Chapter 4
Discussion and Conclusions

In this work, we have studied the gap-to- T_c ratio, R, in the Van Hove singularity density of states based on the BCS framework. The effect of the pairing states both the isotropic s-wave and the anisotropic d-wave which have the influence on the symmetry of the energy gap is examined. The existence of the mixed phase of the (s+d)-wave pairing state in the Van Hove singularity density of states is also investigated.

In our work, we using the weak coupling BCS phonon-mediated pairing theory in the cuprates. We have made the assumption that the two-dimensional energy band dispersion in the cuprates leads to the energy dependent density of states. As a consequence this two dimensional lattice will have a logarithmic singularities in the energy surface and it is well known as the Van Hove singularities (Van Hove, 1953). The two-dimensional tight-binding band, Eq.(3.5),

$$E(\vec{k}) = -2t(\cos k_x + \cos k_y) + 4tr_2 \cos k_x \cos k_y \tag{4.1}$$

consists of two parts; (i) the nearest-neighbor hopping energy $t(tr_1)$ along the a(b) direction, which the parameter r_1 represents the orthorhombic distortion effect, and (ii) the next-nearest-neighbor hopping energy tr_2. In general, the parameter r_2 is less than r_1. The approximate expression for the density of states, Eq.(3.10),

$$N(E) = N_0 \ln \left| \frac{16t\sqrt{1-r_2^2}}{E - E_s} \right| \tag{4.2}$$

has a logarithmic form with the singularity at the saddle point, Eq.(3.6). The success of the Van Hove scenario lies in the fact that the maximum of the critical temperature, T_c, corresponding to the optimum doping concentration, i.e., the Fermi level coincides with the singularity. The enhancement of the transition temperature of high- T_c superconductity in the cuprates was initially proposed by Labbe and Bok (Labbe and Bok, 1987). The superconducting gap ratio within the Van Hove scenario using the BCS phonon-mediated mechanism was performed by Getino, Llano, and Rubio (Getino, Llano, and Rubio, 1993) and Ratanaburi, Udomsamuthirun, and Yoksan (Ratanaburi, Udomsamuthirun, and Yoksan, 1996).

We derive an expression for the superconducting gap-to- T_c ratio R_s in the s-wave pairing state. The BCS equations for the zero-temperature superconducting gap and the transition temperature are combined by the elimination of the constant pairing interaction term. The analytic expression for R_s, Eq.(3.32),

$$R_s = \frac{4E_F}{T_c}\exp -\sqrt{\ln^2\frac{E_F}{2T_c} - 2I_1 - \frac{\pi^2}{6} + \frac{1}{2}\ln^2\frac{\omega_D}{2T_c} + 2\ln\frac{E_F}{2T_c}[F - \ln\frac{\omega_D}{2T_c}]} \quad (4.3)$$

is obtained under the condition $\omega_D \gg T_c$. (Krunavakarn et al., 1998). We find that the superconducting gap-to- T_c, R_s in an isotropic s-wave pairing state decreases with the increase of ω_D/T_c and tends to reach the BCS limit of 3.53 for a very high value of ω_D/T_c. The maximum value of the gap ratio is 4.0 which is achieved only for unrealistically low values of ω_D/T_c. This result indicates that the BCS phonon-mediated pairing theory in an isotropic s-wave state with the Van Hove singularity density of states cannot explain the high values of the gap ratio.

We have investigated the variation of the gap-to- T_c ratio with the shift of the Van Hove singularity from the Fermi energy. The approximate expression for R_s, Eq.(3.36),

$$R_s = \frac{4E_F}{T_c}\exp -\sqrt{\sinh^{-1}\frac{2\delta}{R_0 T_c} + \ln^2\frac{E_F}{\omega_D} - \frac{\pi^2}{6} + A} \quad (4.4)$$

is obtained by the iteration procedure to find the approximate solution. We find that the maximum R_s occurs when the Fermi level shift parameter is zero, in the other words the VHS coincides with the Fermi energy and R_s decreases as the Fermi level shift is displaced from the Fermi energy.

We know that the isotropic s-wave pairing state cannot explain the high values of the gap ratio. The pairing state in a d-wave symmetry has been widely accepted. The behavior of the d-wave state is the node at $k_x = \pm k_y$ in the momentum space of the lattice and it has the highest amplitude along the direction $(k_x, k_y) = (1,0),(0,1)$. In the case of the d-wave pairing, both the pairing interaction and the order parameter, Eqs.(3.46) and (3.47), are assumed to depend on the angular angles in two dimension. When we combine the d-wave pairing and the Van Hove singularity density of state models using the weak coupling BCS phonon-mediated pairing theory to evaluates the d-wave gap-to- T_c ratio R_d, the superconducting gap-to- T_c ratio R_d, Eq.(3.53),

