(1) Superconductors

THE PRESSURE DEPENDENCE OF TRANSITION TEMPERATURE IN SOME SUPERCONDUCTORS *

B. N. GANGULY and K. P. SINHA
National Chemical Laboratory, Poona, India

Received 18 December 1964

In the present paper we discuss a possible mechanism of the pressure dependence of the transition temperature in superconductors having two bands either s - p or s - d. The essential point in the treatment is to envisage such perturbations in the system which can cause interband scattering of the electrons near the Fermi surface. A perturbation theory, analogous to that used by Suhl and Matthias [1] for the impurity scattering, is employed in the formulation.

The Hamiltonian for the system is taken as

$$H = H_0 + H' , \tag{1}$$

where H_0 is the unperturbed BCS-type two band Hamiltonian and the perturbation

$$H' = \sum_{\boldsymbol{kk}'\sigma} M_{\boldsymbol{kk}'} \left(d^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}'\sigma} + c^\dagger_{\boldsymbol{k}'\sigma} d_{\boldsymbol{k}\sigma} \right) , \tag{2}$$

where $c^\dagger$, c and $d^\dagger$, d are the corresponding creation and annihilation operators for s and d (or p) bands respectively. $M_{\boldsymbol{kk}'}$ is the matrix element of the perturbation V_c which causes interband scattering, namely

$$M_{\boldsymbol{kk}'} = \langle \psi_d(\boldsymbol{k}') | V_c | \psi_s(\boldsymbol{k}) \rangle . \tag{3}$$

Next, we apply the Bogoliubov transformation to (1) and then a canonical transformation in order to eliminate the first order term in the transformed Hamiltonian. We get

* Communication No. 743 from the National Chemical Laboratory, Poona-8 (India).

$$H_{\text{new}} = H_{\text{T}}^0 - \sum_{kk'\sigma} |M_{kk'}|^2 \Bigg[\Bigg\{ \Big(\frac{\beta_{kk'}^{\dagger 2}}{E_{\text{s}k'} + E_{\text{d}k}} - \frac{\alpha_{kk'}^{\dagger 2}}{E_{\text{s}k'} - E_{\text{d}k}} \Big) f_{k\sigma}^{\dagger} f_{k\sigma} + \Big(\frac{\beta_{kk'}^{\dagger 2}}{E_{\text{s}k'} + E_{\text{d}k}} + \frac{\alpha_{kk'}^{\dagger 2}}{E_{\text{s}k'} - E_{\text{d}k}} \Big) e_{k'\sigma}^{\dagger} e_{k'\sigma} \Bigg\} +$$

$$+ \frac{\alpha_{kk'}^{\dagger} \beta_{kk'}^{\dagger}}{2} \Bigg\{ \Big(\frac{1}{E_{\text{s}k'} + E_{\text{d}k}} + \frac{1}{E_{\text{s}k'} - E_{\text{d}k}} \Big) \Big(f_{-k\downarrow}^{\dagger} f_{k\uparrow}^{\dagger} - f_{-k\downarrow} f_{k\uparrow} \Big) +$$

$$+ \Big(\frac{1}{E_{\text{s}k'} + E_{\text{d}k}} - \frac{1}{E_{\text{s}k'} - E_{\text{d}k}} \Big) \Big(e_{-k'\downarrow}^{\dagger} e_{k'\uparrow}^{\dagger} - e_{-k'\downarrow} e_{k'\uparrow} \Big) \Bigg\} - 2 \frac{\beta_{kk'}^{\dagger 2}}{E_{\text{s}k'} + E_{\text{d}k}} \Bigg] ,$$

where

$$\alpha_{kk'}^{\dagger} = \cos \tfrac{1}{2}(\theta_{k'} + \varphi_k) \; ; \qquad \beta_{kk'}^{\dagger} = \sin \tfrac{1}{2}(\theta_{k'} + \varphi_k) \tag{4}$$

and

$$E_{\text{s}k} = [\epsilon_{\text{s}k}^2 + \epsilon_{0\text{s}}^2(k)]^{\frac{1}{2}} , \qquad E_{\text{d}k} = [\epsilon_{\text{d}k}^2 + \epsilon_{0\text{d}}^2(k)]^{\frac{1}{2}} ,$$

