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2D VAN HOVE SUPERCONDUCTORS WITH WEAK AND STRONG-COUPLINGS

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The critical temperature (T_c) and the isotope coefficient (α) of two-dimensional van Hove superconductors have been analyzed. The phonon induced superconductors with both weak and strong couplings are considered. For weak coupling, the variation of T_c and α as a function of average phonon frequency, ω_D, for three sets of pairing potential, V, shows that α decreases at nearly same rate with the increase of ω_D; but T_c increases with increasing ω_D but at different rates for different V. For strong coupling, the variation of T_c and α shows that smaller band width produces desirable results that are consistent with observation.

Keywords: 2D superconductor, Critical temperature, Isotope coefficient, Hopping integral, van Hove singularity, Electron-phonon coupling.

1. Introduction

The van Hove singularity (vHs), which originates from the two-dimensional structure, has an effect on critical temperature (T_c) and isotope exponent (α) of two-dimensional superconductors. The occurrence of a logarithmic divergence in the density of states (DOS) near the saddle points of the energy bands, confirmed by the photoemission spectra, has stimulated the use of the model with such an energy dependence. The usual BCS (Bardeen, Cooper and Schrieffer) theory cannot explain the high values of T_c as well as small values of the isotope coefficient (α) of the copper oxide superconductors. For this reason, a simple modification of this theory is needed to account for these properties of the cuprate superconductors. The physical basis for this modification is found in the density of state peaks suggested by band-structure calculations. If the Fermi energy lies near a singularity in the density of states (DOS) then the usual BCS type expressions for T_c and α are modified. This possibility was stressed by Labbe and Bok [1] and by Friedel [2] for the high T_c oxides. In this paper we utilize BCS and Eliashberg [3] approaches to discuss superconductivity in high T_c 2D superconductors.

2. Formalism

The superconducting gap equation is

$$\frac{1}{V} = \int_{-\omega D}^{\omega D} d\varepsilon\, N(\varepsilon) \frac{\tanh\left(\varepsilon / 2kT_c\right)}{2\varepsilon} \qquad (1)$$

The density of state (DOS) is given by, $N(\varepsilon) = \frac{a_1}{t} \ln\left|\frac{\varepsilon}{a_2 t}\right|$

for a two-dimensional square lattice, where a_1 and a_2 are constants. V is the pairing potential, ε is the energy, ω_D is the average phonon frequency, k is the Boltzmann constant and t is the nearest neighbour hopping integral.

After some algebraic manipulation [4, 5] the expressions for T_c and isotope coefficient, α, in the weak coupling case turn out to be

$$k\,T_c = \frac{2e^{\gamma}}{\pi} a_2 t \exp\left[-\left(\frac{\ln^2\left(4e^{\gamma}\pi^{-1}\right)+}{\ln^2 G - 2Q - 2}\right)^{1/2}\right] \qquad (2)$$

with $\gamma = 0.5772$, $Q = t/Va_1$ and

$$\alpha = 0.5 \frac{\ln G}{\left(\ln^2\left(4e^{\gamma}\pi^{-1}\right) + \ln^2 G - 2Q - 2\right)^{1/2}} \qquad (3)$$

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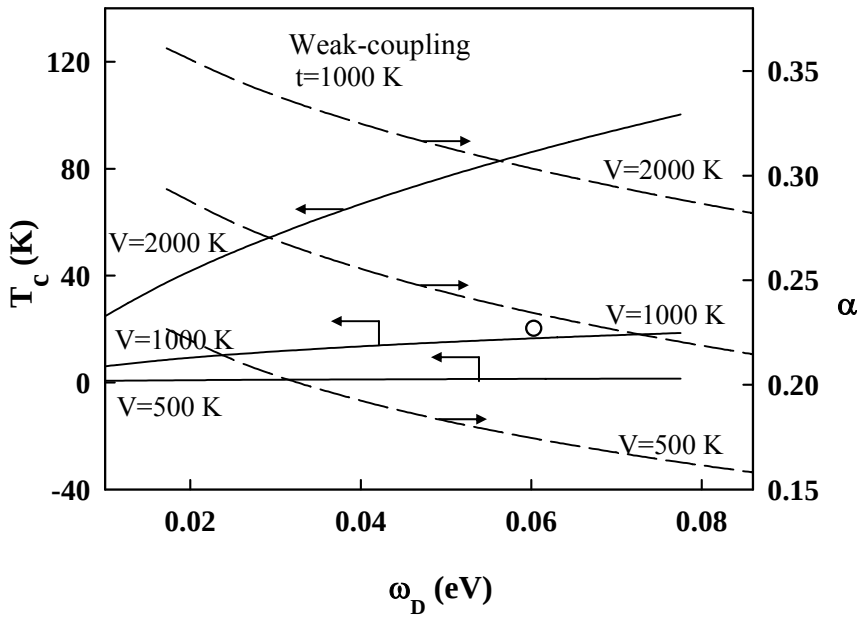

Figure 1. T_c and α as a function of ω_D for different pairing potentials (V) . The point (o) refers to calculation [7] .

where $G = a_2 t/\omega_D$

We would now consider the strong-coupling case. Here T_c can be obtained within the Eliashberg formalism [6] from

$$(kT_C)^{-1} = \frac{1}{\phi(i\omega_n)} \sum_l \frac{\lambda \nu^2}{(l-n)^2 + \nu^2} \int_{-W}^{W} d\varepsilon \quad N(\varepsilon) \frac{\phi(i\omega_l)}{[\omega_l Z(i\omega_l)]^2 + \varepsilon^2} \qquad (4)$$

where, $\phi(i\omega_l)$ is the superconducting order parameter and $Z(i\omega_l)$ represents the wave-function renormalization factor. λ is the electron-phonon coupling function and 2W is the band width and $\nu = \omega_D/(2kT_c)$.