$$R_d = \frac{8E_F}{\sqrt{e}T_c} \exp - \sqrt{\frac{11-\pi^2}{4} - \ln^2\frac{4e^\gamma}{\pi} + \ln^2\frac{2e^\gamma E_F}{\pi T_c}} \qquad (4.5)$$

is found to be larger than the s-wave case and it tends to reach the highest value of 5 for a very low value of ω_D/T_c. We have also studied the dependence of the d-wave gap ratio on the Fermi level shift, the result is that the gap ratio R_d, Eq.(3.58),

$$R_d = \frac{8E_F}{\sqrt{e}T_c} \exp - \sqrt{\frac{3-\pi^2}{4} + \ln^2\frac{E_F}{\omega_D} + 2\left(\frac{2\delta}{R_1 T_c}\right)^2 + A} \qquad (4.6)$$

has a maximum value at the Fermi energy and R_d as well as R_s decrease as the Fermi level shift increases as well as the R_s.

Although the symmetry of pairing state has been widely accepted that the pairing state of the cuprates has a dominant d-wave symmetry, an admixture of s-wave component to the order parameter is still a plausible one. We have studied the existence of a superconducting state of the mixed s- and d-wave supercontor when and the Van Hove singularity density of states has been taken into account. The pairing interaction $V(\vec{k},\vec{k'})$ in the parametric form, Eq.(3.84),

$$V(\vec{k},\vec{k'}) = -V_s 1 + \lambda[\cos 2\phi + \cos 2\phi'] - V_d \cos 2\phi \cos 2\phi' \tag{4.7}$$

contains both the anisotropic s-wave channel, which corresponding to the orthorhombic phase in the cuprates, and the d-wave channel. In the tetragonal phase, the pairing interaction $V(\vec{k},\vec{k'})$ is reduced to the mixing between the pure s-wave and d-wave channels, where the interaction strength of both pure phases have assumed the same magnitude. By using the BCS equation and seperating the equation along the pairing channel, a pair of coupled equations, Eqs.(3.88)

$$\Delta_s = \frac{g_s}{2\pi}\int_0^{2\pi}[1+\lambda\cos 2\phi][\Delta_s + \Delta_d \cos 2\phi]F[E_F,\omega_D,\Delta_s,\Delta_d,\phi] \tag{4.8}$$

and (3.89),

$$\Delta_d = \frac{g_d}{2\pi}\int_0^{2\pi}\cos 2\phi[\Delta_s + \Delta_d \cos 2\phi]F[E_F,\omega_D,\Delta_s,\Delta_d,\phi] \tag{4.9}$$

are obtained. We have shown that our model give the correct form in the case of the pure wave when taking the condition for the pure phase into Eqs.(3.88) and (3.89), i.e., Eq.(3.88) with $\Delta_d = 0$ is reduced to the pure s-wave gap equation, Eq.(3.92), and Eq.(3.89) with $\Delta_s = 0$ is reduced to the pure d-wave gap equation, Eq.(3.95). The following result is that the s-wave gap parameter Δ_s is independent of the orthorhombic distortion parameter.

The mixed phase equation is given by Eq.(3.98), which is obtained by the combination Eqs.(3.88) and (3.89). The solution of Eq.(3.98),

$$(\frac{1}{g_s}-\frac{1}{g_d})2\alpha = \int_0^{\pi}\frac{dx}{\pi}[\alpha+\lambda+2(1+\alpha(\lambda-\alpha))\cos x+(\lambda-\alpha)\cos 2x]F[E_F,\omega_D,\alpha,x] \tag{4.10}$$

as the relative pairing interaction strength g_s/g_d increases, will be the pure d-wave ($\alpha = 0, g_s/g_d = 0$), the mixed (s+d)-wave, and the pure s-wave phases ($\alpha \to \infty, g_s/g_d \to \infty$), respectively, here α is the ratio between the s-wave gap and the d-wave gap. We find that the pure d-wave phase exists at $0 < g_s/g_d < g_{s,min}/g_d$, where $g_{s,min}/g_d$ is given by Eq.(3.108),

$$g_{s,min} = [\frac{2}{g_d} + \frac{3}{8} + \frac{1}{2}\sqrt{\frac{4}{g_d} - \frac{\pi^2 - 3}{4} + \ln^2\frac{E_F}{\omega_D}}]^{-1} \quad (4.11)$$

while the pure s-wave phase exists at $g_s/g_d > g_{s,max}/g_d$, where $g_{s,max}$ is given by Eq.(3.111).

$$g_{s,max} = g_d/2 \quad (4.12)$$

Thus the mixed (s+d) state appears between the pure d-wave and the s-wave states.

In conclusion, we have obtained equations for

1. The s and d superconducting gap-to- T_c ratio of a Van Hove superconductor.
2. The gap ratios for both s-wave and d-wave decrease as ω_D/T_c increases at fixed E_F.
3. Under certain conditions, the mixed (s+d) phase exist.