CHAPTER 5

Discussion and conclusion

In this model, we calculate the two dimensional energy band structure of CuO plane, in the tetragonal phase of La_2CuO_4, by using the tight-binding method. Five Bloch sums are chosen as our bases, they are those of the atomic orbitals s, $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ of copper atoms, and p_x and p_y of oxygen atoms. Using the transformation by Heine[12], the 5x5 interaction matrix can be reduced to a 1x1 matrix and a 4x4 matrix, We discard the 1x1 matrix and solve the secular equation of the 4x4 matrix in terms of some parameters. The four energy bands are found to be

$$E_{\pm\pm} = \left(\frac{E_d+E_p}{2}\right) \pm \left[\left(\frac{E_d-E_p}{2}\right)^2 + \chi_\pm\right]^{1/2} \tag{2.26}$$

$$\chi_\pm = \frac{(\gamma^2+\beta^2+2\alpha_R^2)\left\{(1-e^{ik_xa})(1-e^{-ik_xa})+(1-e^{ik_ya})(1-e^{-ik_ya})\right\}}{2}$$

$$\pm \frac{\left[(\gamma^2+\beta^2+\alpha_R^2)^2\left\{(1-e^{ik_xa})(1-e^{-ik_xa})+(1-e^{ik_ya})(1-e^{-ik_ya})\right\}^2 - 16\gamma^2(\beta^2+\alpha_R^2)(1-e^{ik_xa})(1-e^{-ik_xa})(1-e^{ik_ya})(1-e^{-ik_ya})\right]^{1/2}}{2} \tag{2.24}$$

To make further calculation easier, some approximations have been made by considering only the dominating term of γ. The approximated energy bands are

$$E^{ap}_{\pm\pm}(\vec{k}) = \left(\frac{E_d+E_p}{2}\right) \pm \left[\left(\frac{E_d-E_p}{2}\right)^2 + \chi^{ap}_{\pm}\right]^{1/2} \qquad (2.28)$$

$$\chi^{ap}_{\pm} = \begin{cases} 4\gamma^2\left[\sin^2\left(\frac{k_x a}{2}\right) + \sin^2\left(\frac{k_y a}{2}\right)\right] \\ 0 \end{cases} \qquad (2.29)$$

It can easily be seen that the approximated energy bands $E^{ap}_{\pm-}(\vec{k})$ show no dispersion and, therefore, they will appear as δ-functions in the density of states. This is due to the crudeness of our approximations. If the neglected terms are included, the dispersion should appear and the δ-functions will be replaced by finite peaks.

Next we calculate the density of states of the approximated energy bands $E^{ap}_{\pm+}(\vec{k})$. Instead of calculating the density of states directly, we calculate the reduced density of states, $g(\varepsilon)$, of the reduced energy, ε. The reduced energy is defined by the equation

$$\varepsilon_{\vec{k}} = -\cos(k_x a) - \cos(k_y a) \qquad (3.3)$$

and the reduced density of states per unit cell is found to be

$$g(\varepsilon) = \frac{1}{\pi^2} K\left(\sqrt{1-\left(\frac{\varepsilon}{2}\right)^2}\right) \qquad (3.14)$$

The relation between the reduced density of stated and the density of states is

$$g(\xi) = \frac{\gamma^2}{\left| E - \left(\frac{E_d + E_p}{2}\right)\right|} \rho(E) \qquad (3.16)$$

Therefore, the density of states per unit cell, $\rho(E)$, is

$$\rho(E) = \frac{\left| E - \left(\frac{E_d + E_p}{2}\right)\right|}{\gamma^2} \cdot \frac{1}{\pi^2} K\left(\sqrt{1 - \left(\frac{\epsilon}{2}\right)^2}\right) \qquad (3.18)$$

Replacing the complete elliptic integral by a series representation we can easily see that the density of states shows logarithmic singularities at the energies

$$E_s^{\pm} = \left(\frac{E_d + E_p}{2}\right) \pm \left[\left(\frac{E_d - E_p}{2}\right)^2 + 4\gamma^2\right]^{1/2} \qquad (3.22)$$

of the saddle points $|k_x| = \frac{\pi}{a}$ with $k_y = 0$, and $k_x = 0$ with $|k_y| = \frac{\pi}{a}$, in the reciprocal space. These singularities exhibit the double degeneracy. This enables us to explain the structural phase transition and the existence of superconductivity. In the tetragonal phase of La_2CuO_4, the Fermi level coincides with the logarithmic singularity at the energy E_s^+ of the band $E_{++}^{pp}(\vec{k})$ Due to the double degeneracy of the energy, Jahn-Teller effect occurs and, therefore, lead to the instability of the tetragonal phase. Substituting in small amount of Ba to La, or changing of density of oxygen vacancies, or both, is to shift the Fermi energy a little. As a result the Jahn - Teller effect disappears and the instability of the orthorhombic phase follows, the stable phase is then the tetragonal one. Though the causes of the

instability in the tetragonal phase of La_2CuO_4 may be different, the substitution plays the same role, that is to suppress the instability, as has been pointed out by Mattheiss[18] and Yu[19]. As the Fermi energy E_F in the substituted compound remains close to the singularity, even though it does not exactly coincide with the singularity, the density of states near E_F is large. The tetragonal phase is thus superconducting.

According to the BCS theory, the density of states involved in the calculation of the critical temperature is that in the neighbourhood of the Fermi level. Therefore, we find an approximation for the density of states in the nighbourhood of the Fermi level by considering only the first term of the series representation and taking the limit as E tends to E_s^+. We get, for the whole plane with N unit cells, the density of states as

$$N\rho(E) \cong \frac{N}{2\pi^2 D} \ln(D|E_{++}^{sp}(\vec{k}) - E_s^+|^{-1}) \qquad (3.31)$$

Using eq. (3.31), the critical temperature has been calculated. It is found to be

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

Considering only the dominating term, the equation becomes

$$k_B T_c \cong 1.14\, D\, e^{-\sqrt{4\pi^2 D/v}} \qquad (4.13)$$

The result gives us an explanation for the superconducting at higher temperature. From eq.(4.13) we see that the critical temperature is proportional to $e^{-1/\lambda}$, where $\lambda = \frac{VN}{4\pi^2 D}$, instead of proportional to $e^{-1/\lambda}$ (4.14), where $\lambda = N_0 V$, of the BCS theory. This gives an important enhancement of the critical temperature. The explanation is found to be the same as that of Hirsch and Scalapino[20], in studying an attractive Hubbard model.

An explanation about the isotopic effect is also found. That is the isotopic effect will not exist if the phonon energy $\hbar\omega_0$ is not too small compared to the width D of the logarithmic singularity.

Actually, the tetragonal phase of La_2CuO_4 is unstable and the stability occurs only when μ is a little displaced from E_s by substitution. In that case we find that T_c decreases due to the negative coefficient of the second order term, but the correction is small compared to the leading term.