Consequences of Shiba's theory of magnetic impurities in superconductors, beyond s-wave scattering

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Relations are derived from which all of the thermodynamics and transport properties can be calculated for superconductors with magnetic impurities according to Shiba's theory. Scattering of all partial waves are included, beyond the usual s-wave scattering treatments. A band of local excited states appears for each partial wave which is included. As an example of a thermodynamic property, the discontinuity in the specific heat at the superconducting transition is calculated.

I. INTRODUCTION

Our understanding of the influence of magnetic impurities on the properties of superconductors has been extended in recent years beyond the classic theory of Abrikosov and Gorkov (AG).[1] That theory assumed that the interaction between the magnetic impurities and the conduction electrons is sufficiently weak to be treated in the first Born approximation. A treatment of the magnetic impurity problem which is carried out to all orders of the interaction has been provided by Shiba[2] and, later but independently, by Rusinov.[3] This theory was developed further by Shiba,[4] and has been used to calculate a variety of thermodynamic and transport properties.[5-12] Much of the mathematical treatment which was required for those calculations is similar to that used in calculations based on the AG theory, and has been given by Maki.[13] An alternative "exact" theory of magnetic impurities in superconductors has been devised by Müller-Hartmann and Zittartz (MHZ) and their coworkers,[14] and has recently been improved by extending it to the case of a nonvanishing concentration of magnetic impurities.[15] Unfortunately, it has not been possible yet to carry out calculations of transport properties based on the MHZ theory.

Although Shiba's theory applies to the case where higher-partial-wave electron-impurity scattering is included, the published papers which have been based on the theory have all assumed early in the calculation that only s-wave scattering is present. This assumption is made for simplicity, and is properly used to display the qualitative consequences of the theory. However, accounting for the observed effect of the magnetic impurities on the superconducting transition temperature requires that higher partial waves be included,[16] and the assessment of the results of other detailed experiments has also begun to demand that they be taken into account. It is our purpose to present some of the theoretical predictions of the Shiba theory when the higher partial waves are included. The analysis proceeds along the same lines as that which has already been published for the case of s-wave scattering only, which we will call the restricted case. We use the notation of Nagi and his co-workers.

II. ORDER PARAMETER

The basic equation which we use has been given by Rusinov,[3] and by Chaba and Nagi,[5]

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

where

$$\omega_n = 2\pi T(n+\tfrac{1}{2}) , \quad (2)$$

Δ is the order parameter, T is the temperature, α is the pair-breaking parameter [see Eq. (17) below], l is the orbital angular momentum number of the partial wave, U_n is a renormalized energy defined in Ref. 5,

$$\epsilon_l = \cos(\delta_l^+ - \delta_l^-) , \quad (3)$$

δ_l^+ and δ_l^- are the phase shift of the lth partial wave for spin up or down, respectively,

$$\alpha_l = C(1-\epsilon_l^2)/2\pi N_0 , \quad (4)$$

C is the magentic impurity concentration, and N_0 is the density of states for the conduction electrons (one spin direction only) in the normal state of the pure host metal.

Henceforth, all sums over l go over integers from 0 to ∞. Sums will appear over n; they will also all go over integers from 0 to ∞. Following the methods given in the derivation by Lo and Nagi for the restricted case,[6] we find immediately that

$$\frac{\gamma t(2n+1)}{\delta(\alpha,T)} = U_n\left[1-\sum_l(2l+1)\left(\frac{\alpha_l}{\Delta(\alpha,T)}\right)\times(1+U_n^2)^{1/2}(\epsilon_l^2+U_n^2)^{-1}\right], \quad (5)$$

where

$$\delta(\alpha,T)=\Delta(\alpha,T)/\Delta(0,0)\ , \quad (6)$$

$$\gamma=\pi T_{c0}/\Delta(0,0)\cong 1.781\ , \quad (7)$$

T_{c0} is the transition temperature of the pure host metal, and

$$t=T/T_{c0}\ . \quad (8)$$

Employing the usual self-consistency condition

$$\Delta(\alpha,T)=2\pi T N_0|g|\sum_n(1+U_n^2)^{-1/2}\ , \quad (9)$$

where g is the BCS coupling constant, we continue with Lo and Nagi's methods and find that

