Chapter 3
The Van Hove Superconductors

3.1 Introduction

L.Van Hove (Van Hove, 1953) stressed the crucial role played by topology in the band structure of either electrons or phonons by demonstrating that any nonanalytic behavior in the density of states is caused by a change in the band topology. The singularity now known as Van Hove singularities (VHS).

In materials, the role of a VHS is enhanced, because the density of states N(E) can actually diverge at a VHS. In one dimensional materials, the divergence is power law, N(E) $\propto \Delta E^{-1/2}$. In two dimensional materials, the density of states diverges logarithmically $N(E) \propto \ln(B/\Delta E)$, where $\Delta E = E - E_{VHS}$ is the distance in energy from the VHS and B the bandwidth. The topology of this VHS is the saddle point in the energy surface. The VHS of a two-dimensional metal is the simplest model with a peak in the density of states and can analyze the role of the structure of the density of states in the physics of Fermi liquids.

The review articles are shown in sections (3.2), (3.3), (3.6), and (3.9). The thesis work is given in sections (3.4), (3.5), (3.7), (3.8), and (3.10).

3.2 The Van Hove Scenario

It is well known that the Van Hove scenario can explain many physical properties of high- T_c superconductors such as the high value of T_c, anomalous isotope effect, gap anisotropy, etc. The high- T_c was explained by Labbe' and Bok (Labbe' and Bok, 1987). They proposed a two-dimensional band structure calculation for alkaline-earth-substituted La_2CuO_4 in the tetragonal phase.

Within the framework of the BCS phonon-mediated pairing, Tsuei et al. (Tsuei et al., 1990) showed that a logarithmic (2D) Van Hove singularity in the density of states can provide a basis for understanding the anomalous isotope effects in the $YBa_2Cu_3O_7$ and the BiSrCaCuO systems. The thermodynamic properties such as the specific-heat jump at the transition temperature (T_c), $\Delta C/T_c$, and the zero-temperature critical field $H_c(0)$, of oxygen-deficient $YBa_2Cu_3O_{7-y}$ were analyzed, by Tsuei et al. (Tsuei et al., 1992), to show that the density of states at the Fermi level is peaked at y=0 and the Fermi level lying close to a two-dimensional Van Hove singularity. Pattnaik et al. (Pattnaik et al. 1992) calculated the quasiparticle lifetime broadening $1/\tau$, both for idealized and realistic models of the band structure. The result shows a large lifetime broadening from electron-electron scattering, with the characteristic linear dependence on energy seen in high-temperature superconductors, provided that the Fermi level lies near the Van Hove singularity in the quasi-two-dimensional band structure. Getino et al. (Getino et al., 1993) derived an exact transition temperature (T_c) formula within the Van Hove scenario of BCS phonon-mediated pairing theory consisting of a logarithmic singularity in the density of states at the Fermi energy. Sarkar and Das (Sarkar and Das, 1994) derived an exact expression for the isotope-shift exponent and the pressure coefficient of the transition temperature from the BCS gap equation for a density of states with a Van Hove singularity. The effect of orthorhombic distortion, second-nearest-neighbor hopping, and Coulomb repulsion on the superconducting transition temperature and the isotope-shift exponent were studied, by Sarkar, Basu, and Das (Sarkar, Basu, and Das, 1995), within the Van Hove singularity scenario. Houssa and Ausloos (Houssa and Ausloos, 1996) calculated the electronic contribution κ_e to the thermal conductivity of a two-dimensional superconductor with the saddle points at the Fermi level in the band structure, corresponding to logarithmic Van Hove singularities in the 2D density of states. Wei et al. (Wei et al., 1998) considered the quasiparticle tunneling measurements of the high-temperature superconductors $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ (n=1,2,3) in the context of the $d_{x^2-y^2}$ symmetry of the superconducting order parameter and a two-dimensional Van Hove singularity related to saddle points in the electronic band structure.

3.3 Van Hove Singularity in the Density of States

To investigate the nature of a saddle point in the energy surface which provides the divergence of the electron density of states, we begin with the expression of the density of states

$$N(E) = \frac{1}{(2\pi)^3}\int d^3\vec{k}\delta(E - E(\vec{k})), \tag{3.1}$$

Alternatively, the number of states in the energy interval between E and E+dE is

$$N(E)dE = \int \frac{dS}{(2\pi)^3}\delta\vec{k} \tag{3.2}$$

where S be the energy surface and perpendicular to $\delta\vec{k}$. The infinitesimal change of $E(\vec{k})$ with respect to $\delta\vec{k}$ is given by

$$dE = \nabla_{\vec{k}}E\delta\vec{k} \tag{3.3}$$

here $\nabla_{\vec{k}}$ means the gradient in $\vec{k}-$ space. Thus we obtain the electron density of states in an alternative form:

$$N(E) = \int \frac{dS}{(2\pi)^3}\frac{1}{|\nabla_{\vec{k}}E|} \tag{3.4}$$

When $E(\vec{k})$ approches zero, the density of states diverges. This is known as Van Hove singularities.

In the cuprates, the CuO_2 plane contains three orbitals, $Cud_{x^2-y^2}$ and $O(p_x, p_y)$ orbitals with a lobe pointing towards the Cu. This is the standard three band model. It is sufficient to consider only one band since two of these bands are filled and one is half filled. Thus the energy band dispersion can be modeled by a tight-binding band

$$E(\vec{k}) = -2t(\cos k_x + r_1 \cos k_y) + 2tr_2 \cos k_x \cos k_y, \tag{3.5}$$

where t and tr_1 are the nearest-neighbor hopping energy along the a and b directions, respectively, and tr_2 is the next-nearest-neighbor hopping energy. The parameters r_1 represents the orthorhombic distortion in which the lattice parameters along the a and b directions are slightly different in length. For a square lattice r_1 is unity but smaller than unity for an orthorhombic phase. For parameter r_2 it is resonable to assume that $r_2 < r_1$.

The VHS energy is at

$$E_s = E_\pm = 2t[\pm(1 - r_1) - r_2] \tag{3.6}$$

The standard expressions for the electron density of states (DOS) in two dimension is given by

$$N(E) = \frac{1}{\pi^2}\int_0^\pi dk_x \int_0^\pi dk_y \delta(E - E(\vec{k})), \tag{3.7}$$

the DOS corresponding to the tight-binding energy, Eq.(3.5) is expressed to be

$$N(E) = \frac{1}{2t\pi^2\sqrt{r_1 + r_2(E/2t)}} K[\frac{1}{2}\sqrt{\frac{(1 + r_1)^2 - (E/2t - r_2)^2}{r_1 + r_2(E/2t)}}] \tag{3.8}$$

for $1 + r_1 + r_2 \geq E/2t \geq 1 - r_1 - r_2$, or $-1 + r_1 - r_2 \geq E/2t \geq -1 - r_1 + r_2$, and

$$N(E) = \frac{1}{t\pi^2\sqrt{(1 + r_1)^2 - (E/2t - r_2)^2}} K[2\sqrt{\frac{r_1 + r_2(E/2t)}{(1 + r_1)^2 - (E/2t - r_2)^2}}], \tag{3.9}$$

for $1 - r_1 - r_2 \geq E/2t \geq -1 + r_1 - r_2$, and $K(x) = F(\frac{\pi}{2}, x)$ is the complete elliptic integral of the first kind. Near the singularity E_s, the approximate expression for N(E) is

$$N(E) \doteq N_0 \ln\left| \frac{16t\sqrt{1 - r_2^2}}{E - E_s} \right| \tag{3.10}$$

with $N_0^{-1} = 2t\pi^2\sqrt{1-r_2^2}$ and $E_s = -2tr_2$. Eq.(3.10) was first derived by Xing, Liu and Gong (Xing, Liu, and Gong, 1991). Initiallly, the VHS density of states was proposed as an enhancement of the superconducting transition temperature within the framework of the phonon-mediated paring mechanism by Labbe and Bok (Labbe and Bok, 1987) but not included the orthorhombic distortion and the second-nearest-neighbor hopping paremeters. They calculated the superconducting critical temperature T_c as a function of the position of the Fermi level by using the weak couping BCS theory with a two-dimensional band structure for alkaline-earth- substituted La_2CuO_4 in the tetragonal phase. By using a tight-binding method with a linear atomic orbitals as wave function The structure of the d-p sub-band resulting from the strong hybridization of the $d_{x^2-y^2}$ orbitals with the p_x and p_y orbitals within a CuO_2 plane, leads to the following dispersion relation of the partly occupied antibonding d-p sub-band

$$E(\vec{k}) = \frac{1}{2}[(E_d - E_p) + \sqrt{(E_d - E_p)^2 + 8\gamma^2(2 - \cos k_x - \cos k_y)}] \qquad (3.11)$$

