Chapter 2

Theories of Superconductivity

BCS Theory

The theory of Bardeen, Cooper and Schrieffer (BCS) in 1957 (13), is a model Hamiltonian set up to explain characteristics of the superconducting state that have been already mentioned in Chapter I. In this theory it is assumed that there exist conduction electrons, which are fermions, in superconductors. These electrons are well described by the band theory and consequently they have Fermi surface. An attractive force among conduction electrons combines two electrons with momenta $\vec{p}$ and $-\vec{p}$ into a Cooper pair. A Cooper pair which consists of two fermions behaves like a boson and the Cooper pairs exhibit the Bose condensation in which all the pairs have zero centre-of-mass momentum. This state of many-fermion system exhibits the superconductivity. The electron-lattice interaction is the origin of the attractive force which combines the electrons to form the Cooper pairs. The pair of states $(\vec{k}, -\vec{k})$ is occupied coherently. The Cooper-pair amplitude which is zero by number conservation in the normal state, becomes finite below T_c. The simplest model (39) which permits such behavior is given by the BCS "reduced" Hamiltonian, $\mathcal{H}_o + \mathcal{H}_{red}$, where

$$\mathcal{H}_o = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} \quad , \tag{2.1}$$

$$\mathcal{H}_{red} = -\sum_{k,k'}{}' V_{k',k}(c^{+}_{-k\downarrow}c^{+}_{k\uparrow})(c_{k'\uparrow}c_{-k'\downarrow}) \qquad (2.2)$$

The operator $c_{k\sigma}$ and $c^{+}_{-k\sigma}$ destroys and creates an electron in a Bloch state $k\sigma$ of energy ϵ_k, respectively (measured relative to the chemical potential μ), k is short for k_n (wave number and band index). Interaction (2.2) contains terms that scatter pairs of electrons from one pair state $(k\uparrow,-k\downarrow)$ to a different one $(k'\uparrow,-k'\downarrow)$.

In reality terms also exist that scatter only one of paired electrons , these complicate the Cooper-pair phenomena and they have been omitted. The interaction matrix elements $V_{k',k}$ are at this stage unspecified. Bardeen, Cooper and Schrieffer had in mind the Fröhlich or Bardeen-Pines (40) effective phonon-induced interaction. Because of the minus sign in Eq.(2.2), a positive $V_{k',k}$ corresponds to an attractive interaction.

The BCS solution of this Hamiltonian is exact in the thermodynamic limit and can be derived in many ways. In Gor'kov's Green's function method (41), the field operators c_k are written in the Heisenberg picture, except that time t is replaced by an imaginary time $-i\tau$:

$$c_{k\sigma}(\tau) = e^{\mathcal{H}\tau} c_{k\sigma} e^{-\mathcal{H}\tau} \qquad (2.3)$$

Thermodynamic averages are denoted by

$$\langle A\rangle = Z^{-1}\mathrm{tr}(e^{-\beta\mathcal{H}}A), \qquad (2.4)$$

where Z is $tr(e^{-\beta\mathcal{H}})$ and $\beta=1/Tk_B$. This is actually a grand canonical average. The operator $\mathcal{H}$ implicitly contains the term $-\mu N$ and the trace runs over states with all values of N. Units are used where $\hbar = k_B = 1$. The reason for an imaginary time variable is the similarity of $e^{-\mathcal{H}\tau}$ and $e^{-\mathcal{H}t}$. The Green's function is defined for τ in the range $(-\beta,\beta)$ as

$$G(k,\tau) = -\langle c_{k\sigma}(\tau)c^{+}_{k\sigma}(0)\rangle\theta(\tau)+\langle c^{+}_{k\sigma}(0)c_{k\sigma}(\tau)\rangle\theta(-\tau) \qquad (2.5)$$

where $\theta(\tau)$ is 1 for positive τ and 0 otherwise. This can be written in a concise notation

$$G(k,\tau) = -\langle T_\tau c_{k\sigma}(\tau)c^{+}_{k\sigma}(0)\rangle. \qquad (2.6)$$

where T_τ is the Wick operator, which reorders the operators following it in such a way that τ increases from right to left. Whenever two fermion operators are interchanged in the process, a factor of -1 is introduced. For noninteracting electrons (Hamiltonian $=\mathcal{H}_o$)Eq.(2.6) can be directly evaluated,

$$G_o(k,\tau) = e^{-\epsilon_k\tau}[f_k\theta(-\tau)-(1-f_k)\theta(\tau)], \qquad (2.7)$$

