k}} (C^{\dagger}_{\vec{k},\uparrow} C^{\dagger}_{-\vec{k},\downarrow} + \text{H.c.}) - H_{\vec{Q}} \sum_{k_{\parallel}(<0),\alpha,\beta} (\sigma_z)_{\alpha\beta} (C^{\dagger}_{\vec{k}+\vec{Q},\alpha} C_{\vec{k},\beta} + \text{H.c.}) , \tag{2.1}$$

where $\epsilon_{\vec{k}}$ is the single-particle energy measured from the Fermi level, $C^{\dagger}_{\vec{k},\alpha}$ is the creation operator for the conduction electron, α and β are spin indices, σ_z is a Pauli matrix, Δ is the superconducting order parameter, $H_{\vec{Q}}$ is the AF molecular field (considered temperature independent in this paper), $\vec{Q}$ is the wave vector characterizing the AF order, and $k_{\parallel}$ is the component of the wave vector $\vec{k}$ parallel to $\vec{Q}$. The superconducting order parameter Δ is determined self-consistently by

$$\Delta = g \sum_{\vec{k}} \langle C_{-\vec{k},\downarrow} C_{\vec{k},\uparrow} \rangle , \tag{2.2}$$

where g is the BCS coupling constant and the angular brackets denote the thermal average. We have taken Δ as real and positive.

We introduce the finite-temperature Green's function

$$G_{\vec{k}\vec{k}'}(\tau) = -\langle T_{\tau}[\psi_{\vec{k}}(\tau)\psi^{\dagger}_{\vec{k}'}(0)] \rangle \tag{2.3}$$

having an eight-dimensional base with

$$\psi^{\dagger}_{\vec{k}}=(C^{\dagger}_{\vec{k},\uparrow},C^{\dagger}_{-\vec{k},\downarrow},C_{\vec{k},\uparrow},C_{-\vec{k},\downarrow},C^{\dagger}_{\vec{k}+\vec{Q},\uparrow}C^{\dagger}_{-\vec{k}-\vec{Q},\downarrow},C_{\vec{k}+\vec{Q},\uparrow},C_{-\vec{k}-\vec{Q},\downarrow}) , \tag{2.4}$$

and T_τ as the ordering operator for the imaginary time τ.

The unperturbed Green's function is given by

$$G^0_{\vec{k}}(i\omega_n)=(i\omega_n-\epsilon_s\rho_3-\epsilon_a\tau_3\rho_3-\Delta\rho_2\sigma_2+H_{\vec{Q}}\tau_1\rho_3\sigma_3)^{-1} , \tag{2.5}$$

with

$$\epsilon_s=\tfrac{1}{2}(\epsilon_{\vec{k}}+\epsilon_{\vec{k}+\vec{Q}}) , \tag{2.6}$$

$$\epsilon_a=\tfrac{1}{2}(\epsilon_{\vec{k}}-\epsilon_{\vec{k}+\vec{Q}}) , \tag{2.7}$$

where ω_n is the Matsubara frequency [i.e., $\omega_n=\pi T(2n+1)$, with T as temperature and n as an integer]. Further, σ_i, ρ_i, and τ_i $(i=1,2,3)$ are the 2×2 Pauli matrices operating on the ordinary spin states, the electron-hole states, and the positive- and negative-momentum states, respectively. A direct product such as $\tau_2\rho_2\sigma_1$ means

$$\tau_2\otimes\rho_2\otimes\sigma_1=\begin{bmatrix}0_{4\times4} & -i\rho_2\otimes\sigma_1\\ i\rho_2\otimes\sigma_1 & 0_{4\times4}\end{bmatrix}=\begin{bmatrix}0_{2\times2} & 0_{2\times2} & 0_{2\times2} & -\sigma_1\\ 0_{2\times2} & 0_{2\times2} & \sigma_1 & 0_{2\times2}\\ 0_{2\times2} & \sigma_1 & 0_{2\times2} & 0_{2\times2}\\ -\sigma_1 & 0_{2\times2} & 0_{2\times2} & 0_{2\times2}\end{bmatrix} . \tag{2.8}$$

The interaction of a conduction electron with a nonmagnetic impurity is described by the Hamiltonian

$$\mathcal{H}_{\rm imp}=\frac{1}{N}\sum_{\vec{k},\vec{k}'}\psi^{\dagger}_{\vec{k}}U\psi_{\vec{k}'} , \tag{2.9}$$

with

$$U=(V_1+V_2\tau_1)\rho_3 , \tag{2.10}$$

where V_1 (V_2) is the scattering potential with small (large) momentum transfer. The important role played by V_2 in the similar problem of impurities in charge-density-wave systems is well known.[11,12]

Although the four-dimensional base is enough for treating nonmagnetic impurities in AFS, we use the 8×8 notation for application to the magnetic impurity problem. It should be noted that in the present notation, the momentum $\vec{k}$ is restricted so that $k_{||}<0$ unless specified otherwise.