with γ is the direct transfer integral between the $d_{(x^2-y^2)}$ and the p_x and p_y orbitals located at nearest-neighbouring copper and oxygen sites respectively, E_d and E_p are the inter-atomic energies of these orbitals in the compounds, and $\vec{k} = (k_x, k_y)$ the two-dimentional wave vector within the CuO_2 plane. The logarithmic singularities of N(E), the density of states are obtained in the sub-band at the energies

$$E_s^{\pm} = \frac{1}{2}[(E_d - E_p) + \sqrt{(E_d - E_p)^2 + 16\gamma^2}] \qquad (3.12)$$

the saddle points $\vec{k} = (1,0)$, and (0,1) in the reciprocal space. The dispersion relation, Eq.(3.11) gives a band structure which can be analysed in terms of a small tranfer integral $\gamma^* = \gamma^2(E_d - E_p)^{-1}$ between nearest-neighbouring copper ions only if the difference $E_d - E_p$ would be much large than γ. But in that case, the antibonding sub-band would have a dominant d character, with only a very small contribution from the p states on oxygen, and the electrons in the sub-band would not explore these p states in this band. In the neighbourhood of $E_s^{\pm}$, the density of states per spin has the following approximate expression:

$$N(E) \cong \frac{N}{2\pi B} \ln\left(\frac{B}{E - E_s^{\pm}}\right) \tag{3.13}$$

with $B = \gamma^2[(E_d - E_p)^2 + 16\gamma^2]^{-\frac{1}{2}}$ and N is the number of unit cells contained in the plane. If the inter-atomic energies, E_d, and E_p are chosen at the middle of the sub-band, the dispersion relation, Eq.(3.11), reduces to

$$E(\vec{k}) = -2t(\cos k_x + \cos k_y) \tag{3.14}$$

where t is the parameter which must be adjusted to give the size of the band width and has the same order of magnitude as the direct transfer integral γ between nearest-neighbouring copper and oxygen sites, as long as $E_d - E_p$ is not much larger than γ. The simplified version for the band dispersion does not included the next-nearest-neighbour transfer integral, as stated before. Indeed, the logarithmic divergence of the density of states give rise to a modified form of a BCS result for T_c (Tsuei et al.,1990; Getino, Llano, and Rubio, 1993). The success of the Van Hove scenario lies in the assumption that the maximum T_c corresponding to the optimum doping concentration, the Fermi energy coincides the singularity.

In the weak coupling limit, the BCS equation for T_c is

$$\frac{1}{V} = \int_0^{\omega_D} \frac{dE}{E} N(E) \tanh\left(\frac{E}{2T_c}\right) \tag{3.15}$$

Tsuei et al. assumed the VHS density of states of the form

$$N(E) = N_0 \ln \left| \frac{E_F}{E - E_F} \right| \tag{3.16}$$

and approximated $\tanh x \approx x, (x < 1), \tanh x \approx 1, (x > 1)$, and obtained the transition temperature T_c as

$$T_c = 1.36 E_F \exp - \sqrt{\frac{2}{N_0 V} + \ln^2(\frac{E_F}{\omega_D}) - 1} \tag{3.17}$$

Getino, Llano, and Rubio extended the work of Tsuei et al. further by evaluating the exact T_c formula which has to be solved numerically and found that in the presence of VHS,the implicitly exact T_c formula is given by

$$T_c = \frac{1}{2} E_F \exp - \sqrt{[(\frac{1}{N_0 V} + D) 2 \coth \frac{\omega_D}{2T_c} + \ln^2 \frac{E_F}{\omega_D}]} \tag{3.18}$$

with the function D is defined as

$$D(\frac{\omega_D}{2T_c}, \frac{E_F}{2T_c}) = \int_0^{\frac{\omega_D}{2T_c}} dx [\ln x \ln \frac{E_F}{2T_c x} + \frac{1}{2} \ln^2 x] sech^2 x. \tag{3.19}$$

This T_c formula differed from the standard BCS T_c formula (with constant DOS),

$$T_c = 1.13 \omega_D \exp [-\frac{1}{N_0 V}] \tag{3.20}$$

in two ways. First, the prefactor is the Fermi energy rather than the Debye frequency , secondly, the exponent depends inversely only the square root of N(0)V, and their result gave the smaller values of T_c than the work of Tsuei et al., for given ω_D, E_F, and $N_0 V$ values.

Table 3.1 lists values of the dimensionless conpling constant $N_0 V$ consistent with the two typical values of 40K and 90K along with the ω_D and E_F values. The exact T_c formula, Eq.(3.18), requires values of $N_0 V$ only moderately larger than those of Tsuei et al., Eq.(3.17), and roughly one-quarter of those needed with the BCS T_c formula.

Getino, Llano, and Rubio (Getino, Llano, and Rubio, 1993) evaluated the zero-temperature gap-to-T_c ratio in the VHS DOS, the approximate expression is obtained as

$$\Delta(0) \simeq 2 E_F \exp -[\sqrt{\frac{2}{N_0 V} + \ln^2(\frac{E_F}{\omega_D})} - 1.64] \tag{3.21}$$

Table 3.1: The T_c formula evaluated by using Eqs.(3.17),(3.18), and (3.20) as given by the results of Tsuei et al., Getino et al., and BCS, respectively. (Taken from Getino, Llano, and Rubio, 1993)

			N_0V		
$T_c(K)$	$\omega_D(K)$	$E_F(K)$	Eq.(3.11)	Eq.(3.9)	Eq.(3.10)
	400	5548	0.142	0.093	0.100
40	500	5548	0.378	0.088	0.095
La-Sr-Cu-O	754	5580	0.327	0.082	0.086
	300	8807	0.754	0.148	0.164
90	400	8807	0.620	0.130	0.163
Y-Ba-Cu-O	754	8807	0.445	0.106	0.115

3.4 S-Wave Gap-to-T_c Ratio in the Van Hove Scenario

The zero-temperature superconducting gap ($\Delta(0)$) in the s-wave pairing state and the transition temperature T_c are related for a general DOS N(E) by the relation

$$\int_{E_F-\omega_D}^{E_F+\omega_D} \frac{N(E)}{\sqrt{(E-E_F)^2+\Delta(0)^2}} dE = \int_{E_F-\omega_D}^{E_F+\omega_D} N(E)\tanh\left(\frac{E-E_F}{2T_c}\right)\frac{dE}{E} \qquad (3.22)$$

This equation is obtained by the eliminating the constant pairing potential V between the BCS equation for $T = 0K$ and $T = T_c$.

For the VHS DOS Eq.(3.16), which has a peak at E_F, and Eq.(3.22) give

$$\int_0^{\omega_D} d\epsilon \frac{\ln\left(\frac{E_F}{\epsilon}\right)}{\sqrt{\epsilon^2+\Delta(0)^2}} = \int_0^{\omega_D} \frac{d\epsilon}{\epsilon}\ln\left(\frac{E_F}{\epsilon}\right)\tanh\left(\epsilon/2T_c\right) \qquad (3.23)$$

The numerical calculation of $2\Delta(0)/T_c$ for the VHS DOS Eq.(3.16) for different values of ω_D/T_c ratio along with ω_D, T_c, and E_F values is shown in Table. 3.2 (Ratanaburi et al.,1996). The ratio $2\Delta(0)/T_c$ is found to be larger than 3.53. Table shows that the value of $2\Delta(0)/T_c$ decreases with increase of ω_D/T_c at fixed E_F and tends to reach the BCS limit of 3.53 for a very high value of ω_D/T_c.

Table 3.2: Gap-to-T_c Ratio $2\Delta(0)/T_C$ evaluated by Eq.(3.23) and is compared with Eq.(3.21). Using some typical Debye(ω_D) and Fermi (E_F) characteristic temperature values(Taken from Ratanaburi et al.,1996)

			$2\Delta(0)/T_C$	
$T_c(K)$	$\omega_D(K)$	$E_F(K)$	Eq.(3.21)	Eq.(3.23)
	400	5548	3.64	3.656
40	500	5548	3.66	3.651
La-Sr-Cu-O	754	5580	3.53	3.646
	300	8807	3.60	3.773
90	400	8807	3.63	3.726
Y-Ba-Cu-O	754	8807	3.68	3.670

In order to obtain an analytical exact expression for the superconducting gap-to-T_c ratio $2\Delta(0)/T_c$, we writing Eq.(3.23) as

$$\ln \left| \frac{E_F}{2T_c} \right| [F(\omega_D, T_c) - \sinh^{-1}(2\omega_D/R_sT_c)] - I_1(\omega_D, T_c) + I_2(\omega_D, T_c, R_s) = 0 \quad (3.24)$$

where

$$F(\omega_D, T_c) = \int_0^{\frac{\omega_D}{2T_c}} \frac{dx}{x} \tanh x, \quad (3.25)$$

$$I_1(\omega_D, T_c) = \int_0^{\frac{\omega_D}{2T_c}} \frac{dx}{x} \ln x \tanh x, \quad (3.26)$$

and

$$I_2(\omega_D, T_c, R_s) = \int_0^{\frac{\omega_D}{2T_c}} dx \frac{\ln x}{\sqrt{x^2 + (R_s/4)^2}}, \quad (3.27)$$

with $R_s = 2\Delta(0)/T_c$. Eqs.(3.25)-(3.27) can be evaluated directly and the exact results are

$$F(\omega_D, T_c) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{(2n+1)} \tan^{-1}\left(\frac{\omega_D}{(2n+1)\pi T_c}\right), \quad (3.28)$$

$$I_1(\omega_D, T_c) = \ln\left(\frac{\omega_D}{T_c}\right) F(\omega_D, T_c) - \frac{4}{\pi} \sum_{n,k=0}^{\infty} \frac{(2k)!}{(2n+1)(2k+1)2^{2k}(k!)^2} \left\{K - \sum_{l=1}^{k} \frac{1}{(2k-2l+1)} \tanh^{2p-2l+1} K\right\}, \quad (3.29)$$