$$\ln(t)=\frac{2\gamma t}{\delta}\sum_n\left(\frac{1}{(1+U_n^2)^{1/2}}-\frac{\delta}{2\gamma t(n+\frac{1}{2}+p/4\gamma T)}\right)+\psi(\tfrac{1}{2})-\psi\left(\frac{1}{2}+\frac{p}{4\gamma T}\right), \quad (10)$$

where ψ is the digamma function

$$p=\sum_l p_l\ , \quad (11)$$

$$p_l=(2l+1)\alpha_l/\alpha_{cr}\ , \quad (12)$$

so the factor $(2l+1)\alpha_l/\Delta(\alpha,T)$ in Eq. (1) is equal to $p_l/2\delta$, and where

$$\alpha_{cr}=\tfrac{1}{2}[\Delta(0,0)]\ , \quad (13)$$

which is the critical value of the pair-breaking parameter, that drives T_c down to 0. The order parameter is calculated by finding a value of δ which simultaneously satisfies Eqs. (5) and (10).

III. TRANSITION TEMPERATURE

The transition temperature T_c has the usual dependence on p,

$$\ln(T_c/T_{c0})=\psi(\tfrac{1}{2})-\psi(\tfrac{1}{2}+pT_{c0}/4\gamma T_c)\ . \quad (14)$$

This relation can be used to determine p from an experimental measurement of T_c/T_{c0}. Having found p, one can obtain p_l from the relation

$$p_l=pF_l/\sum_l F_l\ , \quad (15)$$

where

$$F_l=(2l+1)(1-\epsilon_l^2)\ , \quad (16)$$

if one has values for the parameters ϵ_l. Equation (14) is frequently written in the form

$$\ln(T_c/T_{c0})=\psi(\tfrac{1}{2})-\psi(\tfrac{1}{2}+\alpha/2\pi T_c)\ , \quad (17)$$

where

$$\alpha=\tfrac{1}{2}[p\,\Delta(0,0)]=p\,\alpha_{cr}\ . \quad (18)$$

The critical concentration C_{cr} of magnetic impurities, needed to force T_c down to 0, makes $p=1$, and is given by

$$C_{cr}=\pi N_0\Delta(0,0)/\sum_l F_l\ . \quad (19)$$

It is useful to note that

$$p=C/C_{cr}\ . \quad (20)$$

IV. THERMODYNAMIC AND TRANSPORT PROPERTIES

In order to calculate the various thermodynamic and transport properties, one needs to know the reduced, renormalized energy U as a function of ω. The equation which must be solved to find U is related in the usual way to the one which gives U_n, Eq. (5),

$$\frac{\omega}{\Delta}=U\left[1-\sum_l\left(\frac{p_l}{2\delta}\right)(1-U^2)^{1/2}(\epsilon_l^2-U^2)^{-1}\right], \quad (21)$$

where we denote $\Delta(\alpha,T)$ by Δ from here on.

It is interesting, for example, to see what the superconducting density of states N_s looks like. This is given by

$$N_s(\omega)=N_0\,\mathrm{Im}[U/(1-U^2)^{1/2}]\ . \quad (22)$$

As magnetic impurity atoms are added to the superconductor, states appear in the energy gap, forming bands of states. For small impurity concentrations these bands are centered at a series of energies, $\epsilon_l\Delta$. Figure 1 shows an example, where *s*-, *p*-, and *d*-wave scattering are present.