The frequency dependence of the wave-function renormalization factor and the order parameter is assumed. After some manipulation [4, 5] one finally obtains the expression for T_c as

$$kT_c = 2e^{\gamma}\pi^{-1} G \exp\left[-\left(\frac{\ln^2\left(4e^{\gamma}\pi^{-1}\right)+}{\ln^2 G + 2\lambda_{eff}^{-1}}\right)^{1/2}\right] \qquad (5)$$

where

$$\lambda_{eff}^{-1} = -1 - P\lambda^{-1} - 2\pi^{-1}\left[\ln(RG)^{-1} i_1(R) + i_2(R)\right] \qquad (6)$$

with $P = Zt/a_1$; $R = W/Z\omega_D$

The functions i_1 and i_2 represent two fast convergent series [4]. The expression for isotope coefficient is

$$\alpha = \frac{i_1(R) + \ln G \tan^{-1}(R)}{\pi\left[\ln^2\left(4e^{\gamma}\pi^{-1}\right) + \ln^2 G + 2\lambda_{eff}^{-1}\right]^{1/2}} \qquad (7)$$

3. Results and Discussions

For a 2D square lattice with half-filled band and chemical potential $\mu = 0$, $a_1 = -0.04687$ eV and $a_2 = 21.17796$ eV^{-1} [4]. The coupling function λ is tried for $0.5t < \lambda \leq 2t$.

For the weak coupling case, we numerically calculated transition temperature, T_c, and isotope coefficient α. Fig. 1 shows the results of T_c and α as a function of average phonon frequency ω_D. Three sets of curves are drawn for three values of strength of pairing potential V. We observe that the

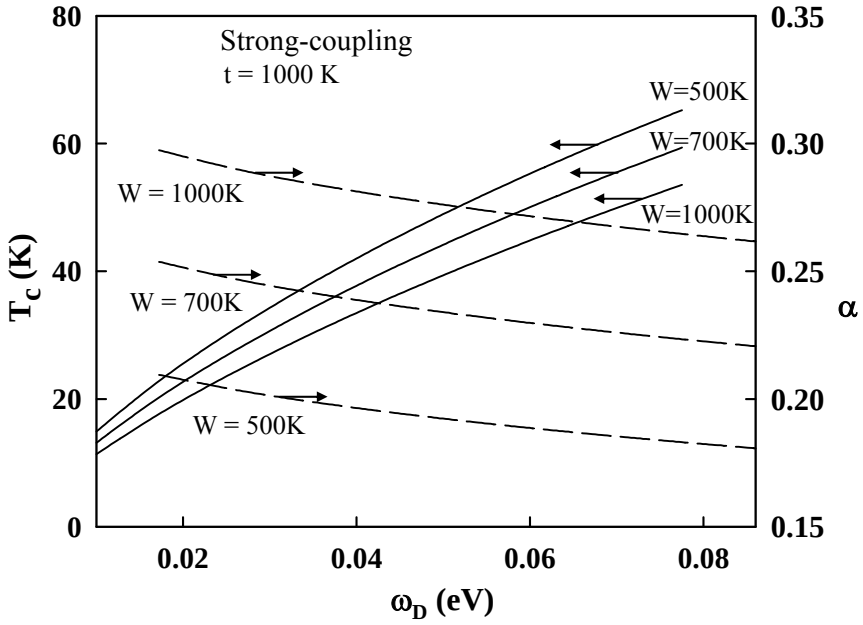

Figure 2. T_c and α as a function of ω_D for different band widths (W).

value of α decreases with the increase of ω_D. Further α is smaller for smaller pairing strength. T_c increases with increase of ω_D. The curve for V = 500 K is nearly flat but the rate of increase of T_c is much faster when V = 2000 K.

For the strong-coupling case we also numerically calculated the superconducting transition temperature (T_c) and the isotope coefficient (α) based on Eqs. (5) and (7), respectively.

From Fig. 2 we observe that, within the Eliashberg formalism, the isotope coefficient gradually decreases with the increasing value of the average phonon frequency ω_D. Three sets of curves are given for three different band widths. In each of the cases the hopping integral is taken as t=1000 K. We find that, for smaller band width (i.e. for smaller R) the value of isotope coefficient gets smaller. On the other hand, T_c increases as a function of ω_D. Larger T_c results when the band width becomes smaller.

We find that for t =1000 K; V = 1000 K, α turns out to be 0.235. Das *et al*. [7] for the same set of values found α to be 0.227. They studied T_c and α for s-wave pairing symmetry within van Hove singularity scenario. The value of minimum α (when the Fermi energy lies at vHs) is found to be 0.33. For s-wave pairing and a square lattice they found that the value of α_{min} could not be reduced below 0.2 even for other reasonable choices of parameters. We should note that in the absence of van Hove singularity in DOS, the isotope coefficient is exactly 0.5. In HTS system the value of α_{min} is lower than that obtained theoretically for s-wave pairing with a square lattice. Das *et al*. [7] tried the orthorhombic distortion when the hopping integrals along x and y axes are different. With the introduction of orthorhombic distortion the singularity in the DOS splits into two and the separation between them is proportional to orthorhombic distortion. The introduction of this type of distortion enhances the value of α_{min} and then pushes the value further away from the observed value. In fact if one considers Coulomb repulsion between the electrons, both the values of T_c and α are expected to be reduced further owing to the Coulomb interaction.

Finally we note that in the strong-coupling case, smaller band width (W = 500 K) would produce the desirable result for both α and T_c (i.e. smaller α and larger T_c) for high T_c superconductors.

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