CHAPTER 4

Calculation of the critical temperature, T_c

In this chapter the critical temperature is calculated. Using the BCS theory, the attractive interaction between electrons comes from the electron-phonon interaction. It is described by a constant attractive matrix element $(-V,\ V > 0)$ in the Hamiltonian when the electrons are in a range of energy $E_F \pm \hbar w_o$ (when E_F is the Fermi level and $\hbar w_o$ a typical phonon energy). The energy gap Δ at temperature T is given[10,16] by

$$\frac{2}{V} = \int_{\mu-\hbar\omega_o}^{\mu+\hbar\omega_o} F(E)n(E)dE \qquad (4.1)$$

where μ is the chemical potential in the superconducting state which can be sometimes different from E_F. μ is determined by the number of electrons in the band, and

$$F(E) = \frac{\tanh\left(\left[(E-\mu)^2+\Delta^2\right]^{1/2}/2k_BT\right)}{\left[(E-\mu)^2+\Delta^2\right]^{1/2}} \qquad (4.2)$$

k_B is the Boltzmann constant, n(E) is the density of state of the electrons in the band, T_c is the temperature at which $\Delta = 0$.

In the tetragonal phase of La_2CuO_4, the band containing Fermi level, $E_{++}^{ap}(\vec{k})$, is a half-filled band, therefore, $\mu = E_s^+$, the position of the logarithmic singularity. At T_c, $\Delta = 0$, and T_c is thus given by

$$\frac{2}{V} = \int_{E_s^+ - \hbar\omega_0}^{E_s^+ + \hbar\omega_0} \frac{\tanh\left(\frac{E-E_s^+}{2k_B T_c}\right)}{E - E_s^+} \frac{N}{2\pi^2 D} \ln(D|E - E_s^+|^{-1}) dE \qquad (4.3)$$

Let $\quad v = VN, \quad x = \dfrac{E - E_s^+}{D}, \quad$ and $\quad a = \dfrac{2k_B T_c}{D} \qquad (4.4)$

The equation, then, becomes

$$\frac{2\pi^2 D}{v} = -\int_0^{x_0 = \frac{\hbar\omega_0}{D}} \frac{\tanh\left(\frac{x}{a}\right)\ln(x)}{x} dx \qquad (4.5)$$

The integration on the right-hand side of eq. (4.5) was found [17] to be

$$-\int_0^{x_0} \frac{\tanh\left(\frac{x}{a}\right)\ln(x)}{x} dx = \frac{1}{2}(\ln a)^2 - 0.819(\ln a) - \frac{1}{2}(\ln x_0)^2 + 1 \qquad (4.6)$$

That is

$$\frac{2\pi^2 D}{v} = \frac{1}{2}(\ln a)^2 - 0.819(\ln a) - \frac{1}{2}(\ln x_0)^2 + 1 \qquad (4.7)$$

Eq. (4.7) is quadratic in ln a, therefore, we can solve the equation by using the quadratic formula. Applying the formula to eq. (4.7), We get

$$\ln a \cong 0.819 \pm \frac{\left[(2)^2(0.819)^2 - 8\left\{1 - \frac{1}{2}(\ln x_0)^2 - \frac{2\pi^2 D}{V}\right\}\right]^{1/2}}{2}$$

$$\ln a \cong 0.819 \pm \frac{\left[8\left\{\frac{2\pi^2 D}{V} + \frac{1}{2}(\ln x_0)^2 - 0.66\right\}\right]^{\frac{1}{2}}}{2}$$

$$\ln a \cong 0.819 \pm \left[2\left\{\frac{2\pi^2 D}{V} + \frac{1}{2}(\ln x_0)^2 - 0.66\right\}\right]^{1/2} \qquad (4.8)$$

Let $$C = \frac{2\pi^2 D}{V} + \frac{1}{2}(\ln x_o)^2 - 0.66 \qquad (4.9)$$

Eq. (4.8) becomes

$$\ln a \cong 0.819 \pm \sqrt{2C}$$

$$\ln a \cong \ln(2.27) \pm \sqrt{2C}$$

i.e. $$a = 2.27\, e^{\pm\sqrt{2C}} \qquad (4.10)$$

From eq. (4.4) and eq. (4.10) , we get

$$\frac{2k_B T_c}{D} \cong 2.27\, e^{\pm\sqrt{2C}}$$

$$k_B T_C = 1.14\, D e^{\pm\sqrt{2C}} \qquad (4.11)$$

Since a is much smaller than 1 (typically 10^{-2} to 10^{-1})[17] , the accepted solution is thus

$$k_B T_c = 1.14\, D e^{-\sqrt{2C}} \qquad (4.12)$$

Eq. (4.12) gives T_c, when the phonon frequency is held fixed,as a function of D. Typical value of D is about an order of magnitude largerthan $\hbar\omega_o$[17], thus we can consider the relation between T_c and D by replacing the constant C with $\frac{2\pi^2 D}{V}$. When this is done the equation becomes

$$k_B T_c \cong 1.14\, D\, e^{-\sqrt{4\pi^2 D/V}} \tag{4.13}$$

and shows the maximum T_c at $D = \frac{V}{\pi^2}$ (Fig.8).

