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STRONG-COUPLING SUPERCONDUCTOR AT NONZERO TEMPERATURE

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The strong-coupling superconductors Pb and Hg have long been considered anomalous in the deviation of their superconducting properties from the law of corresponding states and from the predictions of the simplest form of the BCS theory.[1] Recent calculations of the effective tunneling density of states for Pb are in good agreement with the experimentally measured tunneling anomaly near zero temperature.[2-4] In these calculations, the effective electron-electron interaction was represented by a retarded dressed-phonon exchange and a static Coulomb pseudopotential.

In this Letter we extend these calculations to nonzero temperatures and (1) evaluate the effective electron-phonon coupling constant for Pb using an approximate form of the matrix element suggested by Harrison[5]; (2) determine the frequency dependence of the gap function at nonzero temperature; and (3) discuss an anomaly in the effective tunneling density of states arising from recombination processes.

The electron-electron interaction for energy transfer q_0 and momentum transfer q can be written in the form

$$V(q,q_0)=\frac{4\pi e^2}{q^2\epsilon(q,q_0)}+\sum_\lambda |v_{q\lambda}|^2\frac{1}{q_0^2-\omega_{q\lambda}^2+i\delta}, \quad (1)$$

where $\epsilon(q,q_0)$ is the electron dielectric constant, $\omega_{q\lambda}$ is the dressed-phonon frequency of momentum q and polarization λ, and $v_{q\lambda}$ is the effective electron-phonon coupling matrix element. When q is outside the first Brillouin zone, $\omega_{q\lambda}$ is the frequency corresponding to the appropriate reduced wave vector $q-K$, where K is a reciprocal lattice vector. Using (1) with $q_0=0$ in ϵ, a spherical band approximation, and keeping only the lowest order vertex parts, the integral equation for the energy-gap function $\Delta(\omega)$ at nonzero temperature $T=1/k\beta$ is[6]

$$\Delta(\omega)=\frac{1}{Z(\omega)}\int_0^{\omega_c}d\omega'\,\mathrm{Re}\left\{\frac{\Delta(\omega')}{[\omega'^2-\Delta^2(\omega')]^{1/2}}\right\}[f(-\omega')K_+(\omega,\omega')-f(\omega')K_+(\omega,-\omega')-U_c\tanh(\tfrac{1}{2}\beta\omega')]$$

$$+\frac{i\pi}{Z(\omega)}\int_0^{\omega_c}d\omega'\left\{\frac{\Delta(\omega+\omega')}{[(\omega+\omega')^2-\Delta^2(\omega+\omega')]^{1/2}}+\frac{\Delta(\omega-\omega')}{[(\omega-\omega')^2-\Delta^2(\omega-\omega')]}\right\}\frac{\sum_\lambda a_\lambda^2(\omega')F_\lambda(\omega')}{e^{\beta\omega'}-1}; \quad (2)$$

the renormalization parameter $Z(\omega)$ is given in terms of $\Delta(\omega)$ by the quadrature

$$[1-Z(\omega)]\omega = \int_0^{\omega_C} d\omega' \,\mathrm{Re}\left\{\frac{\omega'}{[\omega'^2-\Delta^2(\omega')]^{1/2}}\right\}[f(-\omega')K_-(\omega,\omega')+f(\omega')K_-(\omega,-\omega')]$$
$$-i\pi\int_0^{\omega_C} d\omega' \left\{\frac{\omega+\omega'}{[(\omega+\omega')^2-\Delta^2(\omega+\omega')]^{1/2}}+\frac{\omega-\omega'}{[(\omega-\omega')^2-\Delta^2(\omega-\omega')]^{1/2}}\right\}\frac{\sum_\lambda a_\lambda^2(\omega')F_\lambda(\omega')}{e^{\beta\omega'}-1}. \quad (3)$$

