Brief Reports

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Free-energy formula for a superconducting alloy with localized states in the energy gap: Eliashberg formalism

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(Received 3 June 1987; revised manuscript received 14 January 1988)

We give a derivation of the formula for calculating the free-energy difference between the superconducting and the normal states of a weak-coupling superconductor with localized states within the energy gap (induced by magnetic impurities) by using the technique of coupling-constant integration. We use the Eliashberg formalism and the square-well model of the electron-phonon interaction.

Recently, Yamamoto and Nagi[1] (YN) derived a formula for calculating the free-energy difference $\Omega_{S\text{-}N}$ between the superconducting and the normal states of a strong-coupling superconductor with localized states within the Bardeen-Cooper-Schrieffer[2] (BCS) energy gap. These localized states arise in the problem of a low concentration of uncorrelated magnetic impurities in a superconductor when the scattering of a conduction electron from an impurity is treated exactly.[3,4] The formula derived in Ref. 1 is a nontrivial modification of the one given by Bardeen and Stephen[5] (for the electron-phonon system) to include the effect of magnetic impurities. The YN formula was used by Zarate and Carbotte[6] to numerically evaluate $\Omega_{S\text{-}N}$, the critical magnetic field, the specific-heat jump at the transition temperature T_c, and the critical-field deviation function. These calculations were done for the case when the host superconductor, containing magnetic impurities, is lead.

In Ref. 1, the single-particle Green's function was written by using the Eliashberg formalism[7,8] (EF) of the theory of superconductivity.[9] For calculating the properties of a strong-coupling superconductor, one needs the electron-phonon spectral density $\alpha^2F(\omega)$ and the Coulomb pseudopotential μ^* for the host metal and usually detailed numerical work is required. For a weak-coupling superconductor, the properties can be calculated analytically within the EF if the square-well model[9] of the electron-phonon interaction (or the $\lambda^{\Theta\Theta}$ model) is used. Although the $\lambda^{\Theta\Theta}$ limit of $\Omega_{S\text{-}N}$ for the superconducting alloy containing magnetic impurities can be written from Eq. (37) of Ref. 1, it is instructive to derive such a formula by using the well-known technique[10] of coupling-constant integration. This derivation is given in the present Brief Report.

The single-particle Green's function for the conduction electrons of a strong-coupling superconductor containing paramagnetic impurities and having localized states within the energy gap is given by[1]

$$G(\mathbf{K},i\omega_n)=(i\tilde{\omega}_n\rho_3-\varepsilon_{\mathbf{K}}-\tilde{\Delta}_n\rho_2\sigma_2)^{-1} , \tag{1}$$

where

$$\tilde{\omega}_n=\omega_n+\delta\tilde{\omega}_n+\sum_{l=0}^{\infty}(2l+1)\Gamma_{1l}\frac{U_n(1+U_n^2)^{1/2}}{\eta_l^2+U_n^2} , \tag{2}$$

$$\tilde{\Delta}_n=\pi T\sum_{m=-\infty}^{\infty}[\lambda(n-m)-\mu^*]\frac{1}{(1+U_m^2)^{1/2}}+\sum_{l=0}^{\infty}(2l+1)\Gamma_{2l}\frac{(1+U_n^2)^{1/2}}{\eta_l^2+U_n^2} , \tag{3}$$

$$\delta\tilde{\omega}_n=\pi T\sum_{m=-\infty}^{\infty}\lambda(n-m)\frac{U_m}{(1+U_m^2)^{1/2}} . \tag{4}$$

In the above equations $\varepsilon_{\mathbf{K}}$ 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); $U_n=\tilde{\omega}_n/\tilde{\Delta}_n$, η_l is the normalized position of a localized state within the BCS energy gap for the lth partial wave, and

$$2\Gamma_{1l}=1/\tau_{1l}+1/\tau_{2l} ,$$
$$2\Gamma_{2l}=1/\tau_{1l}-1/\tau_{2l} , \tag{5}$$

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 related to $\alpha^2F(\omega)$.