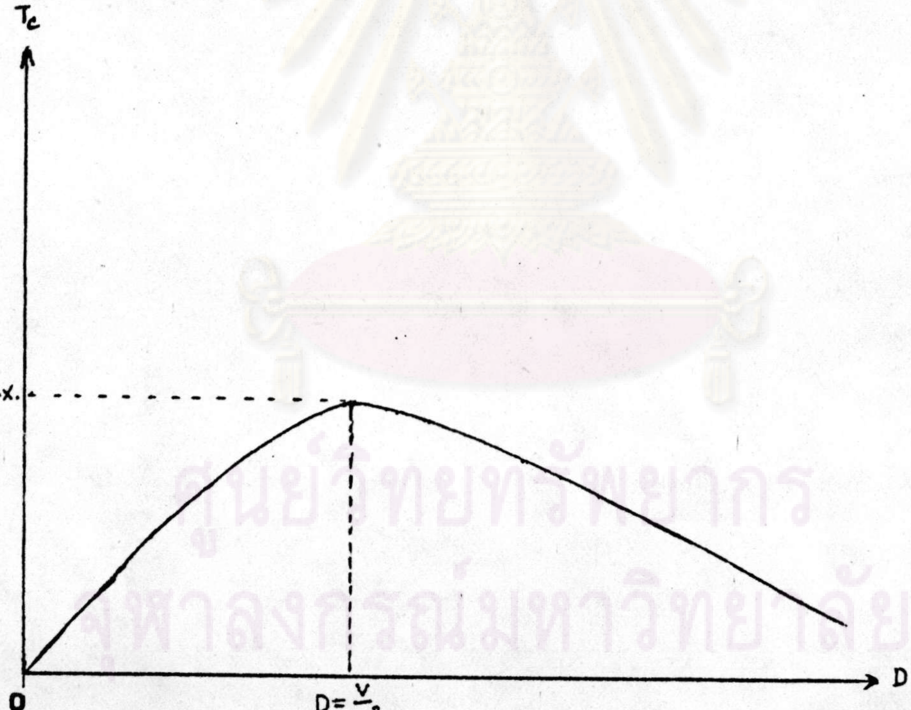

Fig 8 Relation between T_c and D

In the original BCS model, with a constant density of states N_o near the Fermi level, the critical temperature was found to be

$$k_B T_c \simeq 1.14 \hbar\omega_o \exp\left[-\frac{1}{N_o V}\right] \qquad (4.14)$$

keeping in mind that, at any value of D, the density of states in the neighbourhood of the Fermi level is proportional to N (eq.3.31), the total number of unit alls in a CuO_2 plane, and v = VN (eq. 4.4), we are able to compare eq.(4.13) with eq. (4.14). We see that in the BCS model (eq.4.14) T_c is proportional to exp ($-\frac{1}{\lambda}$), where $\lambda = N_oV$, while the logrithmic singularity yields a factor $\frac{1}{\sqrt{\lambda}}$ (4.13), where $\lambda = \frac{NV}{4\pi^2 D}$, instead of $\frac{1}{\lambda}$ in the exponential, giving an important enhancement of the critical temperature. This explains why La_2CuO_4, if it is in the tetragonal phase, can be high - T_c superconductor.

The isotopic effect can also be explained. In the usual BCS theory the energy - range limitation to the attrative interaction between two pairing electrons arises from the narrowness of the phonon spectrum. Since, in our case, the pairing electrons are those in the neighbourhood of the logarithmic singularity the width of which is specified by the parameter D (eq.(3.31)) ,therefore, the isotopic effect will not exist if the phonon energy is not too small compared to the width D of the logarithmic singularity.

Our previous calculation is based on the assumption that $\mu = E_s^+$ (half-filled band). But in that case the crystal becomes unstable and undergoes a tetragonal-to-orthorhombic structural transition. The tetragonal phase is stable only when μ is a little displaced from E_s^+ by substitution. To consider the T_c in this case, we denote the integral on the right-hand side of eq. (4.5) by $I(x_o,a)$: i.e.

$$I(x_o,a) = -\int_0^{x_o} \frac{\tanh\left(\frac{x}{a}\right)\ln(x)}{x}\,dx \tag{4.13}$$

Let us write $u = (\mu - E_s^+)/D$, assume that u is much smaller than 1. The integral $I(x_o,a)$ is now replaced by $I(x_o,a,u)$. Using Taylor's series expansion, we get

$$I(x_o,a,u) = I(x_o,a) + \left(\frac{u^2}{2}\right)I''(x_o,a,0) + O(u^4) \tag{4.14}$$

$$I''(x_o,a,0) \simeq -\frac{(1-\ln x_o)}{x_o^2} \tag{4.15}$$

In general x_o is small thus $\ln x_o < 1$. Therefore, the coefficient of u^2 is negative. Due to the negative coefficient of u^2, T_c is maximum when u = o, we also see that the correction is small