Here the integrations are cut off at a frequency ω_C large compared to the Debye energy,[7] f is the Fermi function, and U_C is a Coulomb pseudopotential which accounts for the Coulomb scattering outside a band of energy $\pm\omega_C$ about the Fermi surface.[8] The kernels $K_\pm(\omega,\omega')$ are given by integrals over the phonon density of states $F_\lambda(\omega)$ of polarization λ:

$$K_\pm(\omega,\omega') = \sum_\lambda \int_0^\infty d\omega_0\, \alpha_\lambda^2(\omega_0)F_\lambda(\omega_0)[D^*(\omega'+\omega+\omega_0)\pm D(\omega'-\omega+\omega_0)], \quad (4)$$

where $D(x)=(x-i0^+)^{-1}$. The effective phonon coupling constant $\alpha_\lambda^2(\omega)$ is the s-wave average of the electron-phonon coupling,

$$\alpha_\lambda^2(\omega) = \frac{q_d^3}{6\pi^2}\left\{\sum_K \int \frac{d\Omega_q}{4\pi}\frac{|v_{q+K\lambda}|^2}{2\omega_{q\lambda}}\frac{m}{2p_F|q+K|}\theta(2p_F-|q+K|)\right\}\Bigg|_{\omega_{q\lambda}=\omega}. \quad (5)$$

Here q_d is the Debye wave vector, p_F the Fermi wave vector, and m is the mass due to the band structure with Coulomb corrections but without corrections for the electron-phonon interaction, which are accounted for in the frequency dependence of Z.[9] θ is a unit step function vanishing when its argument is less than zero and equal to 1 otherwise. The restriction in Eq. (5) to momentum transfer less than $2p_F$ arises because of the large energy denominators associated with scattering away from the Fermi surface. In (5) q is given by $\omega_{q\lambda}=\omega$.

The model for a particular substance is specified by the choice of the phonon density of states $F_\lambda(\omega)$ and the interaction matrix elements U_C and $|v_{q\lambda}|^2$. In our calculation $F_\lambda(\omega)$ was represented by a cut-off Lorentzian

$$F_\lambda(\omega) = A_\lambda\left[\frac{1}{(\omega-\omega_1^\lambda)^2+\omega_2^{\lambda 2}}-\frac{1}{\omega_3^{\lambda 2}+\omega_2^{\lambda 2}}\right], \quad |\omega-\omega_1^\lambda|<\omega_3^\lambda;$$
$$=0 \quad , \quad |\omega-\omega_1^\lambda|>\omega_3^\lambda. \quad (6)$$

Here A_λ normalizes $F_\lambda(\omega)$ to unity, and the ω_1^λ (in meV) are $\omega_1^t=4.4$, $\omega_2^t=0.75$, $\omega_1^l=8.5$, $\omega_2^l=0.5$, and $\omega_3^\lambda=3\omega_2^\lambda$. The values of ω_1^λ and ω_2^λ are the same as those taken in reference 3. This choice is based upon the data obtained from superconducting tunneling experiments which show sudden decreases in the differential conductance at voltages of $\omega_1^\lambda+\Delta$. The choice of ω_3^λ roughly reproduces the high-energy end of the phonon spectrum observed by Brockhouse.[10] The Coulomb pseudopotential U_C is estimated to be 0.11.

The electron-phonon matrix element is given in terms of the form factor $S(q)$:

$$v_{q\lambda} = (N/M)^{1/2} i\vec{q}\cdot\vec{\epsilon}_{q\lambda} S(q). \quad (7)$$

