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Shiba-Rusinov theory of magnetic impurities in superconductors beyond *s*-wave scattering: Eliashberg formalism

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Shiba-Rusinov theory of magnetic impurities in isotropic superconductors beyond the *s*-wave scattering is generalized by using the Eliashberg formalism. The analytical expressions for the transition temperature T_c and the specific-heat jump ΔC are given using the square-well model for the electron-phonon interaction. Taken as a function of the impurity concentration, the quantities T_c/T_{c0} and $\Delta C/\Delta C_0$ depend on the microscopic parameters λ, μ^*, and ω_D of the host material. However, this dependence is absent if one plots the above properties versus the normalized impurity concentration $\alpha/\alpha_{\rm cr}$ or if $\Delta C/\Delta C_0$ vs T_c/T_{c0} is studied. (T_{c0} and ΔC_0 are values of T_c and ΔC, respectively, in the absence of impurities; λ is the electron-phonon interaction parameter, μ^* the Coulomb pseudopotential, and ω_D the Debye cutoff frequency; α is the spin-flip scattering rate; $\alpha_{\rm cr}$ is the value of α for which T becomes zero.)

I. INTRODUCTION

About 15 years ago Shiba[1] and Rusinov[2] independently gave a theory of a low concentration of magnetic impurities in a superconductor. In this theory the electron-impurity scattering is calculated exactly for a single-impurity problem assuming a classical spin. The well-known Abrikosov-Gor'kov[3] (AG) theory is a limiting case of the above model. Several properties of the superconducting alloy in the Shiba-Rusinov (SR) model have been calculated by Nagi and collaborators.[4,5] The consequences of the SR model beyond the *s*-wave scattering have been considered by Ginsberg.[6] The positions of the impurity bound states for the *s*-, *p*-, and *d*-wave scattering for several alloys were calculated by Kunz and Ginsberg[7] by using band theory. The experimental work of Ginsberg and collaborators[8] has confirmed the applicability of the SR model results to the case of transition-metal impurities in superconductors.

The theoretical work described so far is based on the Bardeen-Cooper-Schrieffer[9] (BCS) formalism of the theory of superconductivity and as such the properties do not depend on the microscopic parameters λ, ω_D, and μ^* of the host material (λ: electron-phonon interaction parameter; ω_D: Debye cutoff frequency; μ^*: Coulomb pseudopotential). The case of AG impurities in superconductors using Eliashberg[10] formalism[11] (EF) was considered by Allen,[12] who calculated the transition temperature by using the square-well model (or the $\lambda^{\Theta\Theta}$ model) for the electron-phonon interaction. Detailed numerical study using $\alpha^2F(\omega)$ of lead was done by Schachinger, Daams, and Carbotte[13] [$\alpha^2F(\omega)$: electron-phonon spectral density]. The T_c and some tunneling properties for the case of SR impurities were considered by Schachinger.[14] The quasiparticle density of states for the SR model has been calculated by Schachinger and Carbotte.[15] The Kondo impurities in the strong-coupling superconductors have been described by the present authors.[16] We have also recently investigated the case of SR impurities in anisotropic superconductors using EF.[17]

The purpose of the present paper is to generalize the results of Ref. 6 by using the Eliashberg formalism. We will calculate analytical expressions for T_c and the specific-heat jump at T_c by using the $\lambda^{\Theta\Theta}$ model.

The plan of the paper is as follows. In Sec. II we outline our general formalism. The transition temperature and the specific heat are discussed in Sec. III. Section IV gives a summary.

II. FORMALISM

Using the Eliashberg formalism, the single-particle Green's function for the conduction electrons of a strong-coupling superconductor containing paramagnetic impurities within the Shiba-Rusinov approximation is given by

$$G(\vec{k},i\omega_n)=(i\tilde{\omega}_n\rho_3-\epsilon_{\vec{k}}-\tilde{\Delta}_n\rho_2\sigma_2)^{-1} \ , \tag{2.1}$$

where

$$\tilde{\omega}_n=\omega_n+2\pi T\sum_{m\geqslant 0}\lambda(n-m)\frac{U_m}{(U_m^2+1)^{1/2}} + \sum_{l=0}^{\infty}(2l+1)\Gamma_{1l}\frac{U_n(1+U_n^2)^{1/2}}{\epsilon_l^2+U_n^2} \ , \tag{2.2}$$

$$\tilde{\Delta}_n=2\pi T\sum_{m\geqslant 0}[\lambda(n-m)-\mu^*]\frac{1}{(U_m^2+1)^{1/2}} + \sum_{l=0}^{\infty}(2l+1)\Gamma_{2l}\frac{(1+U_n^2)^{1/2}}{\epsilon_l^2+U_n^2} \ . \tag{2.3}$$