where $f_k = \langle c^{+}_{k\sigma} c_{k\sigma}\rangle_o$ is the Fermi function, $(e^{\beta\epsilon_k}+1)^{-1}$. Within the range $-\beta<\tau<\beta$ Eq.(2.6) has the antiperiodicity property

$$G(k,\tau+\beta) = -G(k,\tau) \qquad (2.8)$$

This property is used as the definition for G outside the range $(-\beta,\beta)$. It follows that G has a Fourier representation

$$G(k,\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}G(k,i\omega_n) , \tag{2.9}$$

$$\omega_n = (2n+1)\pi T , \tag{2.10}$$

where only odd integers 2n+1 appear in the "Matsubara frequencies" $i\omega_n$.

The Fourier coefficients $G(k,i\omega_n)$ are given by inverting Eq.(2.9),

$$G(k,i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau e^{i\omega_n\tau}G(k,\tau). \tag{2.11}$$

For noninteracting electrons, using Eqs.(2.7) and (2.11).

$$G_o(k,i\omega_n) = (i\omega_n-\epsilon_k)^{-1}. \tag{2.12}$$

The analytic continuation of $G(k,i\omega_n)$ to complex values of z, G(k,z), contains full information about the time-dependent thermal Green's function. Furthermore, thermodynamic properties of the systems can be evaluated once the Green's functions $G(k,i\omega_n)$ are known.

To evaluate $G(k,i\omega_n)$ for the BCS model, we calculate the derivative of $G(k,\tau)$, using Eq.(2.1)-(2.5)

$$(-\frac{d}{d\tau}-\epsilon_k)G(k,\tau) = \delta(\tau)-\sum_{k'} V_{k,k'}\langle T_\tau c^{\dagger}_{-k\downarrow}(\tau)c_{k'\uparrow}(\tau)c_{-k'\downarrow}(0)c^{\dagger}_{k\uparrow}(0)\rangle \tag{2.13}$$

The complicated thermal average on the right-hand side of Eq.(2.13) is evaluated using a mean-field argument. In Hartree-Fock mean-field theory, using the Wick's theorem (42), the ensemble averages like $\langle c_1^+ c_2^+ c_3 c_4 \rangle$ are approximated by $\langle c_1^+ c_4 \rangle \langle c_2^+ c_3 \rangle - \langle c_1^+ c_3 \rangle \langle c_2^+ c_4 \rangle$ in the hope that the fluctuations $\langle AB \rangle - \langle A \rangle \langle B \rangle$ are unimportant. However the BCS theory requires a nonzero pair amplitude $\langle c_{k\uparrow} c_{-k\downarrow} \rangle$, namely the possibility that two electrons of opposite spins can form a self-bound Cooper pair. As a model for this phenomenon, we add two extra terms representing the pairing amplitude:

$$\begin{aligned} \langle c_1^+ c_2^+ c_3 c_4 \rangle \approx & \langle c_1^+ c_4 \rangle \langle c_2^+ c_3 \rangle - \langle c_1^+ c_3 \rangle \langle c_2^+ c_4 \rangle \\ & + \langle c_1^+ c_2^+ \rangle c_3 c_4 + c_1^+ c_2^+ \langle c_3 c_4 \rangle \end{aligned} \tag{2.14}$$

Therefore we have the following approximation

$$\langle T_\tau c_{-k\downarrow}^+(\tau) c_{k\uparrow}(\tau) c_{-k\downarrow}(0) c_{k\uparrow}^+(0) \rangle \approx \langle T\, c_{k\uparrow}(\tau) c_{-k\downarrow}(0) \rangle \langle T\, c_{-k\downarrow}^+(\tau) c_{k\uparrow}^+(0) \rangle . \tag{2.15}$$

The other Hartree-Fock-like terms on the right-hand side of Eq.(2.15) are zero unless $\bar{k}=k$, which is an unimportant case. Also, the band energy already includes Hartree-Fock energies, so it would be incorrect to include them again on the right-hand side of Eq.(2.15).