III. SINGLE-IMPURITY PROBLEM

Since this problem has been considered by Machida[10] in connection with the coexistence of spin-density wave and superconductivity in organic conductors, we only sketch it here briefly for use in later sections.

With the use of the definition given in Eq. (2.3) and the Hamiltonians given in Eqs. (2.1) and (2.9), the Green's function for the single-impurity case is obtained as

$$G_{\vec{k}\vec{k}'}(i\omega_n)=G^0_{\vec{k}}(i\omega_n)\delta_{\vec{k}\vec{k}'}+G^0_{\vec{k}}(i\omega_n)t(i\omega_n)G^0_{\vec{k}'}(i\omega_n) , \tag{3.1}$$

where the t matrix $t(i\omega_n)$ is given by

$$t(i\omega_n)=(1-UF^0)^{-1}U , \tag{3.2}$$

with

$$F^0(i\omega_n)=\frac{1}{N}\sum_{\vec{k}}G^0_{\vec{k}}(i\omega_n) . \tag{3.3}$$

In the above we include all terms with respect to V_1 and the even-order terms with respect to V_2. The interaction will be assumed short ranged and we set $V_1=V_2=V$ at the end of the calculation.

The general expression for $F^0(i\omega_n)$ obtained by using Eqs. (3.3) and (2.5) is given in Eq. (A3) of Appendix A. For a general three-dimensional (3D) electron band, the momentum sum can only be evaluated numerically. In order to bring out the essential new results of the present problem, we assume a one-dimensional (1D) electron band which satisfies the nesting condition $\epsilon_{k+Q}=-\epsilon_k$ for k near $-k_F$, that is, $\epsilon_s=0$. The extension to the 3D case is discussed in Sec. VI. Now Eq. (A3) gives

$$F^0(i\omega_n)=-\frac{\pi N_0}{4}\left[\frac{i\omega_n(1+\tau_1\rho_1\sigma_1)+\Delta_+(\rho_2\sigma_2-\tau_1\rho_3\sigma_3)}{(\omega_n^2+\Delta_+^2)^{1/2}}+\frac{i\omega_n(1-\tau_1\rho_1\sigma_1)+\Delta_-(\rho_2\sigma_2+\tau_1\rho_3\sigma_3)}{(\omega_n^2+\Delta_-^2)^{1/2}}\right] , \tag{3.4}$$

with

$$\Delta_{\pm}=\Delta\pm H_Q , \tag{3.5}$$

where N_0 is the density of single-particle states at the Fermi level in the normal metal.

An explicit expression for $t(i\omega_n)$ is not given here as we only discuss the existence of the bound states within the BCS gap. We obtain the poles of the t matrix for the real frequency ω by solving the equation

$$1+v^4+2v^2\frac{\Delta_+\Delta_--\omega^2}{(\Delta_+^2-\omega^2)^{1/2}(\Delta_-^2-\omega^2)^{1/2}}=0 , \tag{3.6}$$

where

$$v=\pi N_0 V \ . \tag{3.7}$$

We find that bound states due to the impurity exist if and only if $H_Q>\Delta$, and get the energy of bound states $\pm\omega_B$ as

$$\omega_B^2=(H_Q-\Delta)^2-\left[\frac{2-\zeta}{2(1-\zeta)}[4(1-\zeta)\Delta^2+\zeta^2H_Q^2]^{1/2}-2\Delta-\frac{\zeta^2}{2(1-\zeta)}H_Q\right]H_Q \ , \tag{3.8}$$

with

$$\zeta=4v^2/(1+v^2)^2 \ . \tag{3.9}$$

The variable ζ characterizes the strength of the electron-impurity scattering and takes the values between 0 and 1. When $\zeta\to 0$, $\omega_B\to(H_Q-\Delta)$. Further, when $\zeta\to 1$, $\omega_B\to 0$. In Fig. 1, the position of bound states is shown for $\zeta=0.5$ (curve *a*), 0.8 (curve *b*), and 0.95 (curve *c*). The cross-hatched area in the figure represents the continuum of states with peaks at $\omega=\Delta+H_Q$ and $|\Delta-H_Q|$.