In the above equations $\epsilon_{\vec{k}}$ is the single-particle energy, σ_i and ρ_i ($i=1,2,3$), respectively, are Pauli matrices operating on the ordinary spin states and the electron-hole spin states, $\omega_n=\pi(2n+1)T$ (T is temperature and n is an integer); $U_n=\tilde{\omega}_n/\tilde{\Delta}_n$, ϵ_l is the normalized position of a bound state within the BCS gap for the lth partial wave, and

$$2\Gamma_{1l}=1/\tau_{1l}+1/\tau_{2l} \ , \qquad 2\Gamma_{2l}=1/\tau_{1l}-1/\tau_{2l} \ , \tag{2.4}$$

where $1/\tau_{2l}(1/\tau_{1l})$ is the spin-flip (non-spin-flip) scattering rate from the magnetic impurities. Further, $\lambda(n-m)$ is the electron-phonon interaction parameter.

In the square-well model (or the $\lambda^{\Theta\Theta}$ model) of the electron-phonon interaction one takes

$$\lambda(n-m)=\lambda\Theta(\omega_D-|\omega_n|)\Theta(\omega_D-|\omega_m|) \ . \tag{2.5}$$

Then Eqs. (2.2) and (2.3) give

$$\frac{\omega_n}{\Delta}=U_n\left[1-\sum_{l=0}^{\infty}(2l+1)\frac{\alpha_l}{\Delta(1+\lambda)}\frac{(1+U_n^2)^{1/2}}{\epsilon_l^2+U_n^2}\right] \ , \tag{2.6}$$

$$\Delta=2\pi T\frac{\lambda-\mu^*}{1+\lambda}\sum_{n=0}^{N}\frac{1}{(U_n^2+1)^{1/2}} \ , \tag{2.7}$$

with

$$N=\frac{\omega_D}{2\pi T}-\frac{1}{2} \ , \tag{2.8}$$

$$\alpha_l=\Gamma_{1l}-\Gamma_{2l}=\frac{c}{2\pi N(0)}(1-\epsilon_l^2) \ , \tag{2.9}$$

where c is impurity concentration and $N(0)$ one spin density of states for the conduction electrons in the normal state of pure host metal.

III. TRANSITION TEMPERATURE AND SPECIFIC-HEAT JUMP

Using Eqs. (2.6) and (2.7) and following a standard procedure, the order parameter Δ for temperature near the transition temperature T_c is given by

$$\ln\left(\frac{T_{c0}}{T}\right)=B_0(c,T)+\tfrac{1}{2}B_1(c,T)\frac{\Delta^2}{4\pi^2T^2} \ , \tag{3.1}$$

with

$$B_0(c,T)=\sum_{n=0}^{N}\left[\left(n+\frac{1}{2}\right)^{-1}-\left(n+\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T}\right)^{-1}\right] \ , \tag{3.2}$$

$$B_1(c,T)=\sum_{n=0}^{N}\left\{\left[\left(n+\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T}\right)^3\right]^{-1}+S\left(\frac{\alpha_\lambda}{2\pi T}\right)\left[\left(n+\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T}\right)^4\right]^{-1}\right\} \ , \tag{3.3}$$

$$\alpha_\lambda=\frac{\alpha}{1+\lambda}=\frac{1}{1+\lambda}\sum_l(2l+1)\alpha_l=\frac{1}{1+\lambda}\frac{c}{2\pi N(0)}\sum_l F_l \ , \tag{3.4}$$

$$F_l=(2l+1)(1-\epsilon_l^2) \ , \tag{3.5}$$

$$S=\frac{\sum_l F_l(1-2\epsilon_l^2)}{\sum_l F_l} \ . \tag{3.6}$$

In writing Eq. (3.1) we have used

$$\frac{1+\lambda}{\lambda-\mu^*}=\sum_{n=0}^{\bar N}\frac{1}{n+\frac{1}{2}}=\psi\left(\frac{\omega_D}{2\pi T_{c0}}+1\right)-\psi(\tfrac{1}{2})\simeq\ln\left(\frac{2\gamma\omega_D}{\pi T_{c0}}\right) \ , \tag{3.7}$$

$$\sum_{n=0}^{N}\frac{1}{n+\frac{1}{2}}=\psi\left(\frac{\omega_D}{2\pi T}+1\right)-\psi(\tfrac{1}{2})\simeq\ln\left(\frac{2\gamma\omega_D}{\pi T}\right) \ , \tag{3.8}$$

where $\bar N=(\omega_D/2\pi T_{c0})-\frac{1}{2}$; $\psi(z)$ is the digamma function[18] and $\ln\gamma=0.577\ldots$ (Euler's constant).