The Gor'kov "anomalous" Green's functions are now defined

$$F(k,\tau) = -\langle T_\tau c_{k\uparrow}(\tau) c_{-k\downarrow}(0) \rangle \tag{2.16}$$

$$F^+(k,\tau) = -\langle T_\tau c_{-k\downarrow}^+(\tau) c_{k\uparrow}^+(0) \rangle \tag{2.17}$$

A careful inspection reveals that these are complex conjugates of each other

$$\overset{+}{F}(k,\tau) = F(k,\tau)^{*} \tag{2.18}$$

Then, using Eqs.(2.15)-(2.17), Eq.(2.14) becomes

$$(-\underline{d}-\epsilon_k)G(k,\tau) = \delta(\tau)-\sum_{k} V_{k,k'}F(k,0)\overset{+}{F}(k,\tau) \tag{2.19}$$
$$d\tau$$

An equation of motion for $F(k,\tau)$ is next generated by similar precedures, giving

$$(-\underline{d}+\epsilon_k)\overset{+}{F}(k,\tau) = -\sum_{k'} V_{k,k'}\overset{+}{F}(k',0)G(k,\tau). \tag{2.20}$$
$$d\tau$$

These are coupled nonlinear differential equations whose solution gives BCS theory. The solution is accomplished by extracting the factor

$$\Delta_k = \sum_{k'} V_{k,k'}F(k',0) \tag{2.21}$$

This will turn out to be the BCS energy gap. It will be treated as an unknown complex parameter that must be constructed self-consistently at the end. Next Eqs.(2.19) and (2.20) are Fourier transformed and we get

$$\begin{bmatrix} i\omega_n-\epsilon_k & \Delta_k \\ \Delta_k & i\omega_n+\epsilon_k \end{bmatrix} \begin{bmatrix} G(k,i\omega_n) \\ F(k,i\omega_n) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{2.22}$$

The determinant of the matrix is $-(\omega_n^2+\epsilon_k^2+|\Delta_k|^2)$ which never vanishes. The combination $\epsilon_k^2+|\Delta_k|^2$ is denoted by

$$E_k^2 = \epsilon_k^2 + |\Delta_k|^2 \tag{2.23}$$

Inverting Eq.(2.22) gives the result

$$G(k,i\omega_n) = (-i\omega_n-\epsilon_k)/(\omega_n^2+E_k^2) \tag{2.24}$$

$$F^{+}(k,i\omega_n) = \Delta_k^{*}/(\omega_n^2 + E_k^2) \tag{2.25}$$

In the limit $\Delta_k \to 0$, the normal state solution $G = (i\omega_n-\epsilon_k)^{-1}$, $F^{+}=0$ is retrieved. The parameter E_k can be interpreted as a quasi-particle energy with Δ_k as an energy gap, because G(k,z) given by Eq.(2.24) has poles at $z_o = \pm E_k$.

Finally, Δ_k must be constructed self-consistently. The F function is computed using the Fourier representation of Eq.(2.10)

$$F(k,T=0) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} F(k,i\omega_n). \tag{2.26}$$

Therefore Eq.(2.21) is written as

$$\Delta_k = \frac{1}{\beta}\sum_{k'}\sum_{n=-\infty}^{\infty} \frac{V_{k,k'}\Delta_{k'}}{\omega_n^2+E_{k'}^2} \tag{2.27}$$

This is the BCS gap equation (43). The more familiar version,

$$\Delta_k = \sum_{k'} V_{k,k'} \Delta_{k'} \tanh(E_{k'}/2k_BT) \qquad (2.28)$$

follows from the identity

$$\sum_{n=-\infty}^{\infty} [(2n+1)^2\pi^2 + a^2]^{-1} = (2a)^{-1}\tanh(a/2) \qquad (2.29)$$

This identity can be derived from the Poisson sum formula (40). BCS theory gives a famous formula for T_c

$$T_c = 1.13\omega_D \exp(-1/N(E_F)V) \qquad (2.30)$$

here ω_D is the Debye cutoff frequency and $N(E_F)$ is the density of states at the Fermi level.

BCS theory explains satisfactorily many properties of conventional superconductors.

Very soon after the discovery of the high T_c copper oxides by Bednorz and Müller, a widely held opinion was that such large values of the superconducting critical temperature T_c could not be explained by a phonon induced attractive mechanism, at least within the framework of a weak coupling theory of the BCS type (13). This opinion is founded on the well known BCS expression of T_c,

$$k_BT_c = 1.13\hbar\omega_D \exp(-1/\lambda) \qquad (2.31)$$

where ω_D is the Debye pulsation and $\lambda = VN(E_F)$ is the product of

the phonon induced attractive coupling constant between the electrons and the electronic density of states $N(E_F)$ at the Fermi energy E_F. As the BCS theory is a weak coupling theory, which is valid only when the effective coupling constant is much smaller than unity, the formula (2.31) gives a value of T_c which is much smaller than the Debye temperature $T_D = h\omega_D/k_B$, and thus it could hardly explain the large values of T_c which are observed at least in the most recently discovered copper oxides, as for instance $YBa_2Cu_3O_7$, $Bi_2Sr_2CaCuO_8$, $Tl_2Ba_2CaCu_2O_8$ or $Tl_2Ba_2Ca_2Cu_3O_{10}$, whose T_c is of the order of 100 K.