It is useful to find the order parameter Δ near T_c in order to find thermodynamic properties, such as the discontinuity in the specific heat (C_s-C_n) at T_c, where s and n refer here to the superconducting and normal state, respectively. Using the methods of Maki,[13] we find, to second order in Δ, a relation for Δ,

$$\ln(T/T_{c0})=\psi(\tfrac{1}{2})-\psi(\tfrac{1}{2}+\alpha/2\pi T)-(\tfrac{1}{2})b(\alpha/2\pi T)(\Delta/2\pi T)^2\ , \quad (23)$$

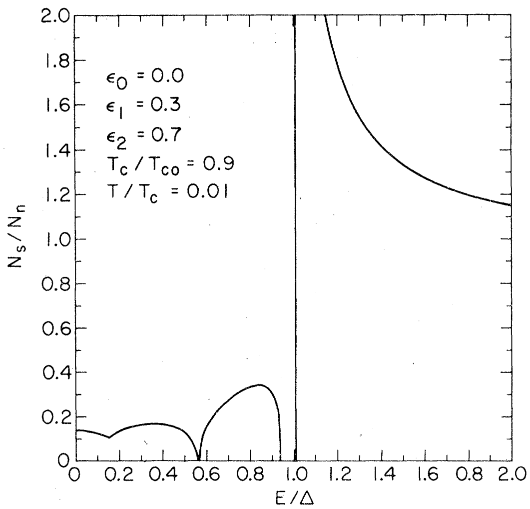

FIG. 1. Density of electron states in the superconducting state, N_s, normalized to that in the normal state, N_n, as a function of energy, E, divided by the order parameter, Δ, for the indicated values of ϵ_0, ϵ_1, ϵ_2, T_c/T_{c0}, and T/T_c.

where

$$b(x) = -(\tfrac{1}{2})\psi^{(2)}(\tfrac{1}{2}+x) + (\tfrac{1}{6}x)S\psi^{(3)}(\tfrac{1}{2}+x) \quad (24)$$

and

$$S = \frac{\sum_l F_l(1-2\epsilon_l^2)}{\sum_l F_l} \, . \quad (25)$$

The function $\psi^{(m)}(x)$ is the polygamma function, $d^m\psi(x)/dx^m$. The discontinuity in the specific heat can then be calculated in the way given by Chaba and Nagi for the restricted case.[5] The result is

$$C_s - C_n = 8\pi^2 N_0 T_c Q^2 / b(\alpha/2\pi T_c) \, , \quad (26)$$

where

$$Q = 1 - (\alpha/2\pi T_c)\psi^{(1)}(\tfrac{1}{2} + \alpha/2\pi T_c) \, , \quad (27)$$

so that

$$(C_s - C_n)/C_n = -\psi^{(2)}(\tfrac{1}{2}) T_c Q^2 / 2b(\alpha/2\pi T_c) T_{c0} \, , \quad (28)$$

where

$$\psi^{(2)}(\tfrac{1}{2}) = -14\zeta(3) \cong -16.83 \, . \quad (29)$$

The factor S in Eq. (25) can be put in the form

$$S = \frac{2\sum_l (2l+1)A_l^2}{\sum_l (2l+1)A_l} - 1 \, , \quad (30)$$

where

$$A_l = 1 - \epsilon_l^2 \, . \quad (31)$$

Since ϵ_l^2 lies between 0 and 1, A_l also lies between 0 and 1 for all l. Looking at the form of S in Eq. (30), it is then obvious what is the smallest possible value of $C_s - C_n$, for given value of $\alpha/2\pi T_c$, and therefore for a given value of T_c/T_{c0}. This smallest value is obtained if at least one ϵ_l is equal to 0 and all the values of ϵ_l are 0 or 1 for all l. In this case, $S = 1$.

V. SUMMARY

We have derived some useful theoretical results for the effect of magnetic impurities on superconductors, according to Shiba's theory.[2] The most useful results are perhaps those for U_n [Eq. (1)], δ [Eqs. (5) and (10)], T_c/T_{c0} [Eq. (17)], U [Eq. (21)], Δ near T_c [Eq. (23)], and $C_s - C_n$ [Eq. (26)]. From these results, all of the thermodynamic and transport properties can be calculated. This should provide good motivation for theoretical calculations of the relative phase shifts $(\delta_l^+ - \delta_l^-)$.

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