IV. FINITE-CONCENTRATION PROBLEM

In this section we consider the finite-impurity-concentration problem. We assume that the impurities are randomly distributed and their concentration n_i is low enough so that the impurity-impurity interaction is negligible. The Green's function averaged over the impurity positions is connected with the self-energy $\Sigma_k(i\omega_n)$ by

$$G_k(i\omega_n)=\bar{G}_{\vec{k}\vec{k}'}(i\omega_n)=[G_k^0(i\omega_n)^{-1}-\Sigma_k(i\omega_n)]^{-1} \ . \tag{4.1}$$

The self-energy is taken as the t matrix, Eq. (3.2), times the impurity concentration n_i, with G_k^0 replaced by G_k. This procedure is the same as that used in the problem of magnetic impurities in usual superconductors.[7–9] We make the ansatz that the Green's function is given by

$$\begin{aligned}G_k(i\omega_n)&=(i\tilde{\omega}_n-\epsilon_k\tau_3\rho_3-\tilde{\Delta}_n\rho_2\sigma_2+i\tilde{\Omega}_n\tau_1\rho_1\sigma_1+\tilde{H}_{Qn}\tau_1\rho_3\sigma_3)^{-1}\\&=-\frac{1}{2}\left[\frac{1}{K_{n+}}[i\tilde{\omega}_{n+}(1+\tau_1\rho_1\sigma_1)+\epsilon_k(\tau_3\rho_3-\tau_2\rho_2\sigma_1)+\tilde{\Delta}_{n+}(\rho_2\sigma_2-\tau_1\rho_3\sigma_3)]\right.\\&\qquad\left.+\frac{1}{K_{n-}}[i\tilde{\omega}_{n-}(1-\tau_1\rho_1\sigma_1)+\epsilon_k(\tau_3\rho_3+\tau_2\rho_2\sigma_1)+\tilde{\Delta}_{n-}(\rho_2\sigma_2+\tau_1\rho_3\sigma_3)]\right] ,\end{aligned} \tag{4.2}$$

with

$$K_{n\pm}=\tilde{\omega}_{n\pm}^2+\epsilon_k^2+\tilde{\Delta}_{n\pm}^2 \ , \tag{4.3}$$

$$\tilde{\omega}_{n\pm}=\tilde{\omega}_n\pm\tilde{\Omega}_n \ , \tag{4.4}$$

$$\tilde{\Delta}_{n\pm}=\tilde{\Delta}_n\pm\tilde{H}_{Qn} \ . \tag{4.5}$$

Then the self-energy $\Sigma_k(i\omega_n)$ is calculated as

$$\Sigma_k(i\omega_n)=\Sigma^{(1)}(i\omega_n)+\Sigma^{(2)}(i\omega_n) \tag{4.6}$$

with

$$\Sigma^{(1)}(i\omega_n)=n_i\frac{v\rho_3}{D}(x-iy\tau_1\sigma_3) \ , \tag{4.7}$$

$$\begin{aligned}\Sigma^{(2)}(i\omega_n)=-n_i\frac{v^2}{2D}\left\{i\left[x\left[\frac{\tilde{\omega}_{n+}}{\lambda_+}+\frac{\tilde{\omega}_{n-}}{\lambda_-}\right]+y\left[\frac{\tilde{\Delta}_{n+}}{\lambda_+}-\frac{\tilde{\Delta}_{n-}}{\lambda_-}\right]\right]-\rho_2\sigma_2\left[x\left[\frac{\tilde{\Delta}_{n+}}{\lambda_+}+\frac{\tilde{\Delta}_{n-}}{\lambda_-}\right]-y\left[\frac{\tilde{\omega}_{n+}}{\lambda_+}-\frac{\tilde{\omega}_{n-}}{\lambda_-}\right]\right]\right.\\-\tau_1\rho_3\sigma_3\left[x\left[\frac{\tilde{\Delta}_{n+}}{\lambda_+}-\frac{\tilde{\Delta}_{n-}}{\lambda_-}\right]-y\left[\frac{\tilde{\omega}_{n+}}{\lambda_+}+\frac{\tilde{\omega}_{n-}}{\lambda_-}\right]\right]\\\left.+i\tau_1\rho_1\sigma_1\left[x\left[\frac{\tilde{\omega}_{n+}}{\lambda_+}-\frac{\tilde{\omega}_{n-}}{\lambda_-}\right]+y\left[\frac{\tilde{\Delta}_{n+}}{\lambda_+}+\frac{\tilde{\Delta}_{n-}}{\lambda_-}\right]\right]\right\} .\end{aligned} \tag{4.8}$$