Theories of High Temperature Layered Superconductors.

The expression (2.31) of T_c holds only when the electronic density of states N(E) has a nearly constant value in the whole energy range from $E_F-\hbar\omega_D$ to $E_F+\hbar\omega_D$, as it is actually the case in most of the superconductors with a tridimensional structure, where the variation of N(E) versus E is very smooth in a large neighbourhood of E_F.

On the contrary, in structures with a lower dimensionality, there exist sharp van Hove singularities in the density of states N(E), and if E_F lies very close to such a singularity, the expression (2.31) is no longer valid, even in the weak coupling limit. Instead, one finds, in that case, a new expression of T_c which is much less sensitive to the cutoff energy $\hbar\omega_D$. The calculated value of T_c is largely enhanced by the fact that the number of electronic states which accumulate in the neighbourhood of E_F is much larger than in the tridimensional case.

Labbe and Bok's Model

Based on this idea J.Labbe and J.Bok(44) (L.B.) have proposed a two dimensional model for the electronic structure of a CuO_2 sheet. As mentioned above, a 2D electronic band always shows a logarithmic singularity in the density of states (45). Assuming that the Fermi level lies near this singularity and using the BCS theory (13) (in the limit of weak coupling), L.B. obtained the following formula for T_c,

$$T_c = T_o \exp(-1/\lambda) \qquad (2.32)$$

where T_o is a characteristic energy of the problem, or Debye temperature for the electron-phonon interaction, and for one sheet,

$$\lambda = \lambda_o = VN(E_F)$$

where $N(E_F)$ is the density of states at the Fermi level averaged over the width of the singularity, and V is the constant attractive matrix element between electron-pairs.

For n sheets, L.B assumed that the interaction V is the same for n coupled layers as for one layer, $\lambda = n\lambda_o$. The L.B formula (2.32) gives for an n-layer sheet,

$$T_c = T_o e^{-1/\sqrt{n\lambda_o}}$$

or

$$\ln(T_c/T_o) = -\frac{1}{\sqrt{n}}\,\frac{1}{\sqrt{\lambda_o}} \qquad (2.33)$$

They plotted a graph between ln T_c and $1/\sqrt{n}$ as shown in Fig. 2.1. They found that the formula (2.33) fits the experiments remarkably well, with

$$\lambda_o = 0.14$$

and $$T_o = 566\ K \approx 600\ K$$

which are reasonable values already obtained in high T_c compounds.

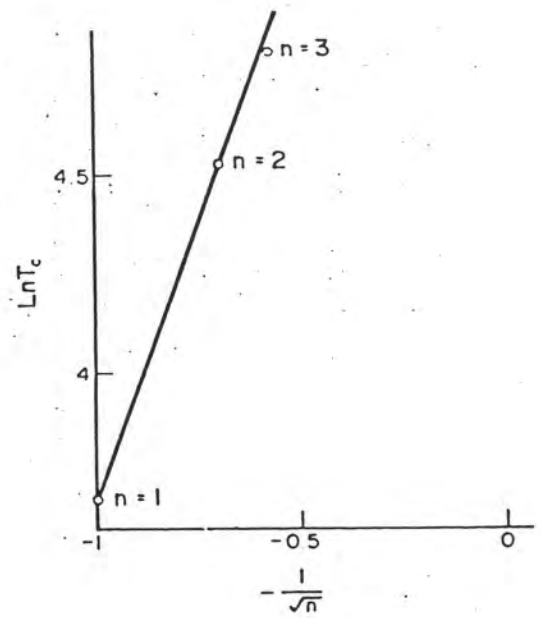

Fig. 2.1 lnT_c versus $-(1/\sqrt{n})$, number of CuO_2 adjacent planes in the unit cell (44).

circle : experimental values

full line : theoretical curve

Ihm and Yu's Model

In view of the fact that most superconducting copper oxides have a layered structure made of weakly coupled CuO_2 planes, or families of CuO_2 planes in the case of the multiple layered structures, J.Ihm and B.D. Yu (46) have shown that the dependence of T_c on the number of layers in the unit cell of high-T_c thallium compounds is quantitatively explained within the BCS framework, irrespective of the precise mechanism responsible for pairing.

