A New Aspect of Superconductivity in A-15 Compounds

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We present a new aspect of superconductivity in A-15 compounds which is able to explain their exceptional role among the high $T_c$ superconductors. The basic idea is that a strong energy dependence of the electronic density of states near the Fermi level may greatly reduce the repulsive part of the frequency dependent electron-phonon interaction. This leads to a large enhancement of $T_c$ which is a maximum when the Fermi energy is comparable to a typical phonon energy. Our findings are based on numerical solutions of the Eliashberg equations where both the retardation of the electron-phonon coupling and the energy dependence of the electronic density of states have been included. For the electronic density of states we use the models of Labbé und Friedel and of Cohen et al., while the shape of the Eliashberg function $\alpha^2 F(\omega)$ is taken from the tunneling results of Shen. We compare our theory to experimental results for ternary A-15 compounds.

1. Introduction

The theoretical investigation of strong-coupling superconductors is based on the Eliashberg equations for the gap function $A(\omega)$ and the renormalization function $Z(\omega)$ [1, 2]. In order to calculate the superconducting transition temperature $T_c$, McMillan [1] has given a solution of these equations in his famous paper of 1968 which has been modified and improved by numerous authors (see, e.g., [3] and references therein). In all these papers, the detailed shape of the phonon spectrum $F(\omega)$ was taken into account, whereas the electronic density of states was assumed to be a constant around the Fermi level. This latter assumption may be good for most of the superconducting materials, but it presumably fails for many of the high $T_c$ A-15 compounds such as Nb$_3$Sn, V$_3$Si, or V$_3$Ga. Here, band structure calculations [4-6] have shown the Fermi level to lie within a narrow peak of the density of states. In addition, for A-15 compounds there is strong experimental evidence of a fast varying density of states near the Fermi level as indicated by the temperature dependence of the paramagnetic susceptibility, of the electrical conductivity and of the elastic constants. (For an extensive review, see, e.g., [5] and [7]). Therefore, any solution of the Eliashberg equations on the line of McMillan’s work or related papers should be regarded cautiously if applied to A-15 compounds.

In 1967, Labbé et al. [8] published a paper on superconductivity in A-15 compounds. Using the one-dimensional electronic density of states of the Labbé-Friedel (LF) model [9], these authors solved the BCS-equation for a constant electron-phonon interaction $V$. Since their calculations were restricted to Fermi energies small compared to phonon energies, i.e. $\varepsilon_F \ll \omega_0$, no phonon cutoff was introduced and the electron-phonon interaction was taken to be strictly non-retarded.

In this work, the energy dependence of the electronic density of states as well as the retardation of the
phonon induced interaction is included when solving the Eliashberg equations. For a density of states of the LF-type (5a) or, more generally, for any density of states which on the scale of phonon energies is rapidly changing around the Fermi level, the combination of these two properties can lead to a considerable enhancement of $T_c$ if the Fermi energy $e_f$ is comparable to a typical phonon energy $\omega_0$. We shall discuss this result in more detail in Section 3, but here limit ourselves to a short explanation: The electron-phonon interaction is attractive for $\omega<\omega_0$, but repulsive for $\omega>\omega_0$. If $e_f<\omega_0$, the repulsive part of the interaction is strongly suppressed by the particular shape of the density of states.

Our paper follows similar lines as that by McMillan [1], the main difference being the consideration of the energy dependence of the electronic density of states. It is arranged as follows: In Section 2 we set up the Eliashberg equations and the models used for the electronic density of states. In Section 3 we present numerical solutions of the $T_c$-equation together with a discussion of the underlying physical picture. In Section 4 we derive an analytical solution which is fitted to the numerical results. The role of the Coulomb repulsion $\mu$ is briefly discussed in Section 5, while an experimental illustration of our theory can be found in Section 6.