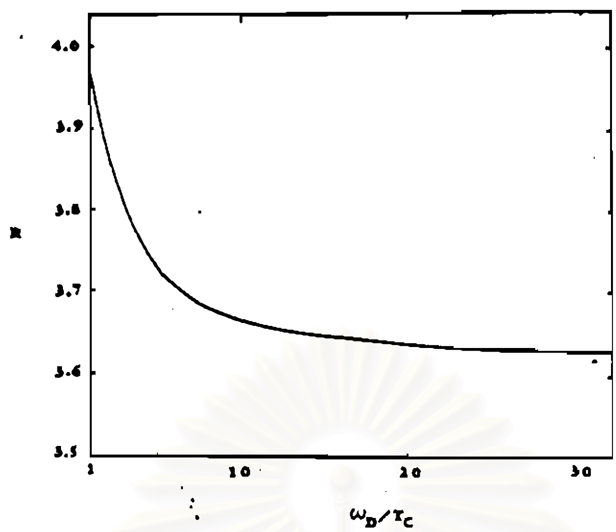

Figure 3.1: Ratio $R = 2\Delta(0)/T_c$ for a VHS DOS that peaks at the Fermi level for different ω_D/T_c values, here $E_F = 4000$K and $\omega_D = 500$K.(Taken from Ratanaburi et al.,1996)

where $K = \sinh^{-1}(\frac{\omega_D}{(2n+1)\pi T_c})$, and

$$I_2(\omega_D, T_c, R_s) = X\ln(R/8) + \frac{1}{2}Li_2[\exp(-2X)] + \frac{1}{2}X^2 - \frac{\pi^2}{12}, \tag{3.30}$$

where $Li_2(x) = \sum_{k=1}^{\infty}\frac{x^k}{k^2}$ is the Euler dilogarithmic function, and $X = \sinh^{-1}(\frac{2\omega_D}{R_sT_c})$

By substituting Eqs.(3.28)-(3.30) in Eq.(3.24) and approximating

$$\sinh^{-1}(\frac{2\omega_D}{R_sT_c}) \cong \ln(\frac{4\omega_D}{R_sT_c}) \tag{3.31}$$

we finally get the analytic expression for R_s as (Krunavakarn et al.,1998)

$$R_s = \frac{4E_F}{T_c}\exp -\sqrt{\ln^2(\frac{E_F}{2T_c}) - 2I_1 - \frac{\pi^2}{6} + \frac{1}{2}\ln^2(\frac{\omega_D}{2T_c}) + 2\ln(\frac{T_F}{2T_c})[F - \ln(\frac{\omega_D}{2T_c})]} \tag{3.32}$$

We remark here that this formula is applicable when $\omega_D \gg T_c$.

From Fig. 3.1, we can see that the superconducting gap-to -T_c ratio is found to be larger than 3.53 for a DOS with a VHS at the Fermi level and that the value decreases with the increase 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. Unfortunately, the high value of the gap ratio (6-8) as observed in some high-T_c cuprate oxide systems can not be explained within the simple VHS model with an isotropic s-wave pairing state (Persson and Demuth, 1990).

3.5 S-Wave Gap-to-T_c Ratio in the Van Hove Scenario with the Fermi Level Shift

As an extension of the VHS DOS at the Fermi level. we will investigate the variation of the gap ratio with the shift of the VHS from the Fermi surface. The form of the density of states is therefore assumed to be

$$N(E) = N_0 \ln \left| \frac{E_F}{E-(E_F-\delta)} \right| \tag{3.33}$$

here δ is the position of the saddle points in the energy surface, which is not far from the Fermi level, i.e., δ has a small value. The exact equation for the s-wave gap ratio is given by

$$\int_0^{\omega_D/2T_c} \frac{dx}{x} \tanh x \ln \left| \frac{(E_F/2T_c)^2}{x^2-(\delta/2T_c)^2} \right| = \int_0^{\omega_D} \frac{dx}{\sqrt{x^2+(R_sT_c/2)^2}} \ln \left| \frac{E_F^2}{x^2-\delta^2} \right| \tag{3.34}$$

The integration can be performed directly and has the following result

$$\sum_{n=0}^{\infty} \frac{1}{(n+\frac{1}{2})\pi} \{4tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}] \ln [\frac{(E_F/2T_c)\cos\alpha}{(n+1/2)\pi}] + Cl_2[tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}]+2\alpha] + Cl_2[tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}]-2\alpha] + 2Cl_2[\pi - 2tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}]]\}$$

$$= 2\sinh^{-1}(\frac{2\omega_D}{R_sT_c}) \ln (\frac{4E_F}{R_sT_c}) - [\sinh^{-1}(\frac{2\omega_D}{R_sT_c})]^2 - [\sinh^{-1}(\frac{2\delta}{R_sT_c})]^2 + \frac{\pi^2}{6} - \sum_{n=1}^{\infty} \frac{1}{n^2} \cosh[2n\sinh^{-1}(\frac{2\delta}{R_sT_c})] \exp[-2n\sinh^{-1}(\frac{2\omega_D}{R_sT_c})] \tag{3.35}$$

where $\tan\alpha = \frac{\delta/2T_c}{(n+1/2)\pi}$ and $Cl_2(z) = -\int_0^z \ln|\,2\sin(x/2)\,|dx$ is the Clausen's integral.

With the condition $\omega_D/T_c \gg 1$, the approximate expression for R_s is

$$R_s = \frac{4E_F}{T_c}\exp-\sqrt{\sinh^{-1}(\frac{2\delta}{R_0T_c}) + \ln^2(\frac{E_F}{\omega_D}) - \frac{\pi^2}{6} + A} \qquad (3.36)$$

where

$$R_0 = \frac{4E_F}{T_c}\exp-\sqrt{\ln^2(\frac{E_F}{\omega_D}) - \frac{\pi^2}{6} + A} \qquad (3.37)$$

and A is the expression on the left-hand side of Eq.(3.35). When we compare the result between the exact and the approximate values, we find that for given E_F/ω_D and ω_D/T_c values, as seen from Fig. 3.2, the approximate R_s values is always less than the exact one. Clearly, the maximum R_s occurs when the Fermi level shift, δ coincides at the Fermi surface and R_s decreases as the Fermi level shift is displaced away from the Fermi level.

3.6 D-Wave Gap Ratio

It is well known that the high value of the gap ratio cannot be achieved within an isotropic s-wave pairing state. The question about the symmetry of the pairing state arises to resolve this problem and it plays an important role in the investigation the several properties of the cuprate superconductors. Experiments have been reported that most of the high-T_c cuprates have d-wave pairing symmetry (Tsuei et al.,1994; Kirtley et al.,1995), the behavior of this state is the node at $k_x = \pm k_y$ in momentum space of lattice or $\phi = \pi/4$ in the first quadrant of the $\vec{k}$ space where ϕ is defined by the relation $\phi = \tan^{-1}(k_y/k_x)$ and it has the highest amplitude along the directions $(k_x, k_y) = (1,0)$ and (0, 1).
Musaelian et al.,(Musaelian et al.,1996) studied the weak coupling BCS theory of a d-wave gap superconductor with a constant density of states and showed that the d-wave gap ratio can give the value of 4.28 which is larger than 3.53 of the s-wave one. They start from the finite temperature gap equation,