Putting $\Delta=0$ in Eq. (3.1) we obtain the T_c equation

$$\ln\left(\frac{T_{c0}}{T_c}\right)=B_0(c,T_c)=\psi\left(\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T_c}\right)-\psi(\tfrac{1}{2}) \ , \tag{3.9}$$

where $B_0(c,T_c)$ has been evaluated by taking the upper limit on the summation to be infinity. Comparing Eq. (3.9) with Eq. (14) of Ref. 6, we note that the pair breaking parameter has been reduced by a factor of $1/(1+\lambda)$.

For a low impurity concentration, Eq. (3.9) gives

$$\frac{T_c}{T_{c0}}=1-4\lambda(2)\frac{\alpha_\lambda}{2\pi T_{c0}} \ , \tag{3.10}$$

where

$$\lambda(l)=\sum_{n=0}^{\infty}\frac{1}{(2n+1)^l}=\frac{1}{2^l(-1)^l(l-1)!}\psi^{(l-1)}(\tfrac{1}{2}) \ . \tag{3.11}$$

The critical value of α needed to make $T_c=0$ as obtained from Eq. (3.9) is

$$\alpha_{\rm cr}=\frac{\pi T_{c0}}{2\gamma}(1+\lambda) \ . \tag{3.12}$$

Defining $p=\alpha/\alpha_{\rm cr}$, we can write

$$\frac{\alpha_\lambda}{2\pi T_c}=\frac{P}{4\gamma}\frac{T_{c0}}{T_c} \ . \tag{3.13}$$

Equation (3.9) can be used to plot T_c/T_{c0} versus the impurity concentration α/T_{c0}. This curve will depend on the parameter λ. However, Eq. (3.13) indicates that a plot of T_c/T_{c0} vs p will be independent of λ.

The specific-heat jump at T_c is obtained by following the procedure used in Refs. 4 and 6 as in the $\lambda^{\Theta\Theta}$ model the electron-phonon interaction parameter is independent of temperature. We get

$$\Delta C=C_s-C_n=\frac{8\pi^2N(0)T_c(1+\lambda)}{B_1(c,T_c)}\left[1-\frac{\alpha_\lambda}{2\pi T_c}\psi^{(1)}\left(\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T_c}\right)\right]^2 \ . \tag{3.14}$$

Denoting the value of ΔC in the absence of impurities as ΔC_0 and evaluating $B_1(c,T_c)$ by taking the upper limit on the summation to be infinity, we get

$$\frac{\Delta C}{\Delta C_0}=8\lambda(3)\frac{T_c}{T_{c0}}\left\{\left[1-\frac{\alpha_\lambda}{2\pi T_c}\psi^{(1)}\left(\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T_c}\right)\right]^2\Big/\left[-\tfrac{1}{2}\psi^{(2)}\left(\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T_c}\right)+\left(\frac{\alpha_\lambda}{2\pi T_c}\right)\frac{S}{6}\psi^{(3)}\left(\frac{1}{2}+\frac{\alpha_\lambda}{2\pi T_c}\right)\right]\right\} \ , \tag{3.15}$$

with

$$\Delta C_0=\frac{8\pi^2N(0)T_{c0}(1+\lambda)}{8\lambda(3)} \ . \tag{3.16}$$

Equation (3.15) agrees[19] with Eq. (28) of Ref. 6 except that now the pair breaking parameter has been reduced by the

