BARDEEN-COOPER-SCHRIEFFER THEORY OF SUPERCONDUCTIVITY IN THE CASE OF OVERLAPPING BANDS

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The purpose of this note is to point out an extension of the Bardeen-Cooper-Schrieffer theory of superconductivity[1] to the case where two bands with more or less itinerant electrons overlap. Such a situation arises in the transition elements, in which s-d scattering supposedly contributes considerably to the resistivity in the normal state.[2] We discuss here the corresponding result for the superconducting state in some of the transition elements, though one may speculate if such effects do not also occur in some cases of superconductors with s-p bands.

By analogy with the BCS theory, we write down the electron portion of the Hamiltonian resulting from emission and reabsorption of a phonon. This virtual process may take place in four ways, since an s or a d electron may emit the phonon, and then, an s or a d electron may reabsorb it independently. The phonon involved must have a wave number equal to the difference in wave numbers of the two electrons, both of which must be in the same vicinity of the Fermi level as in the BCS theory. For an s-d process the phonon involved must therefore have a certain minimum momentum, the same minimum as in the corresponding resistivity theory.

The portion of the Hamiltonian that is amenable to formation of ss and dd pairs now takes the form

$$H=\sum_{k\sigma}\epsilon_{ks}c_{k\sigma}^*c_{k\sigma}+\sum_{k\sigma}\epsilon_{kd}d_{k\sigma}^*d_{k\sigma}-\sum_{kk'}V_{ss}c_{k\uparrow}^*c_{-k\downarrow}^*c_{-k'\downarrow}c_{k'\uparrow}-V_{dd}\sum_{kk'}d_{k\uparrow}^*d_{-k\downarrow}^*d_{-k'\downarrow}d_{k'\uparrow}$$
$$-V_{sd}\sum_{kk'}(c_{k\uparrow}^*c_{-k\downarrow}^*d_{-k'\downarrow}d_{k'\uparrow}+d_{k\uparrow}^*d_{-k\downarrow}^*c_{-k'\downarrow}c_{k'\uparrow}), \qquad (1)$$

where ϵ_{ks}, ϵ_{kd} are s- and d-band kinetic energies, and c^*, c and d^*, d the corresponding annihilation and creation operators. V_{ss}, V_{dd}, and V_{sd} are the averaged interaction energies resulting from phonon emission and absorption by s-s, d-d, and s-d processes, minus the corresponding shielded Coulomb interaction terms. As in the BCS theory, we assume that the summations extend only over $\vec{k}$ values (quite different $\vec{k}$ values in the two bands) corresponding to energies within a distance $\pm\hbar\omega$ of the Fermi surface. ($\hbar\omega$ is of the order of the maximum available phonon energy.)

Following Bogoliubov,[3] we introduce the new operators e and f by the transformations

$$c_{k\uparrow}=\cos(\theta_k/2)e_{k\uparrow}+\sin(\theta_k/2)e_{-k\downarrow}^*;$$

$$d_{k\uparrow}=\cos(\varphi_k/2)f_{k\uparrow}+\sin(\varphi_k/2)f_{-k\downarrow}^*,$$

$$c_{k\downarrow}=\cos(\theta_k/2)e_{k\downarrow}-\sin(\theta_k/2)e_{-k\uparrow}^*;$$

$$d_{k\downarrow}=\cos(\varphi_k/2)f_{k\downarrow}-\sin(\varphi_k/2)f_{-k\uparrow}^*.$$

The parameters θ, φ are determined by substituting for c and d in (1), and equating to zero the coefficients of $e_k^*e_{-k}^*$ and $e_{-k}e_k$, and similarly for the f terms. The resulting equations are

$$\epsilon_{ks}\sin\theta_k-[V_{sd}D+V_{ss}S]\cos\theta_k=0,$$
$$\epsilon_{kd}\sin\varphi_k-[V_{dd}D+V_{sd}S]\cos\varphi_k=0, \qquad (2)$$

with

$$D=\tfrac{1}{2}\sum_k\sin\varphi_k[1-2f_d(E_{kd})],$$
$$S=\tfrac{1}{2}\sum_k\sin\theta_k[1-2f_s(E_{ks})]. \qquad (3)$$