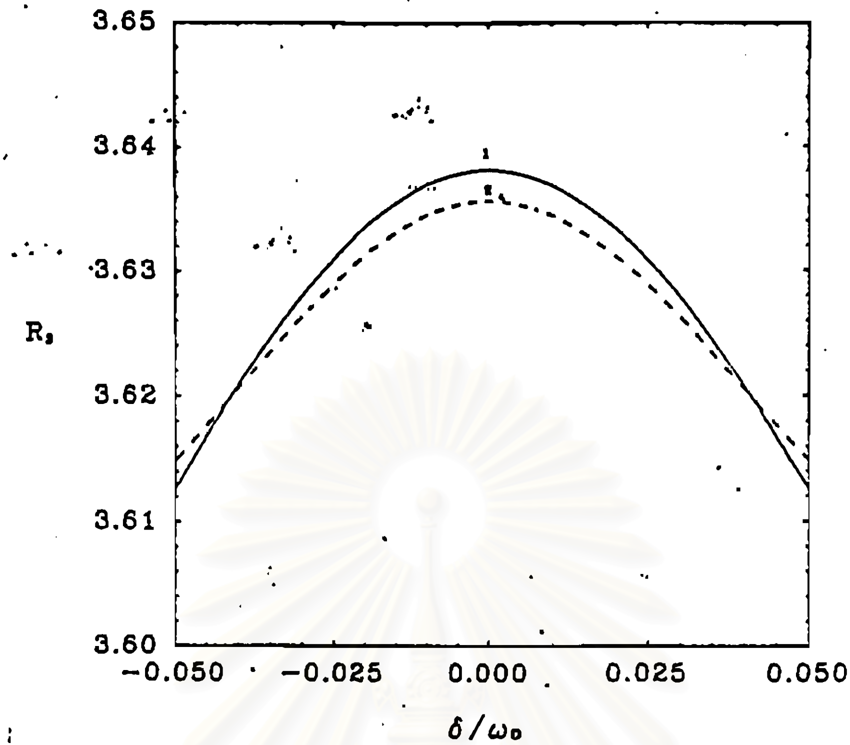

Figure 3.2: Variation of reduced gap-to-T_c ratio $R_s = 2\Delta(0)/T_c$ with δ/ω_D, where δ is the Fermi level shift and ω_D is the Debye cutoff energy. Curve 1 and 2 correspond to exact R_s and approximate R_s. Here $E_F/\omega_D = 10$ and $\omega_D/T_c = 20$.

$$\Delta_{\vec{k}} = \sum_{k'} V_{\vec{k}\vec{k}'} \frac{\Delta_{\vec{k}'}}{2\sqrt{\epsilon_{\vec{k}'}^2 + \Delta_{\vec{k}'}^{\ 2}}} \tanh\left(\frac{\sqrt{\epsilon_{\vec{k}'}^2 + \Delta_{\vec{k}'}^{\ 2}}}{2T}\right) \qquad (3.38)$$

and assume the order parameter and the

$$\Delta_{\vec{k}} = \Delta_d(T)\cos(2\phi), \qquad (3.39)$$

and the interaction

$$V_{\vec{k}\vec{k}'} = V_d(k_F, k_F')\cos(2\phi)\cos(2\phi') \qquad (3.40)$$

respectively. Here $V_d(k_F, k_F')$ is the constant pairing potential at the Fermi level. The d-wave gap at the zero-temperature satisfies the equation

$$1 = g_d \int_0^{2\pi} \frac{d\phi}{2\pi}\cos^2(2\phi) \int_0^{\omega_D} \frac{d\epsilon}{\sqrt{\epsilon^2 + [\Delta_d \cos(2\phi)]^2}} \qquad (3.41)$$

where $g_d = N(0)V_d$. After performing the integrations, the solution is given by

$$\Delta_d = \frac{\omega_D}{\sqrt{e}} \exp\left(-\frac{1}{g_d}\right) \tag{3.42}$$

At the same time, the critical temperature is obtained as

$$T_c = \frac{e^{\gamma}\omega_D}{2\pi} \exp\left(-\frac{1}{g_d}\right) \tag{3.43}$$

where $e^{\gamma} \approx 1.781$, Thus

$$\frac{2\Delta_d}{T_c} = \frac{4\pi}{\sqrt{e}e^{\gamma}} \approx 4.28 \tag{3.44}$$

as stated above.

3.7 D-Wave Gap-to- T_c Ratio in the Van Hove Scenario

In the previous section the constant density of states has been used to evaluate the d-wave gap-to-T_c ratio, but this is not the realistic density of states of the cuprates. To enhance the gap-to-T_c ratio above 4, the d-wave gap parameter and the Van Hove singularity DOS are combined together to explain the high values of the gap ratio $2\Delta_d(0)/T_c$.

We start with the usual BCS gap equation

$$\Delta_{\vec{k}} = \sum_{k'} V_{\vec{k}\vec{k'}} \frac{\Delta_{\vec{k'}}}{2\sqrt{\epsilon_{\vec{k'}}^2 + \Delta_{\vec{k'}}^2}} \tanh\left(\frac{\sqrt{\epsilon_{\vec{k'}}^2 + \Delta_{\vec{k'}}^2}}{2T}\right) \tag{3.45}$$

The pairing potential $V_{\vec{k}\vec{k'}}$ is now not a constant but has the form

$$V_{\vec{k}\vec{k'}} = V_d \cos(2\phi)\cos(2\phi') \tag{3.46}$$

in the range $-\omega_D \leq \epsilon_{\vec{k}} - E_F \leq \omega_D$, and zero otherwise. Here V_d is a constant pairing potential and ϕ is the two-dimensional angle which is defined as $\tan^{-1}(\frac{k_y}{k_x})$.

Of the same form as $V_{\vec{k}\vec{k'}}$, the d-wave order parameter takes the form

$$\Delta_{\vec{k}} = \Delta_d(T)\cos(2\phi). \tag{3.47}$$

Introduce Eqs.(3.16), (3.46), and (3.47) into Eq.(3.45), the following equation is obtained

$$\frac{1}{N_0V_d} = \int_0^{2\pi}\frac{d\phi}{2\pi}\cos^2(2\phi)\int_{-\omega_D}^{\omega_D} d\epsilon\frac{\ln|\frac{E_F}{\epsilon}|}{2W}\tanh(\frac{W}{2T}) \tag{3.48}$$

where $W = \sqrt{\epsilon^2 + [\Delta_d(T)\cos(2\phi)]^2}$. By eliminating the coupling constant N_0V_d, one finds the relation between the zero-temperature superconducting gap $\Delta_d(0)$ and the transition temperature T_c,

$$\int_0^{2\pi}\frac{d\phi}{2\pi}\cos^2(2\phi)\int_0^{\omega_D}\frac{d\epsilon}{\epsilon}\ln(\frac{E_F}{\epsilon})\tanh\frac{\epsilon}{2T_c} = \int_0^{2\pi}\frac{d\phi}{2\pi}\cos^2(2\phi)\int_0^{\omega_D} d\epsilon\frac{\ln(\frac{E_F}{\epsilon})}{\sqrt{\epsilon^2 + [\Delta_d(0)\cos(2\phi)]^2}} \tag{3.49}$$

Performing the integration over the energy on the right-hand side we obtain

$$\int_0^{\frac{\omega_D}{2T_c}}\frac{dx}{x}\ln(\frac{E_F}{2T_cx})\tanh x = \frac{2}{\pi}\int_0^{\pi} d\theta\cos^2\theta\{X\ln(\frac{4E_F}{R_dT_c\cos\theta}) - \frac{1}{2}Li_2[\exp(-2X)] - \frac{1}{2}X^2 + \frac{\pi^2}{12}\} \tag{3.50}$$

where $R_d = 2\Delta_d(0)/T_c$, and $X = \sinh^{-1}(\frac{2\omega_D}{R_dT_c\cos\theta})$. One is interested in the approximate expression for R_d. By approximating $X = \sinh^{-1}(\frac{2\omega_D}{R_dT_c\cos\theta}) \cong \ln(\frac{4\omega_D}{R_dT_c\cos\theta})$, and neglecting the Euler dilogarithmic function $Li_2(x)$, then Eq.(3.50) is reduced to

$$2 - \ln^2(\frac{4e^\gamma}{\pi}) - \ln^2(\frac{E_F}{\omega_D}) + \ln^2(\frac{2e^\gamma E_F}{\pi T_c}) = \frac{1}{\pi}\int_0^{\pi} d\theta\cos^2\theta[\frac{\pi^2}{6} - \ln^2(\frac{E_F}{\omega_D}) + \ln^2\frac{4E_F}{R_dT_c\cos\theta}] \tag{3.51}$$

where the integration on the left-hand side of Eq.(3.50) is performed in the BCS limit. Once the angular integration is evaluated, we get the equation

$$\ln^2\frac{8E_F}{\sqrt{e}R_dT_c} = \frac{11-\pi^2}{4} - \ln^2(\frac{4e^\gamma}{\pi}) + \ln^2(\frac{2e^\gamma E_F}{\pi T_c}) \tag{3.52}$$

Solving this equation, we finally obtain the approximate equation for R_d (Pakokthom et al., 1998)

$$R_d = \frac{8E_F}{\sqrt{e}T_c}\exp[-\sqrt{\frac{11-\pi^2}{4} - \ln^2(\frac{4e^\gamma}{\pi}) + \ln^2(\frac{2e^\gamma E_F}{\pi T_c})}], \tag{3.53}$$

where $\gamma = 0.5772....$ is the Euler' constant. In the limit $E_F/T_c \to \infty$, $R_d \approx (\frac{8E_F}{\sqrt{e}T_c})(\frac{\pi T_c}{2e^\gamma E_F})$ we find that Eq.(3.53) gives $R_d = 4.28$ which is the same as that obtained by Musaelian et al. where the condition $\omega_D/T_c \gg 1$ was considered.