Here N is the number density of ions, M the ionic mass, and $\vec{\epsilon}_{q\lambda}$ the polarization vector of the phonons. Harrison[5] has shown that $S(q)$ can be approximated by a Coulomb attraction and a repulsive δ function (representing the effects of orthogonalization to the core electrons), all screened by a Hartree dielectric constant. In this calculation the dielectric constant is approximated by the Fermi-Thomas form so that

$$S(q) = \frac{-(4\pi e^2 Z/q^2)+\beta}{1+(K_s/q)^2}. \quad (8)$$

Here K_s is the Fermi-Thomas screening fac-

tor, Z is the ionic charge, and β characterizes the strength of the repulsive core. β is approximately 60 Ry × atomic units of volume for Pb.[5] Using this value, the effective coupling constants $\alpha_\lambda^2(\omega)$ are calculated from Eq. (5). The q dependence of the dressed-phonon frequency $\omega_{q\lambda}$ is obtained from the phonon density of states $F_\lambda(\omega)$, Eq. (6). We restrict the summation over K in (5) to the 14 shortest reciprocal lattice vectors and neglect the condition $\theta(2p_F - |q+K|)$. A phase-space estimation shows that this may lead to some 20% error in α_λ^2 (overestimation). The results are given in Fig. 1. These turn out to be smoothly varying functions of ω in the neighborhood of the peaks of $F_\lambda(\omega)$ with $\alpha_t^2(\omega_1^t) = 1.05$ meV and $\alpha_l^2(\omega_1^l) = 1.98$ meV.

We have solved the gap equation with $\alpha_l^2/\alpha_t^2 = 2$, $U_C = 0.11$, and the phonon density of states, Eq. (6). In this calculation α_t^2 was taken as a constant and adjusted to give the correct zero-temperature value of the gap at the gap edge [$\Delta_0 = \Delta(\Delta_0) = 1.34$ meV]. The value of α_t^2 obtained in this manner was 0.807 meV, about 20% smaller than the calculated value of $\alpha_t^2(\omega_1^t)$.

The frequency dependence of Δ at $T/T_C = 0$ and $T/T_C = 0.98$ is shown in Fig. 2. The general resonance shape is maintained and scaled down.[11] At $T = 0$, resonant peaks in Δ_2 associated with phonon emission appear at energies $\omega_1^\lambda + \Delta_0$. Because of the nonlinearity of the gap equation, additional structure associated with these resonances is observed at higher

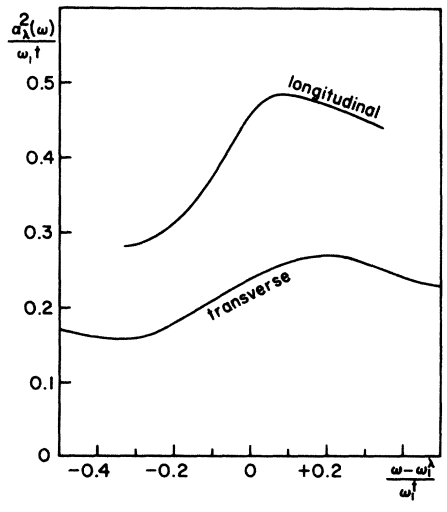

FIG. 1. The energy dependence of the effective electron-phonon coupling constants $\alpha_\lambda^2(\omega)$ in the unit of typical transverse phonon energy ω_1^t. $\beta = 60$ Rydberg × atomic units of volume.

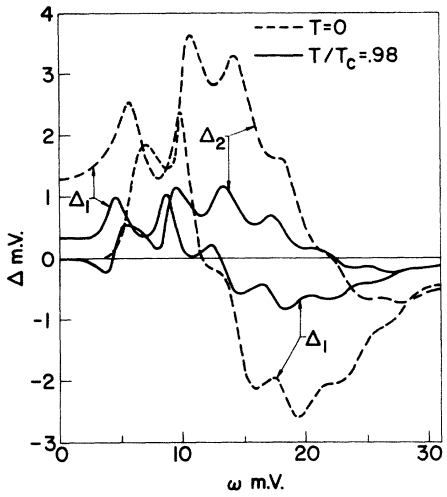

FIG. 2. Computed real and imaginary parts of the complex gap function $\Delta = \Delta_1 + i\Delta_2$ as a function of energy. The dashed curves are for $T = 0$, and the solid curves for a reduced temperature $T/T_C = 0.98$. For this calculation $\alpha_t^2 = (\alpha_l^2/2) = 0.807$.