Here $f_s(E_{ks})$, $f_d(E_{kd})$, respectively, denote the number of quasi-particles deriving from the s and d bands that are excited to energies E_{ks}, E_{kd}, respectively. These energies are

$$E_{ks}=(\epsilon_{ks}^2+A^2)^{1/2},\quad E_{kd}=(\epsilon_{kd}^2+B^2)^{1/2},$$

where

$$A=V_{sd}D+V_{ss}S,\quad B=V_{dd}D+V_{sd}S.$$

The self-consistency conditions for (2) and (3) give two simultaneous equations for A and B:

$$A[1-V_{ss}N_sF(A)]=BV_{sd}N_dF(B),$$
$$B[1-V_{dd}N_dF(B)]=AV_{sd}N_sF(A), \qquad (4)$$

where

$$F(A)=\int_0^{\hbar\omega}d\epsilon\tanh\left[\frac{(\epsilon^2+A^2)^{1/2}}{2kT}\right]\Big/(\epsilon^2+A^2)^{1/2},$$

and where N_s, N_d are the densities of states in the s and d bands near the Fermi level.

The transition temperatures are given by the quadratic

$$[V_{ss}+N_d(V_{sd}^2-V_{ss}V_{dd})F(0)][V_{dd}+N_s(V_{sd}^2-V_{ss}V_{dd})F(0)]=V_{sd}^2.$$

When this equation is solved for $F(0)$, and use is made of the BCS expression for $F(0)$, the transition temperature is found to be

$$kT_c=1.14\hbar\omega\exp\left\{-\left[\frac{[V_{sd}^2/N_sN_d+\frac{1}{4}(V_{dd}/N_s-V_{ss}/N_d)^2]^{1/2}}{V_{sd}^2-V_{ss}V_{dd}}-\frac{\frac{1}{2}(V_{dd}/N_s+V_{ss}/N_d)}{V_{sd}^2-V_{ss}V_{dd}}\right]\right\},$$

and both A and B go to zero there. In the special case of interband scattering only ($V_{ss}=V_{dd}=0$) one obtains the same transition temperature as BCS, with a state density $(N_sN_d)^{1/2}$, but, unless $N_s=N_d$, there are still two gaps. Figures 1 and 2 show the gaps for a variety of values of the parameters.

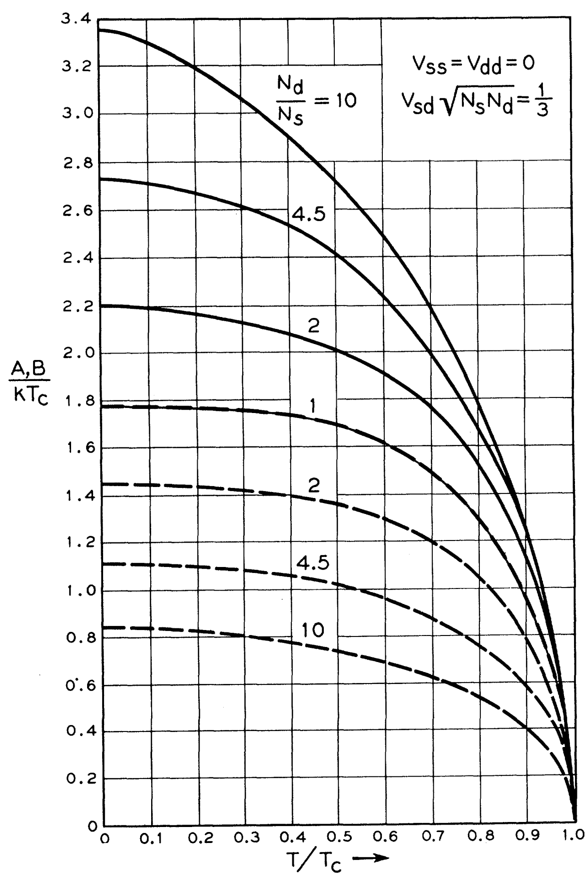

FIG. 1. The gap-pairs for $V_{ss}=V_{dd}=0$ and various densities of state. The curves for V_{ss}, $V_{dd}\neq 0$ are very similar to those shown, except when $V_{sd}^2 \ll V_sV_d$.