3.8 D-Wave Gap-to-T_c Ratio in the Van Hove Scenario with the Fermi Level Shift

In the s-wave case, the dependence of the gap ratio on the Fermi level shift is studied. One finds that the gap ratio decreases as δ increases. When the VHS is at the Fermi level, the gap ratio has the maximum value. In this section, the dependence of the gap ratio on the Fermi level shift will be examined in the context of the d-wave pairing state. If the saddle point is not lying at the Fermi level, the density of states will be

$$N(E) = N_0 \ln|\frac{E_F}{E-(E_F-\delta)}|. \tag{3.54}$$

here δ be the shift of the Fermi level from the VHS. The finite temperature d-wave gap equation, Eq. (3.48), is modified to be

$$\frac{1}{N_0V_d} = \int_0^{2\pi}\frac{d\phi}{2\pi}\cos^2(2\phi)\int_{-\omega_D}^{\omega_D}\frac{d\epsilon}{2W}\ln|\frac{E_F}{\epsilon+\delta}|\tanh(\frac{W}{2T}) \tag{3.55}$$

where $W = \sqrt{\epsilon^2 + [\Delta_d(T)\cos(2\phi)]^2}$. The elimination of N_0V_d from the zero-temperature and the transition temperature equations gives

$$\int_0^{2\pi}\frac{d\phi}{2\pi}\cos^2(2\phi)\int_0^{\omega_D}\frac{d\epsilon}{\epsilon}\ln(\frac{E_F}{\epsilon^2-\delta^2})\tanh\frac{\epsilon}{2T_c} =$$

$$\int_0^{2\pi}\frac{d\phi}{2\pi}\cos^2(2\phi)\int_0^{\omega_D}d\epsilon\frac{\ln(\frac{E_F}{\epsilon^2-\delta^2})}{\sqrt{\epsilon^2+[\Delta_d(0)\cos(2\phi)]^2}} \tag{3.56}$$

Manipulating the energy integral on the right-hand side and writing $\Delta_d(0)$ in term of $R_d = 2\Delta_d(0)/T_c$ yields

$$\int_0^{\omega_D/2T_c} \frac{dx}{x} \tanh x \ln \left| \frac{(E_F/2T_c)^2}{x^2 - (\delta/2T_c)^2} \right|$$
$$= \frac{2}{\pi} \int_0^{\pi} d\theta \cos^2\theta \{2\sinh^{-1}(\frac{2\omega_D}{R_d T_c \cos\theta}) \ln(\frac{4E_F}{R_d T_c \cos\theta}) - [\sinh^{-1}(\frac{2\omega_D}{R_d T_c \cos\theta})]^2$$
$$- [\sinh^{-1}(\frac{2\delta}{R_d T_c \cos\theta})]^2 + \frac{\pi^2}{6} - \sum_{n=1}^{\infty} \frac{1}{n^2} \cosh[2n\sinh^{-1}(\frac{2\delta}{R_d T_c \cos\theta})]$$
$$\times \exp[-2n\sinh^{-1}(\frac{2\omega_D}{R_d T_c \cos\theta})]\} \qquad (3.57)$$

A numerical computation for R_d of Eq.(3.57) is shown in Fig.(3.3) as a function of δ/ω_D. An approximate formula for R_d is evaluated as

$$R_d = \frac{8E_F}{\sqrt{e}T_c} \exp[-\sqrt{\frac{3-\pi^2}{4} + \ln^2(\frac{E_F}{\omega_D}) + 2(\frac{2\delta}{R_1 T_c})^2 + A}], \qquad (3.58)$$

with

$$R_1 = \frac{8E_F}{\sqrt{e}T_c} \exp[-\sqrt{\frac{3-\pi^2}{4} + \ln^2(\frac{E_F}{\omega_D})}], \qquad (3.59)$$

where the expression for A is given by

$$A = \sum_{n=0}^{\infty} \frac{1}{(n+\frac{1}{2})\pi} \{4tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}] \ln[\frac{(E_F/2T_c)\cos\alpha}{(n+1/2)\pi}]$$
$$+Cl_2[tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}] + 2\alpha] + Cl_2[tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}] - 2\alpha]$$
$$+2Cl_2[\pi - 2tan^{-1}[\frac{\omega_D/2T_c}{(n+\frac{1}{2})\pi}]]\} \qquad (3.60)$$

here $\tan\alpha = \frac{\delta/2T_c}{(n+1/2)\pi}$ and $Cl_2(z) = -\int_0^z \ln|2\sin(x/2)|dx$ is the Clausen's integral.

From Fig.(3.3), we can see that the R_d as well as R_s has the maximum value at the Fermi level and it decreases as the ratio δ/T_c increases.

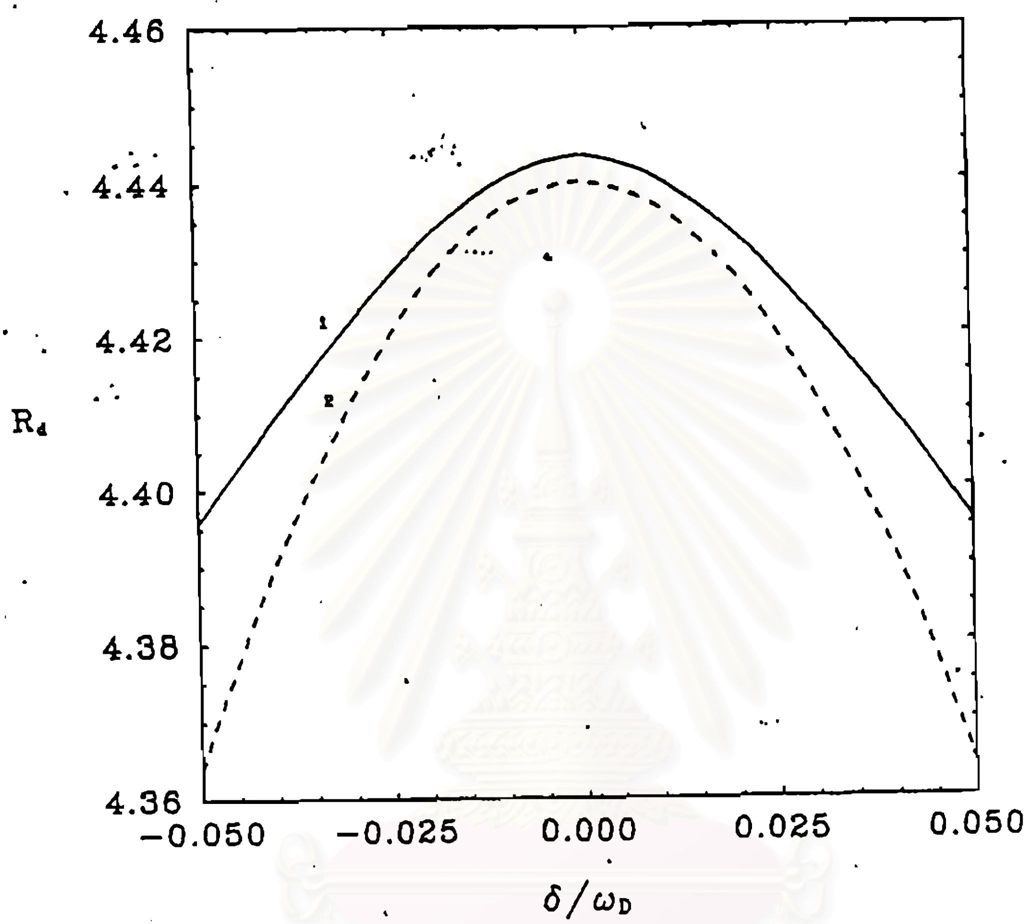

Figure 3.3: Variation of d-wave gap-to-T_c ratio $R_d = 2\Delta_d(0)/T_c$ with δ/ω_D, where δ is the Fermi level shift and ω_D is the Debye cutoff energy. Curve 1 and 2 correspond to exact R_s and approximate R_s. Here $E_F/\omega_D = 10$ and $\omega_D/T_c = 20$.