Here we have used

$$\lambda_\pm=(\tilde{\omega}_{n\pm}^2+\tilde{\Delta}_{n\pm}^2)^{1/2} \ , \tag{4.9}$$

$$x=1+v^2\frac{\tilde{\omega}_{n+}\tilde{\omega}_{n-}+\tilde{\Delta}_{n+}\tilde{\Delta}_{n-}}{\lambda_+\lambda_-}\ , \tag{4.10}$$

$$y=v^2\frac{\tilde{\omega}_{n-}\tilde{\Delta}_{n+}-\tilde{\omega}_{n+}\tilde{\Delta}_{n-}}{\lambda_+\lambda_-}\ , \tag{4.11}$$

$$D=x^2+y^2=1+v^4+2v^2\frac{\tilde{\omega}_{n+}\tilde{\omega}_{n-}+\tilde{\Delta}_{n+}\tilde{\Delta}_{n-}}{\lambda_+\lambda_-}\ . \tag{4.12}$$

In Eq. (4.9), the branch of the square root of $\lambda_\pm$ is chosen such that the real part of this function is positive. The self-energy part $\Sigma^{(1)}(i\omega_n)$ given in Eq. (4.7) contains odd-order terms with respect to v and is related to the shift of the chemical potential or the deviation from the complete nesting. This shift has an interesting effect on the property of AFS.[13] This problem, however, will be left for a separate investigation, so that we discard $\Sigma^{(1)}(i\omega_n)$ hereafter.

Using Eqs. (4.1), (4.6), and (4.8), we can set up the self-consistency equations for $\tilde{\omega}_{n\pm}$ and $\tilde{\Delta}_{n\pm}$,

$$\tilde{\omega}_{n\pm}-\omega_n=\frac{n_i}{\pi N_0}\frac{v^2}{D}\frac{1}{\lambda_\mp}(x\tilde{\omega}_{n\mp}\mp y\tilde{\Delta}_{n\mp})\ , \tag{4.13}$$

$$\tilde{\Delta}_{n\pm}-\Delta_\pm=\frac{n_i}{\pi N_0}\frac{v^2}{D}\frac{1}{\lambda_\mp}(x\tilde{\Delta}_{n\mp}\pm y\tilde{\omega}_{n\mp})\ . \tag{4.14}$$

Defining $u_{n\pm}=\tilde{\omega}_{n\pm}/\tilde{\Delta}_{n\pm}$, Eqs. (4.13) and (4.14) can be combined to give

$$\omega_n=u_{n\pm}\Delta_\pm\pm\frac{1}{\tau_1}\left[\frac{(u_{n+}-u_{n-})(1+u_{n\pm}^2)^{1/2}}{(2-\zeta)(1+u_{n+}^2)^{1/2}(1+u_{n-}^2)^{1/2}+\zeta(1+u_{n+}u_{n-})}\right]\ , \tag{4.15}$$

where

$$\frac{1}{\tau_1}=\frac{1}{\tau_1^0}\frac{1}{(1+v^2)^2}=\frac{2n_iv^2}{\pi N_0}\frac{1}{(1+v^2)^2}\ . \tag{4.16}$$

Equation (4.15) is our generalized equation for $u_{n\pm}$ and Eq. (3.1) of Ref. 5 is retrieved from it by setting $\zeta=0$ and replacing τ_1 by τ_1^0.

Now we comment on the "dirty"-limit behavior of the system. We follow a method similar to the one used by Fulde and Maki[14] while considering the spin-orbit scattering in usual superconductors in a magnetic field. We introduce two quantities u_A, u_B defined by

$$u_A=\tfrac{1}{2}(u_{n+}+u_{n-}),\quad u_B=\tfrac{1}{2}(u_{n+}-u_{n-})\ . \tag{4.17}$$

Expanding Eq. (4.15) in powers of u_B, we have

$$\frac{\omega_n}{\Delta}=u_A\left[1-\frac{\tau_1H_Q^2/\Delta}{(1+u_A^2)^{1/2}}\right]+O(\tau_1^2H_Q^2)\ . \tag{4.18}$$

This equation has the same structure as the one obtained in Ref. 6 for the case of magnetic impurities in the usual superconductors. For the present case of the AFS in the short mean-free-path limit, the effective pair-breaking parameter α_s is given by

$$\alpha_s=\tau_1H_Q^2/\Delta\ . \tag{4.19}$$

In deriving Eq. (4.18) one must pay special attention to the branch of the square root. In the extremely dirty limit, $\alpha_s\to 0$, and Eq. (4.18) gives the BCS result.