$\epsilon_{0\text{s}}(k)$ and $\epsilon_{0\text{d}}(k)$ being the energy gaps in the s- and d- (or p) bands respectively; θ_k and φ_k are the angle variables involved in the Bogoliubov transformation. In the present study only the zero point shift term i.e. the last term of (4) is important; others in the square bracket are disregarded on the basis of the arguments similar to those put forward by Suhl and Matthias [1].

Assuming that the transition temperature decreases on the application of pressure which in turn involves change in volume of the system, we can write

$$\eta = \frac{\Delta V}{V} = \frac{F_{\text{n}}(T_{\text{c}}^*) - F_{\text{s}}(T_{\text{c}}^*)}{\delta F_{\text{n}}(T_{\text{c}}^*) - \delta F_{\text{s}}(T_{\text{c}}^*)} , \tag{5}$$

where T_{c}^* represents the new transition temperature and suffixes n and s refer to the normal and superconducting phases $F_{\text{n, s}}$ being the free energy of the corresponding phases. Then following the method of Suhl and Matthias [1] we get,

$$\epsilon_0^{\text{eff}}(\eta) = \hbar\omega \left[\frac{\epsilon_0^{\text{eff}}(0)}{\hbar\omega} \right] \exp \left\{ \frac{4\,|M_{kk'}|^2}{\hbar\omega} [N_{\text{s}}(0) \cdot N_{\text{d}}(0)]^{\frac{1}{2}} \cdot \frac{P}{K} \right\} \tag{6}$$

where

$$\epsilon_0^{\text{eff}}(0) = [\epsilon_{0\text{s}} \cdot \epsilon_{0\text{d}}]^{\frac{1}{2}}$$

and

$$\epsilon_0^{\text{eff}}(\eta) = [\epsilon_{0\text{s}}(\eta) \cdot \epsilon_{0\text{d}}(\eta)]^{\frac{1}{2}} .$$

In deriving (6) we have used the relation [2] $\eta = \Delta V/V = -P/K$, where P is the pressure and $1/K$ the constant of hydrostatic compression. It is to be noted that we have the relation

$$\epsilon_0^{\text{eff}}(\eta) = 1.75\; kT_{\text{c}}^* \quad \text{and} \quad \epsilon_0^{\text{eff}}(0) = 1.75\; kT_{\text{c}} .$$

Now

$$\epsilon_0^{\text{eff}}(0)/\hbar\omega \approx 1.75\; kT_{\text{c}}/\Theta_{\text{D}} = 1/n ,$$

where Θ_{D} is the Debye temperature of the system. The value of $1/n$ is derived from the known superconducting transition (T_{c}) and Debye (Θ_{D}) temperatures of each system. K is taken to be of the order of 10^{12} dynes per cm^2 and $[N_{\text{s}}(0) \cdot N_{\text{d}}(0)]^{\frac{1}{2}} \approx 3.05 \times 10^{12}$ (erg. atom)$^{-1}$, $|M_{kk'}|^2$ is estimated to be of the order of 10^{-27} (erg)^2 from one experimental point of each system. In the figure we give the theoretical curve along with experimental points for In [3], Sn [3] and Nb_3Sn [4] systems which involves two overlapping s and d (or p) bands. It is to be noted that the cyrstal field around Nb atoms due to nearest neighbours has axial symmetry and mixes s and d states. It will be seen that the experimental points fall all along the theoretical curves.

The estimated value of $|M_{kk'}|^2$ is of the order of 10^3 cm^{-1} i.e. 0.2 eV. If the origin of the perturbation is of the crystal field type, one can attempt to have a rough idea from some earlier studies. In this context, we have to take into account two types of interband transitions. One is the mixing of states on