3.9 Mixed (S+D)-Wave Superconductivity

The symmetry of an energy gap parameter, $\Delta_{\vec{k}}$, in high-temperature superconductivity is the central issue whether the pairing symmetry is conventional or unconventional. An order parameter in the classical BCS theory occurs when electrons with opposite momenta and spins form bound pairs, which is the so-called Cooper pairs with a definite relative angular momentum. Conventional metallic superconductors all have s-wave symmetry (angular momentum $l = 0$). We know that if Cooper pairs also occur in high-temperature superconductors then there is a possibility that the strong on-site Coulomb repulsion among the electrons may prevent the formation of pairs with s-wave symmetry . Since the Cu^{2+} ion in the parent compounds, La_2CuO_4, have nine d electrons per copper ion and the very strong Coulomb repulsion between electrons forces them to be localized on individual ionic sites. Upon doping, the dopant holes that are introduced onto the copper ions destroy the magnetic order and then the doped compounds become superconductors with an unusual high transition temperature of the order 100K. This is in contrast to the conventional metallic superconductor . However, Cooper pair can form in a higher angular momentum state and the candidate for unconventional pairing is the d-state (angular momentum $l = 2$). This symmetry is supported by the phenomenological theory in which the pairing is mediated by the exchange of spin fluctuation (Monthoux et al., 1991) . While some photoemission experiments are inconsistent with the pure d-wave but more consistent with a mixture of s-wave and d-wave pairings. (Ma et al.,1995 ; Ding et al.,1995)

The s-d mixing superconducting state was first discussed by Ruckenstein, Hirschfeld, and Appel (Ruckenstein, Hirschfeld, and Appel,1987) and independently by Gotliar (Gotliar,1988) for the possibility of inducing transition between the different superconducting states . Musaelian et al. (Musaelian et al.,1996) studied the model of and isotropic two-dimensional Fermi liquid with attractive interaction in both s-and d-channels and with the free particles dispersion relation to investigate the possibility of a superconducting state with the mixed s-wave and d-wave order parameters. It was shown that a mixed (s+id) symmetry gap is stable in a certain range of interaction while a mixed (s+d) state does not occur. However, the model they considered is oversimplified because the realistic parameters such as the tight-binding dispersion relation, the orthorhombic distortion, and the second nearest-neighbor hopping integral have not been taken into account. These parameters lead to the Van Hove singularity in the density of states . Liu, Xing, and Wang (Liu, Xing, and Wang, 1997) applied the Van Hove scenario to the superconducting state with a mixed (s+id)-wave symmetry. They found that both s-wave and d-wave states can coexist in a small range of relative strength of the two attractive interactions.

In the work of Musaelian et al.,they considered the gap equation at the zero-temperature:

$$\Delta(\vec{k}) = \sum_{\vec{k}'} V(\vec{k}, \vec{k}') \frac{\Delta(\vec{k})}{2E_{\vec{k}'}} \tag{3.61}$$

where $E_{\vec{k}} = \sqrt{\epsilon_{\vec{k}}^2 + |\Delta(\vec{k})|^2}$ and assuming the interaction of the following form,

$$V(\vec{k}, \vec{k}') = V_s(k_F, k_F') + V_d(k_F, k_F') \cos[2(\phi - \phi')] \tag{3.62}$$

which contains both s and d pairing components. The two-dimensional angle ϕ is defined as $\phi = \tan^{-1}(k_y/k_x)$. Since the interaction dominates on the Fermi surface, $|\vec{k}| = |\vec{k}'| = k_F$. Then the order parameter, $\Delta(\vec{k})$ depends only through the angle, ϕ, and is supposed to be

$$\Delta(\phi) = \Delta_s + \Delta_d \cos(2\phi). \tag{3.63}$$

Inserting Eqs.(3.62) and (3.63) in Eq.(3.61) and seperating the s and d components, the coupled equations are

$$\Delta_s = N_0 V_s \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{\omega_D} dE \frac{[\Delta_s + \Delta_d \cos(2\phi)]}{\sqrt{E^2 + [\Delta_s + \Delta_d \cos(2\phi)]^2}} \tag{3.64}$$

$$\Delta_d = N_0 V_d \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{\omega_D} dE \frac{\cos(2\phi)[\Delta_s + \Delta_d \cos(2\phi)]}{\sqrt{E^2 + [\Delta_s + \Delta_d \cos(2\phi)]^2}} \tag{3.65}$$

where N_0 is the constant density of states at the Fermi level.By using the approximation $\Delta(\phi) \ll \omega_D$,

$$\int_0^{\omega_D} \frac{dE}{\sqrt{E^2 + \Delta^2(\phi)}} \approx \ln \left| \frac{2\omega_D}{\Delta(\phi)} \right| \tag{3.66}$$

Performing the integration of Eqs.(3.64) and (3.65) over the angle, and eliminating the logarithmic term, the result is

$$(1 - \frac{2g_s}{g_d})\alpha = g_s f(\alpha) \tag{3.67}$$

where $g_s = N_0 V_s, g_d = N_0 V_d, \alpha \equiv \Delta_s/\Delta_d$, and the function $f(\alpha)$ is given by

$$\begin{aligned} f(\alpha) &= \int_0^{\pi} \frac{dx}{\pi}(2\alpha\cos x - 1)(\alpha + \cos x)\ln(\alpha + \cos x) \\ &= [\frac{\alpha}{2} + (\alpha^2 - 1)(\alpha - \sqrt{\alpha^2 - 1})] \end{aligned} \tag{3.68}$$

In the limit $\alpha \to \infty, f(\alpha) \approx \frac{\alpha}{2}$, and the solution of Eq.(3.67) is given by

$$g_s^{(1)} = \frac{2g_d}{4 + g_d}. \tag{3.69}$$

This state is the pure s-wave symmetry, the pure d-wave state does not exists at this point. In the limit $\alpha \to 0, f(\alpha) \approx -\frac{\alpha}{2}$ (i.e., pure d-wave state), Eq.(3.67) gives

$$g_d^{(2)} = \frac{2g_d}{4 - g_d}. \tag{3.70}$$

Because $g_s^{(1)} < g_s^{(2)}$, and therefore $0 < g_s < g_s^{(1)}$ is the region for the (s+d)-wave, $g_s > g_s^{(1)}$ for the s-wave, while $g_s^{(1)} < g_s^{(2)}$ for the d-wave, and $g_s > g_s^{(2)}$ for the (s+d)-wave. From this statement, it shows that the (s+d) state does not occur.

Beal-Monod and Maki (Beal-Monod and Maki,1996) studied some of the superconducting properties of anisotropic hybrid (s+d)- and (d+s)-wave superconductor models (depending whether the s or d component predominates). The anisotropy is contained in the fermion-fermion pairing interaction as reflecting the structural anisotropies of layers in high-T_c cuprates, particularly the orthorhombic distortion.In the case of the (d+s) model, they proposed the anisotropic pairing interaction:

$$V(\vec{k},\vec{k'}) = \\ -V\{\cos(2\phi)\cos(2\phi') + g[\cos(2\phi) + \cos(2\phi')]\} + \frac{\mu}{N_0} \tag{3.71}$$

where V is the positive constant, $\phi(\phi')$ is the angle of $\vec{k}(\vec{k'})$ on the circular Fermi surface, N_0 is the constant density of states at the Fermi level in the normal phase, g measures the anisotropy between the a and b directions within the layer, and μ is the Coulomb repulsion. In absence of the orthorhombic distortion, the small s component vanishes, that includes the parameter g. The gap function $\Delta(\vec{k})$ is taken to be

$$\Delta(\vec{k}) = \Delta[r + \cos(2\phi)] \tag{3.72}$$

where r is the small component of the s-wave pairing due to the orthorhombic distortion effect. $\Delta_M = \Delta(r+1)$ be the maximum gap. The T_c formula obeys

$$\ln\frac{1.134E_F}{T_c} = \frac{\mu - \lambda + \sqrt{(\mu+\lambda)^2 + 8(g\lambda)^2}}{2\lambda(\mu + 2g^2\lambda)} \tag{3.73}$$

In the absence of anisotropy, g=0, $\ln(1.134E_F/T_c)$ is just $1/\lambda$, where $\lambda = N_0V/2$. Also, the value of r at T_c reads

$$r_{T_c} = \frac{\sqrt{(\mu+\lambda)^2 + 8(g\lambda)^2} - (\mu+\lambda)}{4g\lambda} \tag{3.74}$$

with the equation for the anisotropy, g, is given by

$$g = \frac{\sqrt{1 - 2r^2\lambda + 4r^2(\mu+\lambda)(1-2r^2)^{-1}} - 1}{2r\lambda} \tag{3.75}$$

Table 3.3: Various parameters computed for different values of the anisotropy g with $\lambda = 0.5, \mu = 0.2$ and E_F =600K.(Taken from Beal-Monod and Maki ,1996)

g	r_{T_c}	r	T_c	Δ	Δ_M/T_c	T_c/T_c^{pd}
0	0	0	92.08	197.00	2.14	1
0.13	0.09	0.1	96.59	202.76	2.31	1.05
0.20	0.10	0.15	102.38	210.11	2.36	1.11

The gap equation is found to be

$$\ln \frac{4E_F}{\Delta} = 1 + \frac{\lambda^{-1} + r^2 - 0.5}{1 + 2gr} \tag{3.76}$$

In this model, the Coulomb repulsion does not affect the critical temperature in the absence of anisotropy. The gap-to-T_c ratio at this limit (pure d-wave) yields $2\Delta/T_C = 4.28$, which is the same value as that studied by Musaelian et al. Table 3.3 shows the values of g, r (at T=0), $r_{T_c}, T_c, \Delta, \Delta_M/T_c$, and T_c/T_c^{pd} (T_c^{pd} is the value of T_c for g=0, the pure d-wave, and $\Delta_M = \Delta(r+1)$).