These results may obviously be generalized to more complicated band structures. When there are n distinct Fermi surfaces in $\vec{k}$ space, the pair of equations (4) is replaced by the set

$$A_i=\sum_{j=1}^{n}V_{ij}A_jN_jF(A_j), \qquad (n=1,2\ldots)$$

determining the n energy gaps A_i. We suggest

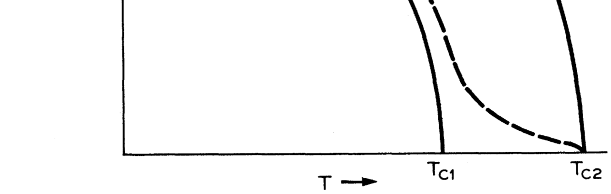

FIG. 2. When $V_{sd}=0$, there are two transition temperatures. When V_{sd}^2 is finite but much less than $V_{ss}V_{dd}$, the lower transition temperature disappears in the manner shown.

these results as a possible explanation of the fine structure observed by Tinkham and co-workers[4,5] in their infrared absorption measurements in some superconductors. They may also partly account for the rules according to which maximal transition temperatures for s - d superconductors are observed at conduction electron concentrations corresponding to at least some of the maxima in the N_d curve. Even though the d electrons may not participate directly in the phenomenon of superconductivity ($V_d = 0$), the s electrons can benefit from the higher density of states in the d band.

[1]Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957); hereafter referred to as BCS.

[2]E.g., A. H. Wilson, The Theory of Metals (Cambridge University Press, Cambridge, 1953), second edition, Sec. 9.51.

[3]N. N. Bogoliubov, J. Exptl. Theoret. Phys. U.S.S.R. 34, 65 (1958) [translation: Soviet Phys. JETP 7, 41 (1958)].

[4]Ginsberg, Richards, and Tinkham, Phys. Rev. Letters 3, 337 (1959).

[5]P. L. Richards, thesis, Berkeley, 1959 (to be published).

RESONANT ABSORPTION OF THE 14.4-kev γ RAY FROM 0.10-μsec Fe^{57}†

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We wish to report experiments on the resonant scattering of a recoil-free γ ray[1] which appears to be sharp enough to be used for an experimental determination of the "gravitational red-shift," as proposed in our recent note.[2]

Our initial work has been with the 14.4-kev γ ray of 0.10-microsecond Fe^{57}. Although we first worked with a source of the 270-day parent Co^{57} extracted from an iron foil kindly irradiated for us with the deuteron beam at the MIT cyclotron, an intense background of Co^{56} rendered that source poor for our purposes. Most of our work has been with Co^{57} obtained commercially.

About 50 microcuries of Co^{57} was electroplated together with added iron onto one face of a one-centimeter square of thin Armco iron.

Initial studies of the absorption of a 0.001-in. thick iron foil at temperatures of liquid nitrogen and at room temperature indicated that the desired resonant absorption was present, that the ratio of about 3:2 of the magnitudes at the two temperatures was in reasonable agreement with theory, but that the absorption was small and the line was broad compared to its natural breadth. In these experiments crude 60-cycle magnetic vibrators were used to destroy resonance and to observe the line widths. The increase in intensity available by the use of low temperatures is so small that we henceforth operated at room temperature, in the interest of stability.

The supposition that the hyperfine structure splittings of the ferromagnetic source and absorber were not fully equivalent led us to try heat treatments of the source and absorber foils. A dramatic improvement resulted after the source had been held at 950°C for an hour, which treatment was expected to result in diffusion of the cobalt, if it were retained on the surface initially, into the lattice a mean distance of about 3×10^{-5} cm, or 1000 lattice spaces. We have discovered that there was probably about 0.1 mg of stable cobalt carrier present in our source which may be important in making such treatment necessary. With the absorber foil first used, which was found to contain 3% silicon, replaced by one rolled from Armco iron to 11.5 mg/cm^2 thickness, and annealed, the line shown in Fig. 1 was obtained.

These data represent counts above background of the 14.4-kev γ ray as made with a scintillation spectrometer, using a 0.040-in. by $\frac{3}{4}$-in. NaI(Tl) crystal[3] and a single-channel pulse-height analyzer set to accept most of the full-energy peak.

All but about fifteen percent of the counts in the channel arose from the γ ray, from evidence obtained with absorbing foils. Each point is based on about 2.3×10^5 counts shared equally between conditions with the source fixed and with it moving toward and away from the absorber at constant speed. The motion was produced by a moving-coil magnetic transducer on which the source was cemented and which was supplied with a ten-cycle-per-second triangular waveform of current of adjustable amplitude.

The resonant absorption is halved by a Doppler speed of $|v_{1/2}| = 0.017$ cm/sec (which, incidentally,