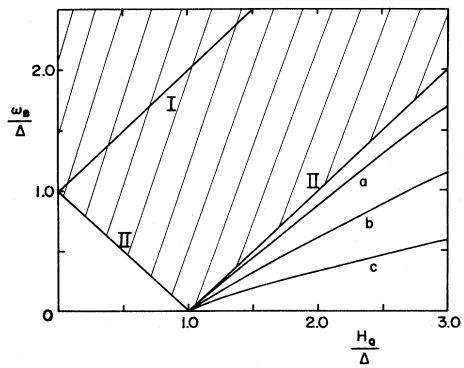

FIG. 1. Position of bound states due to single nonmagnetic impurity for $\zeta=0.5$ (curve *a*), 0.8 (curve *b*), and 0.95 (curve *c*). Cross-hatched area shows the continuum of states, which has two peaks at $\omega=\Delta+H_Q$ (line I) and $|\Delta-H_Q|$ (line II).

V. DENSITY OF STATES

Several thermodynamic and transport properties can be calculated by using the u_n equation (4.15). Here we consider the superconducting density of states $N(\omega)$, which is given by

$$N(\omega)=\frac{N_0}{2}\mathrm{Im}\left[\frac{u_+}{(1-u_+^2)^{1/2}}+\frac{u_-}{(1-u_-^2)^{1/2}}\right]\ , \tag{5.1}$$

where Im stands for the imaginary part of the function. Here $u_\pm$ is the analytically continued value of $u_{n\pm}$ and it satisfies an equation obtained from Eq. (4.15) by replacing $iu_{n\pm}\to u_\pm$ and $i\omega_n\to\omega$. In the present paper we consider the order parameter Δ as given and scale various quantities with respect to Δ.

The density of states is qualitatively different for the

cases $H_Q < \Delta$ and $H_Q > \Delta$. As an example of the former case, the $N(\omega)$ for $H_Q = 0.4\Delta$, $\zeta = 0$, 0.5, and 1.0, and $(\tau_1\Delta)^{-1} = 0.2$, 1.0, and 5.0, respectively, are shown in Figs. 2(a)–2(c). The ζ dependence in various figures should be noted. The large-concentration behavior shown in Fig. 2(c) is easily understood by the dirty-limit analysis given at the end of the last section.

Now we consider the case $H_Q > \Delta$ where the impurity bound states arise. In Fig. 3 we show the density of states $N(\omega)$ for $H_Q = 2.5\Delta$. The arrow indicates the position of the single-impurity bound state. One may note that the impurity band grows and that the gaplessness appears as the impurity concentration increases. It may be mentioned that for a much larger impurity concentration the $N(\omega)$ is governed by Eq. (4.18). Thus for such concentrations the gap would appear again and the overall behavior of the density of states will become AG-like (ultimately BCS-like). This behavior has been numerically demonstrated for a quasi-3D model by NLG within the lowest-order Born approximation (Fig. 6 of Ref. 5).