harmonics. At nonzero temperature, the gap at the gap edge is reduced and the phonon-emission resonances at $\omega_1^\lambda + \Delta_0(T)$ are shifted down in energy. The overall amplitude of the gap function is scaled down by roughly $\Delta_0(T)/\Delta_0(0)$. Δ vanishes at $\omega = 0$ due to the nonvanishing damping of the excitations, although it cannot be seen in Fig. 2. Moreover, new resonance structure occurs near the frequencies $\omega_1^\lambda - \Delta_0(T)$. This is most evident at $\omega_1^t - \Delta_0(T)$ (Fig. 2, $\omega = 3.9$ meV), where $\Delta_2(\omega, T)$ goes through a negative resonance peak. These new resonances are associated with recombination processes. At nonzero temperatures there are excited quasiparticles and there is a high density of states for quasiparticles at the gap edge $\Delta_0(T)$. The injected electron can combine with an excited quasiparticle, emit a phonon, and form a ground-state pair. The rate of this process is a maximum when the total energy ω of the injected electron and excited quasiparticle at $\Delta_0(T)$ are equal to a frequency corresponding to a peak in the phonon density of states ω_1^λ [i.e., $\omega + \Delta_0(T) = \omega_1^\lambda$].

This additional structure in Δ is reflected in the effective tunneling density of states

$$\frac{N(\omega)}{N(0)} = \mathrm{Re}\left\{\frac{\omega}{[\omega^2 - \Delta^2(\omega, T)]^{1/2}}\right\}.$$

However, the differential conductance dI/dV

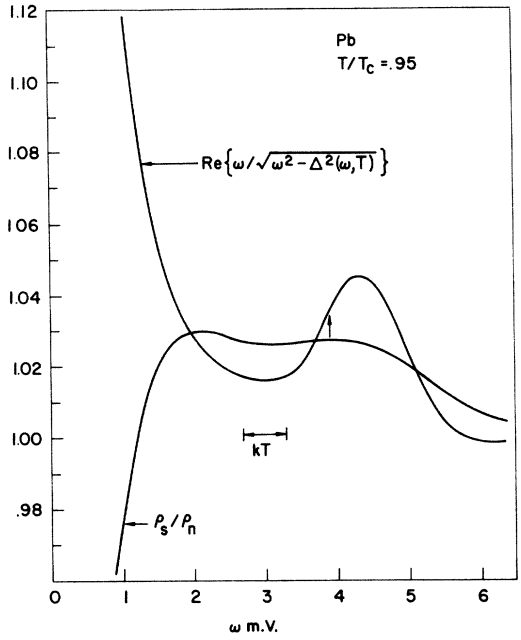

FIG. 3. Normalized density of states $N(\omega)/N(0) = \mathrm{Re}\{\omega/[\omega^2-\Delta^2(\omega,T)]^{1/2}\}$, and normalized differential conductance $\rho_S/\rho_n = (dI/dV)_S/(dI/dV)_n$ versus energy for a reduced temperature $T/T_c = 0.95$. The subscripts n and s refer to normal and superconducting. The arrow indicates $\omega = \omega_1^t - \Delta_0(T)$.

is proportional to

$$\int dE\, N(E)\left[-\frac{df(E+V)}{dE}\right],$$

and the additional structure present at nonzero temperature is smeared out. Our present calculations indicate that this recombination structure should nevertheless be observable above $T/T_c = 0.7$ with the maximum effect occurring near $T/T_c = 0.95$. Figure 3 is a plot of the density of states and of dI/dV at $T/T_c = 0.95$ in the energy region near $\omega_1^t - \Delta_0 = 3.9$ meV.

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$$\tfrac{1}{2}\alpha_\lambda^2 \ln\left[\frac{(\omega+\omega_1^\lambda+\omega_c)^2+\omega_2^{\lambda 2}}{(\omega-\omega_1^\lambda-\omega_c)^2+\omega_2^{\lambda 2}}\right]$$

is obtained for each polarization branch.

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