2. $T_c$-Equation for A-15 Compounds

Our basic equations are the Eliashberg equations in the dirty limit [2]. For low temperatures such that $k_B T=1/\beta$ is small compared to typical phonon energies the equations for the superconducting gap $\Delta(e, k_0)$ and for the renormalization function $Z(e, k_0)$ are

$$\phi(e, k_0) = \int_0^\infty \frac{dk_0}{\pi} \int_{-\infty}^{\infty} d\epsilon' \frac{\phi(\epsilon', k_0')}{(Z(k_0')^2 - \epsilon'^2 - \phi'^2)}$$

$$k_0(1 - Z(e, k_0)) = \int_0^\infty \frac{dk_0}{\pi} \int_{-\infty}^{\infty} d\epsilon' \left[ \frac{Z(e', k_0') \phi'(k_0')}{(Z(k_0')^2 - \epsilon'^2 - \phi'^2)} \right] K_\perp(e', e; k_0, k_0').$$

(1a)

(1b)

Here, $\phi = \Delta \cdot Z$ (for $\phi'=\phi(\epsilon', k_0')$ etc) $k_0$ and $k_0'$ are frequency variables and $e$ and $\epsilon'$ are the single particle energies which in the dirty limit replace the momentum variables. The kernels $K_\perp$ in (1a, b) may be written as

$$K_\perp(e, e'; k_0, k_0') = N(\epsilon') V_\perp(e, \epsilon'; k_0, k_0').$$

(2)

where $N(\epsilon')$ denotes the electronic density of states and $V_{\perp}$ describes the interaction (electron-phonon and Coulomb) between the electrons averaged over surfaces of constant energies $e$, $\epsilon'$ in momentum space. Usually, for $e_f \gg \omega_0$, the dependence of $V_{\perp}$ on the single particle energies $e$, $\epsilon'$ is neglected and the density of states is taken to be a constant near the Fermi level. For the phonon part of the interaction one then gets the kernel

$$\lambda_\perp(k_0, k_0') = K_{\perp, \text{phon}}(0, 0; k_0, k_0')$$

$$K_{\perp, \text{phon}}(0, 0; k_0, k_0') = \int_0^\infty d\omega \omega^2 F(\omega)$$

$$\cdot \left[ \frac{1}{(k_0 + k_0' + \omega - i\delta)} \pm \frac{1}{(k_0 - k_0' + \omega - i\delta)} \right]$$

(3)

where $\lambda_\perp(0, 0)$ is the electron-phonon coupling constant of McMillan and $\omega^2 F(\omega)$ the Eliashberg function. In our work we shall take account of the energy dependence of the electronic density of states, but also neglect the dependence of $V_{\perp}$ on $e$, $\epsilon'$. The assumption that the interaction $V_{\perp}$ does not depend on the single particle energies $e$, $\epsilon'$ seems to be rather speculative for a nearly empty $d$-band. A definite answer to this problem can only be given on the basis of a microscopic calculation of the electron-phonon coupling in A-15 compounds. In an earlier paper [10] one of the authors (P.H.) performed such calculations for the case of interchain scattering. For this case it turned out that $V_{\perp}$ was independent of $e$, $\epsilon'$ and that $\lambda_\perp \sim N(0)$. For intrachain scattering a more general discussion of the electron-phonon coupling can be found in [11, 12], but to our knowledge no explicit calculation of $V_{\perp}$ has so far been performed.

For the kernel of (1a, b) we make the ansatz

$$K_{\perp, \text{phon}}(\epsilon'; k_0, k_0') = \left( \frac{N(\epsilon')}{N(0)} \right)^2 \lambda_\perp(k_0, k_0')$$

(4)

with the electronic density of states $N(\epsilon)$ given in the LF-model by

$$N_{\text{LF}}(\epsilon) = N(0) \frac{1}{\epsilon_f} (\epsilon_f + \epsilon)^k \theta(\epsilon + \epsilon_f)$$

(5a)

while for the model of Cody, Cohen and Halloran [13] (CCH-model) it reads

$$N_{\text{CCH}}(\epsilon) = N(0) \theta(\epsilon + \epsilon_f).$$

(5b)

Here, $\epsilon_f$ is the Fermi level counted from the lower edge of the $d$-band and used as zero of the energy scale. Although still approximative, the ansatz (4) for $K_{\perp, \text{phon}}$ has the essential property to combine phonon retardation with a fast variation of the electronic density of states near $e_f$. For the Coulomb contribution to $K_\perp$ we write

$$K_{\perp, \text{Coul}}(\epsilon') = -\mu N(\epsilon')/N(0).$$

(6)