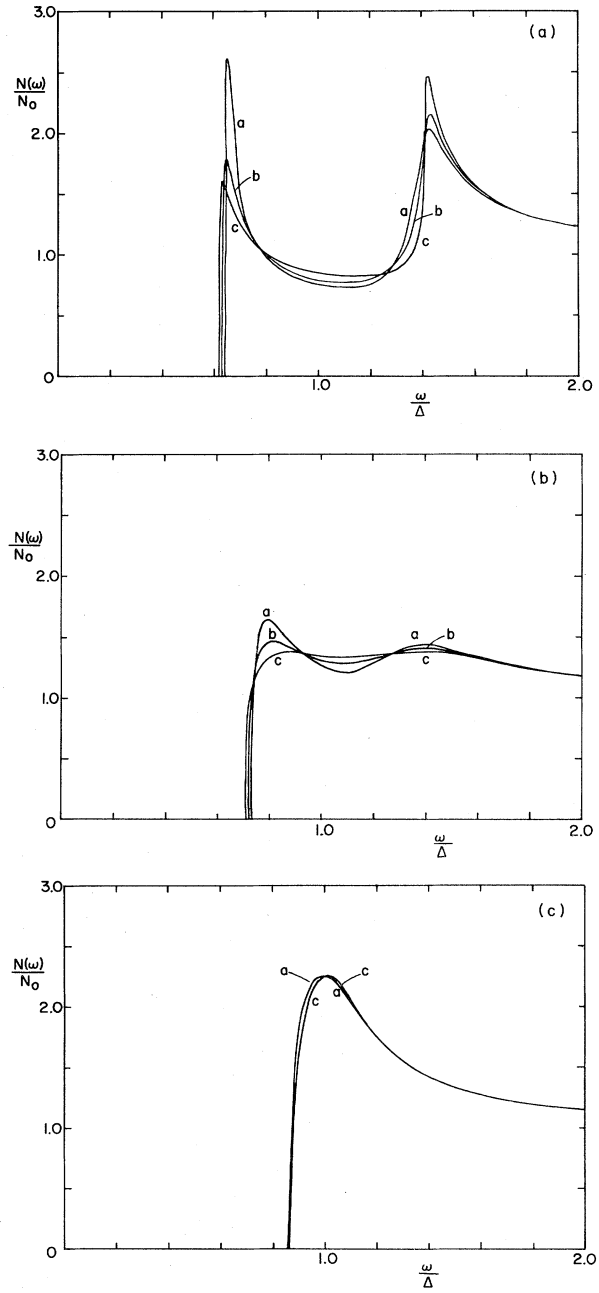

FIG. 2. (a) Density of states $N(\omega)$ for $H_Q = 0.4\Delta$, $(\tau_1\Delta)^{-1} = 0.2$, and $\zeta = 0$ (curve *a*), 0.5 (curve *b*), and 1.0 (curve *c*). Same values of H_Q and ζ are used in (b) and (c). (b) $N(\omega)$ for $(\tau_1\Delta)^{-1} = 1.0$. (c) $N(\omega)$ for $(\tau_1\Delta)^{-1} = 5.0$.

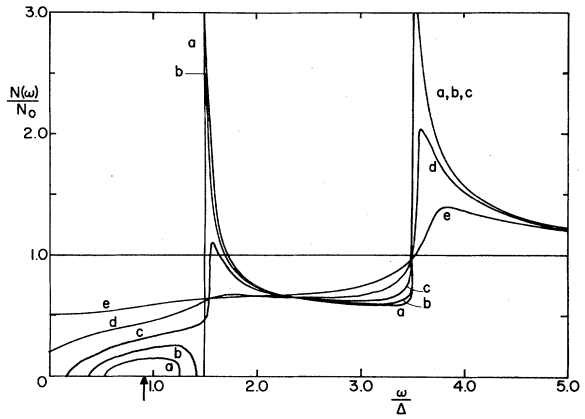

FIG. 3. Impurity concentration dependence of the density of states $N(\omega)$ for $H_Q = 2.5\Delta$ and $\zeta = 0.8$. Value of $(\tau_1\Delta)^{-1}$ is taken as 0.05 (curve *a*), 0.1 (curve *b*), 0.2 (curve *c*), 0.5 (curve *d*), and 1.0 (curve *e*). The arrow indicates the position of one-impurity bound state.

Next we consider the condition for the appearance of the gaplessness in more detail. We note that from the analytical properties of the Green's function, the real part of $u_\pm$ is zero at $\omega = 0$. Then the density of states at $\omega = 0$ becomes finite only if the imaginary part of $u_\pm$ is nonzero. Investigating Eq. (4.15), we find that the condition for a finite density of states at $\omega = 0$ is

$$\frac{H_Q^2 - \Delta^2}{H_Q \Delta} 1 - \zeta < \frac{1}{\tau_1 \Delta} < \frac{H_Q^2 - \Delta^2}{\Delta^2} \tag{5.2}$$

for $H_Q > \Delta$. Of course, there is no possibility of the gaplessness, for $H_Q < \Delta$, which was already pointed out by NLG. The derivation of the condition (5.2) is given in Appendix B. In Fig. 4 we show the condition for the gaplessness graphically.

VI. SUMMARY AND DISCUSSION

We have studied the effect of nonmagnetic impurities on AF superconductors by considering the electron-impurity scattering exactly. The bound states due to nonmagnetic impurities appear when $H_Q > \Delta$. The growth of the impurity band and the existence of gaplessness with the increase in the impurity concentration have been investigated. The dirty-limit behavior of the system has been analyzed. We have also studied the condition for the gaplessness analytically.