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

$$\lambda(n-m)=\lambda\Theta(\omega_D-|\omega_n|)\Theta(\omega_D-|\omega_m|)\ , \quad (6)$$

where ω_D is the Debye cutoff frequency. In this model, Eq. (4) gives $\delta\tilde{\omega}_n=\lambda\omega_n$ and Eqs. (2) and (3) are combined to give

$$U_n\phi=\omega_n(1+\lambda)+\sum_{l=0}^{\infty}(2l+1)\alpha_l\frac{U_n(1+U_n^2)^{1/2}}{\eta_l^2+U_n^2}\ , \quad (7)$$

$$\phi=2\pi TgN(0)\sum_{n=0}^{N}\frac{1}{(1+U_n^2)^{1/2}}\ , \quad (8)$$

$$\alpha_l=\Gamma_{1l}-\Gamma_{2l}=\frac{n_i}{2\pi N(0)}(1-\eta_l^2)\ , \quad (9)$$

$$g=\lambda-\mu^*\ , \quad (10)$$

$$N=\frac{\omega_D}{2\pi T}-\frac{1}{2}\ , \quad (11)$$

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

The free-energy difference $\Omega_{S\text{-}N}$ can be calculated from the relation[10]

$$\Omega_{S\text{-}N}=\int_0^g\delta\left[\frac{1}{g}\right]\phi^2\ . \quad (12)$$

Substituting $(1/g)$ from Eq. (8) in Eq. (12) and doing partial integration, we obtain

$$\Omega_{S\text{-}N}=2\pi TN(0)\sum_{n(\geq 0)}\left[\frac{\phi}{(1+U_n^2)^{1/2}}+2\int_{U_n}^{\infty}\frac{dU_n}{(1+U_n^2)^{1/2}}\frac{d\phi}{dU_n}\right]\ . \quad (13)$$

Evaluating $d\phi/dU_n$ from Eq. (7), substituting it in Eq. (13) and after integration, we get

$$\Omega_{S\text{-}N}=-2\pi TN(0)\sum_{n(\geq 0)}\left\{-\frac{\phi}{(1+U_n^2)^{1/2}}+2\omega_n(1+\lambda)\left[\frac{(1+U_n^2)^{1/2}}{U_n}-1\right]+\sum_{l=0}^{\infty}(2l+1)\alpha_l\left[\frac{2}{\eta_l^2+U_n^2}+\frac{1}{1-\eta_l^2}\ln\left[\frac{\eta_l^2+U_n^2}{1+U_n^2}\right]\right]\right\}\ . \quad (14)$$

Substituting ϕ and α_l from Eqs. (7) and (9), respectively, Eq. (14) gives

$$\Omega_{S\text{-}N}=-2\pi TN(0)\sum_{n(\geq 0)}\left[\omega_n(1+\lambda)\left[\frac{(1+U_n^2)^{1/2}}{U_n}+\frac{U_n}{(1+U_n^2)^{1/2}}-2\right]\right]-n_iT\sum_{n(\geq 0)}\sum_{l=0}^{\infty}(2l+1)\left[\frac{1-\eta_l^2}{\eta_l^2+U_n^2}+\ln\left[\frac{\eta_l^2+U_n^2}{1+U_n^2}\right]\right]\ , \quad (15)$$

which is our final result. Ignoring the difference between $\delta\tilde{\omega}_n$ and its normal-state value $\delta\tilde{\omega}_n^0$, which in the $\lambda^{\Theta\Theta}$ model is at most of the order $(\Delta_0/\omega_D)^2$ (Δ_0 being the gap edge for the system with no magnetic impurities), the $\lambda^{\Theta\Theta}$ limit of Eq. (37) of Ref. 1 agrees with Eq. (15).

Summarizing, we have derived a formula [Eq. (15)] for calculating the free-energy difference $\Omega_{S\text{-}N}$ for a weak-coupling superconductor with localized states within the energy gap by using the well-known technique[10] of coupling-constant integration. We have used the Eliashberg formalism and the square-well model of the electron-phonon interaction.

Financial support provided by the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

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