3.10 Mixed (S+D)-Wave in the Van Hove Scenario

We see that in the works of Musaelian et al., and Beal-Monod and Maki the density of states is assumed to be constant value along the Fermi surface where it arises from the presence of the free particle dispersion. Indeed in the layers of high-T_c cuprates, the moving of the electrons must encounter the interaction between it and the host atoms (e.g., Cu and O atoms). Then the free perticle dispersion is made irrelevant for high-T_c cuprates. The more appropriate form of the energy dispersion will be the tight-binding band energy and is given by

$$E(\vec{k}) = -2t(\cos k_x + r\cos k_y) \tag{3.77}$$

where t is the hopping energy and r is the orthorhombic distortion parameter which measures the anisotropy between the a and b directions of the lattice. For the square lattice, r=1,and nearly unity for the rectangular lattice. The standard expression for the density of states (DOS) is defined as

$$N(E) = \sum_{\vec{k}} \delta[E - E_{\vec{k}}] \tag{3.78}$$

After the two-dimensional band dispersion relation is introduce in the DOS. The DOS is evaluated approximately as

$$N(E) = N_0 \ln \left| \frac{E_F}{E - E_F} \right| \tag{3.79}$$

where N_0 is the constant DOS at the Fermi level. The two-particle interaction, which is responsible for the superconductivity, is assumed to be of the following form

$$V(\vec{k}, \vec{k'}) = -V[a\cos(k_x - k_{x'}) + b\cos(k_y - k_{y'})] \tag{3.80}$$

where the parameters a and b represent the anisotropy within the layer, due to the orthorhombic distortion effect. For the square lattice, a=b, the orthorhombic distortion disappears. Here V is the strength of the pairing interaction and has the positive value. The pairing interaction is obtained by means of the short range nature of the attractive interaction which has the non-zero value only among the nearest neighbors of the lattice sites. Because the interaction plays a role at the Fermi surface, $|\vec{k}| = |\vec{k'}| = k_F$. Then the interaction $V(\vec{k}, \vec{k'})$ will depend only through the angle ϕ, where ϕ is the two-dimensional angular angle of $\vec{k}$ in reciprocal space. Using the transformation in the parametric form,

$$k_x = k_F \cos\phi, \quad k_y = k_F \sin\phi, \tag{3.81}$$

since the $\sin k_x \sin k_{x'}$ and $\sin k_y \sin k_{y'}$ terms contribute to the p-wave interaction, the relevant interaction will be

$$V(\vec{k}, \vec{k'}) = -V[a\cos k_x \cos k_{x'} + b\cos k_y \cos k_{y'}] \tag{3.82}$$

Expressing the cosine function in terms of the Bessel function, we have

$$\cos[k_F\cos\phi] = J_0(k_F) + 2\sum_{n=1}^{\infty}(-1)^n J_{2n}(k_F)\cos[2n\phi],$$
$$\cos[k_F\sin\phi] = J_0(k_F) + 2\sum_{n=1}^{\infty} J_{2n}(k_F)\cos[2n\phi] \qquad (3.83)$$

Inserting Eq.(3.83) into Eq.(3.82) with the higher order terms $n \geq 2$ will be omitted, the interaction $V(\vec{k},\vec{k}')$, is given by

$$\begin{aligned} V(\vec{k},\vec{k}') &= V_s(\phi,\phi') + V_d(\phi,\phi') \\ &= -V_s\{1+\lambda[\cos(2\phi)+\cos(2\phi')]\} - V_d\cos(2\phi)\cos(2\phi') \end{aligned} \qquad (3.84)$$

where $V_{s,d} \propto b+a$ represents the strength of the interaction along the s(d) chennel, $\lambda \propto (b-a)/(b+a)$ represents the anisotropic s-wave pairing interaction which corresponds to the orthorhombic distortion effect in cuprates. The attractive interactions which contain both the anisotropic s-wave and d-wave channels are energy independent in an energy range bounded by the cut off energy ω_D, and zero for $|\epsilon_{\vec{k}}| \geq \omega_D$. This equation shows that the main interaction is V_s and V_d while the small component is the λV_s. In the tetragonal phase, a=b, $\lambda = 0$. the anisotropic pairing interaction $V(\vec{k},\vec{k}')$ reduces to the mixing between the pure s-wave and d-wave pairing interaction. Consequently, the order parameter for the mixed (s+d)-wave pairing is assumed in the form

$$\Delta(\vec{k}) = \Delta_s + \Delta_d\cos(2\phi) \qquad (3.85)$$

Using the BCS framework, the (s+d)-wave pairing will consist of the phase regions of the pure s- and d-wave pairing as well as the (s+d)-wave pairing. In the weak coupling theory, the gap parameter at the zero-temperature satisfies

$$\Delta(\vec{k}) = -\sum_{\vec{k}'} V(\vec{k},\vec{k}')\frac{\Delta(\vec{k})}{2E_{\vec{k}'}} \qquad (3.86)$$

where $E_{\vec{k}} = \sqrt{(\epsilon_{\vec{k}} - E_F)^2 + |\Delta_{\vec{k}}|^2}$ is the excitation energy in the superconducting state.

Substituting Eqs.(3.79),(3.84), and (3.85), in Eq.(3.86). We arrive at the equation

$$\begin{aligned}\Delta_s + \Delta_d \cos(2\phi) &= N(0)\int_0^{2\pi} \frac{d\phi'}{2\pi}[V_s(\phi,\phi') + V_d(\phi,\phi')][\Delta_s + \Delta_d \cos(2\phi')] \\ &\times \int_0^{\omega_D} \frac{dE}{\sqrt{E^2 + [\Delta_s + \Delta_d \cos(2\phi')]^2}} \ln(\frac{E_F}{E}) \qquad (3.87)\end{aligned}$$

where N(0) is the constant density of states per spin at the Fermi surface.

Seperating this equation along the pairing channel. We obtain the pair of coupled equations

$$\Delta_s = g_s \int_0^{2\pi} \frac{d\phi}{2\pi}[1 + \lambda \cos(2\phi)][\Delta_s + \Delta_d \cos(2\phi)]F[E_F, \omega_D, \Delta_s, \Delta_d, \phi] \qquad (3.88)$$

$$\Delta_d = g_d \int_0^{2\pi} \frac{d\phi}{2\pi} \cos(2\phi)[\Delta_s + \Delta_d \cos(2\phi)]F[E_F, \omega_D, \Delta_s, \Delta_d, \phi] \qquad (3.89)$$

with the function $F[E_F, \omega_D, \Delta_s, \Delta_d, \phi]$ is defined as

$$F[E_F, \omega_D, \Delta_s, \Delta_d, \phi] = \int_0^{\omega_D} \frac{dE}{\sqrt{E^2 + [\Delta_s + \Delta_d(\cos 2\phi)]^2}} \ln(\frac{E_F}{E}) \qquad (3.90)$$

and it has the approximate result,

$$F[E_F, \omega_D, \Delta_s, \Delta_d, \phi] = \frac{1}{2}[\ \frac{\pi^2}{6} - \ln^2|\ \frac{E_F}{\omega_D}\ | + \ln^2|\ \frac{2E_F}{\Delta_s + \Delta_d \cos(2\phi)}\ |\ ] \qquad (3.91)$$

here $g_{s(d)} = N(0)V_{s(d)}$ is the dimensionless coupling constant of the phonon interaction in the s(d) channel.

In the case of the pure s-wave. Eq.(3.88) with $\Delta_d = 0$ is reduced to an s-wave gap equation

$$\begin{aligned}\Delta_s &= g_s\Delta_s \int_0^{2\pi} \frac{d\phi}{2\pi}[1 + \lambda \cos(2\phi)]F[E_F, \omega_D, \Delta_s, \Delta_d = 0, \phi] \\ &= g_s\Delta_s F[E_F, \omega_D, \Delta_s, \Delta_d = 0, \phi] \qquad (3.92)\end{aligned}$$

From Eq.(3.91), $F[E_F, \omega_D, \Delta_s, \Delta_d = 0, \phi]$ is given by

$$F[E_F, \omega_D, \Delta_s, \Delta_d = 0, \phi] = \frac{1}{2}[\ \frac{\pi^2}{6} - \ln^2(\frac{E_F}{\omega_D}) + \ln^2(\frac{2E_F}{\Delta_s})\ ] \tag{3.93}$$

Combining Eq.(3.93) with Eq.(3.92) we have

$$\frac{2}{g_s} = \frac{\pi^2}{6} - \ln^2(\frac{E_F}{\omega_D}) + \ln^2(\frac{2E_F}{\Delta_s}) \tag{3.94}$$

We see that the orthorhombic distortion parameter λ does not affecte the s-wave gap parameter Δ_s.