Now we comment on the magnitudes of H_Q and Δ. In a pure AFS with a 1D electron band at $T = 0$ K, the coex-

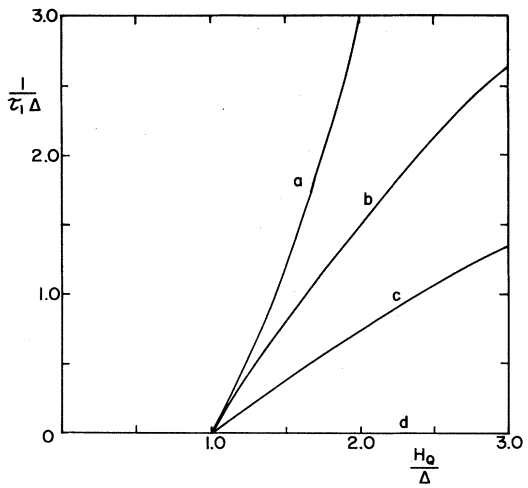

FIG. 4. Condition for gaplessness, Eq. (5.2). Curve a represents the upper bound $(H_Q^2-\Delta^2)/\Delta^2$ for $(\tau_1\Delta)^{-1}$. Values of lower bound $(H_Q^2-\Delta^2)(1-\zeta)/H_Q\Delta$ for $\zeta=0.0$, 0.5, and 1.0 are denoted by curves b, c, and d, respectively.

isting state becomes unstable for $H_Q>\Delta_0$, where Δ_0 is the zero-temperature superconducting order parameter in the absence of H_Q.[4] However, for temperatures near the superconducting transition temperature, Δ becomes small and $H_Q/\Delta>1$ is permitted.[4] The latter condition should also apply in the present case where Δ depends on the temperature, the impurity concentration, and H_Q. In the present paper we have kept H_Q as a constant which is especially valid for materials having a superconducting transition temperature below the AF ordering temperature.[15]

Nass, Levin, and Grest[5] have employed the quasi-3D model in their study. In this model, the Fermi surface is divided into two regions designated I and II. It is assumed that in region I the nesting condition is satisfied and H_Q is important. In region II the effects of H_Q are neglected. Machida[10] has used essentially the same approximation for treating highly anisotropic materials. The extension of the present work to the above-mentioned scheme is straightforward. The pair breaking due to nonmagnetic impurities only belongs to region I. Therefore, the main results of the present study, which are the existence of impurity bands and the appearance and disappearance of gaplessness in AFS, will be valid also in the quasi-3D model. We also note that our mean-field Hamiltonian, Eq. (2.1), has a 1D character in itself because we consider only one characteristic wave vector $\vec{Q}$.

Next we comment briefly on the deviation from the complete nesting condition. Now ϵ_s defined in Eq. (2.6) is nonzero and the renormalized Green's function has a form

$$G_k(i\omega_n)=(i\tilde{\omega}_n-\tilde{\epsilon}_{sn}\rho_3-\epsilon_a\tau_3\rho_3-\tilde{\Delta}_n\rho_2\sigma_2 +i\tilde{\Omega}_n\tau_1\rho_1\sigma_1+\tilde{H}_{Qn}\tau_1\rho_3\sigma_3+\tilde{\xi}_{sn}\tau_1\sigma_3)^{-1} . \quad (6.1)$$

The necessity of $\tilde{\epsilon}_{sn}$ and $\tilde{\xi}_{sn}$ is understood by noting the structure of $F^0(i\omega_n)$ given in Appendix A. The self-consistent calculation in this case is quite involved and is left to a planned future study.

ACKNOWLEDGMENT

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APPENDIX A: CALCULATION OF $F^0(i\omega_n)$

Using Eq. (2.5) for the unperturbed Green's function $G^0_{\vec{k}}(i\omega_n)$, we obtain

$$G^0_{\vec{k}}(i\omega_n)=-\frac{1}{L_n^0}\{(i\omega_n+\epsilon_s\rho_3+\epsilon_a\tau_3\rho_3+\Delta\rho_2\sigma_2-H_Q\tau_1\rho_3\sigma_3)(\omega_n^2+\epsilon_s^2+\epsilon_a^2+\Delta^2+H_Q^2-2\epsilon_s\epsilon_a\tau_3) +[(i\omega_n+\epsilon_s\rho_3+\epsilon_a\tau_3\rho_3+\Delta\rho_2\sigma_2)\tau_1\rho_3\sigma_3-H_Q]2(\epsilon_sH_Q\rho_3+\Delta H_Q\rho_2\sigma_2)\} , \quad (A1)$$

where

$$L_n^0=(\omega_n^2+\epsilon_s^2+\epsilon_a^2+\Delta^2+H_Q^2)^2-4(\epsilon_s^2\epsilon_a^2+\epsilon_s^2H_Q^2+\Delta^2H_Q^2) . \quad (A2)$$