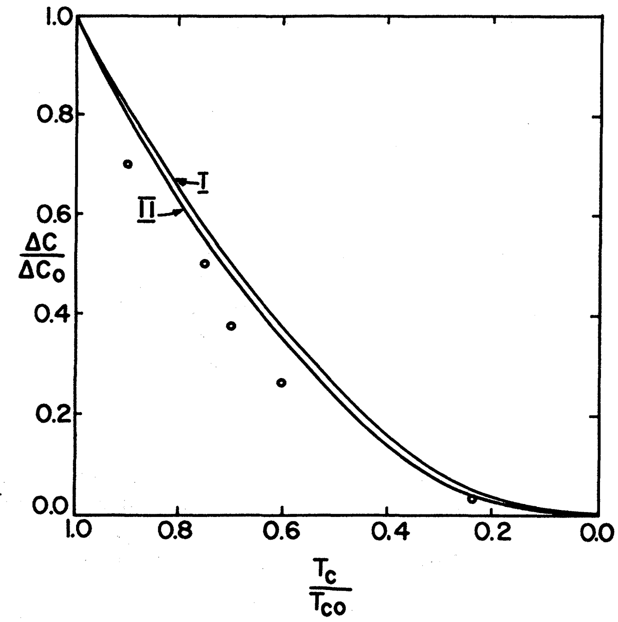

FIG. 1. Normalized specific-heat jump at T_c vs the normalized transition temperature. For curve I: $\epsilon_0=1.0$, $\epsilon_1=0.53$, $\epsilon_2=0.94$. Curve II corresponds to $\epsilon_0=0.25$, $\epsilon_1=0.50$, $\epsilon_2=1.00$. These sets of ϵ_l are suggested by the tunneling experiment of Terris and Ginsberg (Ref. 20) on Zn-Mn. The circles are the experimental points of Smith (Ref. 21) for Zn-Mn.

factor $1/(1+\lambda)$.

The initial depression of $\Delta C/\Delta C_0$ in the limit of $c\rightarrow 0$ can be written by using Eqs. (3.15) and (3.10) and we obtain

$$\frac{\Delta C}{\Delta C_0}=1-12\lambda(2)\frac{\alpha_\lambda}{2\pi T_{c0}}+\frac{2\lambda(4)}{\lambda(3)}(3-S)\frac{\alpha_\lambda}{2\pi T_{c0}} \quad . \quad (3.17)$$

One should note the dependence of Eq. (3.17) on the parameter λ.

Defining the quantity

$$c^*=\lim_{c\rightarrow 0}\frac{(\Delta C-\Delta C_0)/c\Delta C_0}{(T_c-T_{c0})/cT_{c0}} \quad , \quad (3.18)$$

one can calculate it from Eqs. (3.10) and (3.17). We obtain

$$c^*=3-\frac{\lambda(4)}{2\lambda(2)\lambda(3)}(3-S) \quad . \quad (3.19)$$

We note that c^* is independent of λ.

The detailed dependence of $\Delta C/\Delta C_0$ on the impurity concentration α/T_{c0} can be obtained from Eqs. (3.15) and (3.9). This curve will depend on the parameter λ. However, in view of Eq. (3.13) the $\Delta C/\Delta C_0$ vs p curve will be independent of λ. Similarly, a plot of $\Delta C/\Delta C_0$ vs T_c/T_{c0} does not depend on λ. In Fig. 1, we show the normalized specific-heat jump versus the normalized transition temperature. Curve I corresponds to $\epsilon_0=1.0$, $\epsilon_1=0.53$, and $\epsilon_2=0.94$. For curve II, $\epsilon_0=0.25$, $\epsilon_1=0.50$, and $\epsilon_2=1.00$. These sets of ϵ_l are suggested by the tunneling experiment of Terris and Ginsberg[20] on Zn-Mn. The circles are the experimental points of Smith[21] for Zn-Mn. In passing we may mention that the curve II is closer to the experimental data.

IV. SUMMARY

Using the Eliashberg formalism and the $\lambda^{\theta\theta}$ model we have given some theoretical results for the effect of magnetic impurities on isotropic superconductors according to the Shiba-Rusinov theory beyond the s-wave scattering. Our results are generalization of Ref. 6.

The transition temperature and the specific-heat jump are discussed in Sec. III. The initial depression in T_c [Eq. (3.10)], the critical value of the spin-flip scattering rate α_{cr} [Eq. (3.12)], and the initial depression in ΔC [Eq. (3.17)] depend on the microscopic parameters λ, μ^*, and ω_D of the host material. Taken as a function of the impurity concentration α/T_c, the quantities T_c/T_{c0} and $\Delta C/\Delta C_0$ also depend on the material parameters. However, this dependence disappears if one plots the above properties versus α/α_{cr} or if $\Delta C/\Delta C_0$ vs T_c/T_{c0} is studied.

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