In the pure d-wave case, by taking $\Delta_s = 0$ in Eq.(3.89), we get

$$\Delta_d = g_d\Delta_d \int_0^{2\pi} \frac{d\phi}{2\pi}\cos^2(2\phi)F[E_F, \omega_D, \Delta_s = 0, \Delta_d, \phi] \tag{3.95}$$

Now from Eq.(3.91), $F[E_F, \omega_D, \Delta_s = 0, \Delta_d, \phi]$ is given by

$$F[E_F, \omega_D, \Delta_s = 0, \Delta_d, \phi] = \frac{1}{2}[\ \frac{\pi^2}{6} - \ln^2(\frac{E_F}{\omega_D}) + \ln^2(\frac{2E_F}{\Delta_d\cos 2\phi})\ ] \tag{3.96}$$

Inserting Eq.(3.96) in Eq.(3.95) and integrating over the angular variable, the result is

$$\frac{4}{g_d} = \frac{\pi^2 - 3}{4} - \ln^2(\frac{E_F}{\omega_D}) + \ln^2|\ \frac{4E_F}{\sqrt{e}\Delta_d}\ | \tag{3.97}$$

Eqs.(3.94) and (3.97) are the gap parameter equations in the pure s-wave and d-wave, respectively.

In order to obtain the equation of the mixed phase. Dividing Eqs.(3.88) and (3.89) by Δ_d and subtract them, we obtain the mixed phase equation

$$(\frac{1}{g_s} - \frac{1}{g_d})2\alpha = \int_0^{\pi} \frac{dx}{\pi}[\alpha + \lambda + 2[1 + \alpha(\lambda - \alpha)]\cos x + (\lambda - \alpha)\cos 2x]F[E_F, \omega_D, \alpha, x] \tag{3.98}$$

where $\alpha \equiv \Delta_s/\Delta_d$ is the ratio of the superconducting gap between the s-wave and the d-wave, and

$$F[E_F, \omega_D, \alpha, x] = \frac{1}{2}[\frac{\pi^2}{6} - \ln^2(\frac{E_F}{\omega_D}) + \ln^2|\ \frac{2E_F}{\Delta_d(\alpha + \cos x)}\ |] \tag{3.99}$$

The solution of Eq.(3.98) is obtained in three regions, the pure d-wave for $\alpha = 0$ or $g_s = 0$, the pure s-wave for $\alpha \to \infty$ or $g_s \to \infty$ and the (s+d)-wave which is the intermediate region between the pure waves. To show the existence of the mixed (s+d) state, we will examine the stable phases for the pure states. We remark here that in the limiting cases, $\alpha \to \infty$ and $\alpha \to 0$, the form of $F[E_F, \omega_D, \alpha, x]$ in Eq.(3.99), has reduced to

$$F[E_F, \omega_D, \alpha, x] = \frac{1}{2}[\frac{\pi^2}{6} - \ln^2|\frac{E_F}{\omega_D}| + \ln^2|\frac{2E_F}{\Delta_s}|], \quad \alpha \to \infty \qquad (3.100)$$

$$= \frac{1}{2}[\frac{\pi^2}{6} - \ln^2|\frac{E_F}{\omega_D}| + \ln^2|\frac{2E_F}{\Delta_d \cos x}|], \quad \alpha \to 0 \qquad (3.101)$$

For the pure d-wave case, $\alpha \to 0$, the mixed phase equation, Eq.(3.98), becomes

$$(\frac{1}{g_s} - \frac{1}{g_d})4\alpha = (\alpha + \lambda)[\frac{\pi^2}{6} - \ln^2|\frac{E_F}{\omega_D}| + I_0] + 2[1 + \alpha(\lambda - \alpha)]I_1 + (\lambda - \alpha)I_2 \qquad (3.102)$$

where

$$I_n = \int_0^{\pi} \frac{dx}{\pi} \cos(nx) \ln^2|\frac{2E_F}{\Delta_d \cos x}|, \quad n = 0, 1, 2. \qquad (3.103)$$

Integration can be performed directly and we find

$$I_0 = \frac{\pi^2}{12} + \ln^2|\frac{4E_F}{\Delta_d}|,$$

$$I_1 = \pi,$$

$$I_2 = -\frac{1}{2} - \ln|\frac{4E_F}{\Delta_d}|. \qquad (3.104)$$

Using Eq.(3.104) in Eq.(3.102), we get

$$(\frac{1}{g_s} - \frac{1}{g_d})4\alpha = [\frac{\pi^2 - 1}{4} + 2\pi\lambda + \ln^2\frac{4\sqrt{e}E_F}{\Delta_d} - \ln^2\frac{E_F}{\omega_D}]\alpha + [\frac{\pi^2 - 3}{4} - \ln^2\frac{E_F}{\omega_D} + \ln^2\frac{4E_F}{\sqrt{e}\Delta_d}]\lambda + 2\pi(1 - \alpha^2) \qquad (3.105)$$

If we start out with $g_s = 0$, then Eq.(3.105) has no solution. The pure d-wave phase is confined in the range $0 < g_s < g_{s,min}$ where $g_{s,min}$ satisfies the condition

$$4(\frac{1}{g_s} - \frac{1}{g_d}) - \frac{\pi^2 - 1}{4} - 2\pi\lambda - \ln^2\frac{4\sqrt{e}E_F}{\Delta_d} + \ln^2\frac{E_F}{\omega_D} = 0 \tag{3.106}$$

With the help of Eq.(3.97), Eq.(3.106) can be written as

$$\frac{1}{g_s} - \frac{2}{g_d} = \frac{3}{8} + \frac{1}{2}\sqrt{\frac{4}{g_d} - \frac{\pi^2 - 3}{4} + \ln^2\frac{E_F}{\omega_D}} \tag{3.107}$$

Thus $g_{s,min}$ is given by

$$g_{s,min} = [\ \frac{2}{g_d} + \frac{3}{8} + \frac{1}{2}\sqrt{\frac{4}{g_d} - \frac{\pi^2 - 3}{4} + \ln^2\frac{E_F}{\omega_D}}\ ]^{-1} \tag{3.108}$$

For the case of the pure s-wave, $\alpha \rightarrow \infty$, or $\Delta_d = 0$, in this limit Eq.(3.100), $F[E_F, \omega_D, \alpha \rightarrow \infty, x]$, does not depend on the angular variable. Thus Eq.(3.98) becomes

$$(\frac{1}{g_s} - \frac{1}{g_d})4\alpha = (\alpha + \lambda)[\ \frac{\pi^2}{6} - \ln^2\frac{E_F}{\omega_D} + \ln^2\frac{2E_F}{\Delta_s}\ ] \tag{3.109}$$

At this limit, the orthorhombic distortion effect does not have influences on the pure s-wave phase. Thus λ can be negligible and Eq.(3.109) is reduced to

$$4(\frac{1}{g_s} - \frac{1}{g_d}) = [\ \frac{\pi^2}{6} - \ln^2\frac{E_F}{\omega_D} + \ln^2\frac{2E_F}{\Delta_s}\ ] \tag{3.110}$$

By using Eq.(3.94), we obtain

$$g_{s,max} = g_d/2 \tag{3.111}$$

Eq.(3.111) shows that the pure s-wave phase starts out at $g_{s,max}$.

Therefore we can see from Eq.(3.108) that, $g_{s,min}$, the pure d-wave solution exists at $0 < g_s < g_{s,min}$, while the pure s-wave solution, Eq.(3.111), exists at $g_s > g_{s,max}$. Since $g_{s,min} < g_{s,max}$, then the intermediate region $g_{s,min} < g_s < g_{s,max}$, belongs to the mixed (s+d)- wave. In an intermediate region, $g_{s,min} < g_s < g_{s,max}$, both phases exist together.

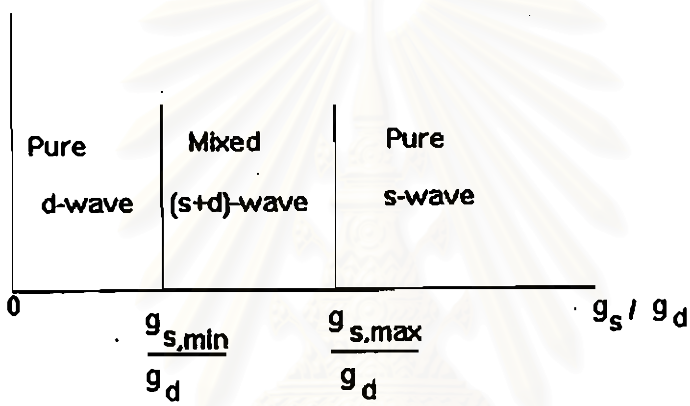

Figure 3.1: The phase diagram shows the existence of the mixed (s+d)-wave in the Van Hove singularity superconductor, here $g_{s,min} < g_s < g_{s,max}$, where $g_{s,min}$ and $g_{s,max}$ are given by Eqs.(3.107) and (3.111), respectively.