Then $F^0(i\omega_n)$, Eq. (3.3), is calculated as

$$F^0(i\omega_n)=-\frac{1}{N}\sum_{\vec{k}}\frac{1}{L_n^0}(i\omega_na_1+\epsilon_sa_2\rho_3+\Delta a_3\rho_2\sigma_2-H_Qa_4\tau_1\rho_3\sigma_3-i\omega_na_5\tau_1\rho_1\sigma_1+\epsilon_sa_6\tau_1\sigma_3) , \quad (A3)$$

where

$$a_1=\omega_n^2+\epsilon_s^2+\epsilon_a^2+\Delta^2+H_Q^2,\quad a_2=\omega_n^2+\epsilon_s^2-\epsilon_a^2+\Delta^2-H_Q^2 ,$$
$$a_3=\omega_n^2+\epsilon_s^2+\epsilon_a^2+\Delta^2-H_Q^2,\quad a_4=\omega_n^2-\epsilon_s^2+\epsilon_a^2-\Delta^2+H_Q^2,\quad a_5=2\Delta H_Q,\quad a_6=2i\omega_nH_Q .$$

In deriving Eq. (A3), we have considered the symmetry of ϵ_a.

APPENDIX B: CONDITION FOR GAPLESSNESS

For the real frequency ω, the functions $u_{\pm}$ satisfy the equation

$$\omega = u_{\pm}\Delta_{\pm} \pm \frac{1}{\tau_1}\left[\frac{(u_+ - u_-)(1-u_{\pm}^2)^{1/2}}{(2-\zeta)(1-u_+^2)^{1/2}(1-u_-^2)^{1/2}+\zeta(1-u_+u_-)}\right] . \tag{B1}$$

In the above, the branch of the square root should be chosen such that $\mathrm{Im}[u_{\pm}/(1-u_{\pm}^2)^{1/2}]$ is not negative.

At $\omega=0$, the real part of $u_{\pm}$ is zero because of the symmetry condition $u(\omega)=-u^*(-\omega)$. Thus we set

$$u_+(\omega=0)=ip_1u_1 , \tag{B2}$$

$$u_-(\omega=0)=ip_2u_2 , \tag{B3}$$

where $u_{1,2}$ is real and nonnegative, and $p_{1,2}=\pm 1$. The coupled equations for u_1 and u_2 are

$$\frac{u_1\Delta_+}{(1+u_1^2)^{1/2}} = -\frac{u_2\Delta_-}{(1+u_2^2)^{1/2}} = \frac{1}{\tau_1}\frac{p_1u_2-p_2u_1}{(2-\zeta)(1+u_1^2)^{1/2}(1+u_2^2)^{1/2}+\zeta(p_1p_2+u_1u_2)} . \tag{B4}$$

In (B4), the positive branch is taken for the square root.

For $H_Q<\Delta$ one can easily show that the only permitted solution is $u_1=u_2=0$, which indicates no possibility of gaplessness. On the other hand, the nontrivial solution with $u_1\neq 0$ and $u_2\neq 0$ is possible for $H_Q>\Delta$. After some algebra, we obtain the condition for the nontrivial solution as

$$\alpha_1 < \frac{1}{\tau_1\Delta} < \alpha_2 , \tag{B5}$$

with

$$\alpha_1 = \frac{H_Q^2-\Delta^2}{H_Q\Delta}1-\zeta , \tag{B6}$$

$$\alpha_2 = \frac{H_Q^2-\Delta^2}{\Delta^2} . \tag{B7}$$

It should be noted that $p_1=+1$ for all the regions $\alpha_1<(\tau_1\Delta)^{-1}<\alpha_2$. However, p_2 is $+1$ for $\alpha_1<(\tau_1\Delta)^{-1}<\alpha_3$ and p_2 is -1 for $\alpha_3<(\tau_1\Delta)^{-1}<\alpha_2$, where α_3 is given by

$$\alpha_3 = \frac{(H_Q-\Delta)[H_Q+(1-\zeta)\Delta]}{\Delta(H_Q\Delta)^{1/2}} . \tag{B8}$$

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