In Ihm and Yu's model, it has been assumed that the pairing interaction within a CuO_2 layer is strong enough to exhibit superconductivity by itself and a weak interlayer interaction enhances T_c further. They predicted the limit of T_c attainable by stacking more CuO_2 layers ($n\to\infty$), to be no more than 150 K (providing each layer has the same density of states).

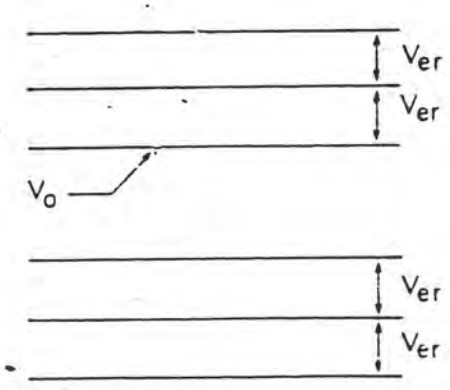

Fig. 2.2 Schematic diagram of the coupling interactions in Ihm and Yu's model for n=3. Each horizontal line presents a CuO layer. V_a exists in each layer (46).

Applying the standard Bogoliubov transformation, they obtained a T_c equation

$$kT_c \cong 1.13\hbar\omega \exp(-F) \qquad (2.34)$$

where $F = 1/(\lambda_a + p(n)\lambda_{er})$ and $\lambda_a = NV_a$, $\lambda_{er} = NV_{er}$, the geometrical factor $p(n) = 0, 1, \sqrt{2}, (\sqrt{5}+1)/2$, 3 and 2 for n=1,2,3,4,5, and ∞ , respectively, N is the density of states.

In Tl compounds, the reported (47) T_c's were $\approx$ 80, 108 and 125 K for n=1, 2 and 3, respectively. Ihm and Yu varied $\hbar\omega$ in a wide range and obtained λ_a and λ_{er} which fitted the measured T_c's. Results are presented in Table 2.1 for $\hbar\omega$ = 0.1 and 0.2 eV.

$\hbar\omega$ (eV)	λ_a	λ_{er}	n=1 T_c (K)	n=2 T_c (K)	n=3 T_c (K)	n=4 T_c (K)	n=5 T_c (K)	n$\rightarrow\infty$ T_c (K)
0.1	0.356	0.049	80	111	125*	132	136	145
0.1	0.339	0.060	70	108*	125*	133	138	150
0.2	0.277	0.036	71	108*	125*	134	139	151

TABLE 2.1 The calculated T_c for $Tl_2Ca_{n-1}Ba_2Cu_nO_x$ and the parameters used in Eq.(2.34). In each row $\hbar\omega$ is first chosen and λ_o and λ_{er} are determined to fit experimental values (*)(46).

An interesting question is how far T_c can go up as n increases, as shown in table 2.1, Ihm and Yu got $T_c \approx 138$ K for n=5,

and 150 K for a large n limit. Therefore, their model makes a pessimistic prediction that fabricating higher n compounds, even if successful, does not enhance T_c much further (unless λ_a or λ_{er} is strengthened simultaneously). In any case, as the prefactor increases from the phonon energy to near the Fermi energy of the carriers, relatively weak coupling parameter λ_o and λ_{er} are capable of accounting for T_c as high as 125 K.

Recently M.Crisan and D.Vacaru (48) calculated the dependence of the critical temperature of the layered high-T_c materials as a function of the distance between layers. Using the BCS model they considered the influence of the neighbour layers on CuO_2 layer. In their calculation they used the layered electronic gas approach, and considered the main contribution to be given by the screened Coulomb interaction between neighbouring layers.

Their equation for the critical temperature is of the form

$$T_c = \omega_o \exp(-1/\Lambda(d)) \qquad (2.35)$$

where $\Lambda(d)$ is the effective coupling constant which depends on "d", the distance between the layers. In a model of ν layers they obtained the critical temperature as

$$\ln(T_c(\nu)/T_o) = \ln(\omega_o/T_o) + \ln[1+\rho_\nu e^{-\delta}] - \left[\lambda - \frac{\mu - ce^{-\delta}}{1+\chi(\mu-ce^{-\delta})}\right]^{-1} \qquad (2.36)$$

where T_o=1 K and ρ_ν, c are constants, $\chi = \ln E_F/\omega_o$, E_F being the Fermi energy and ω_o the energy cut-off, λ is the electron-phonon coupling constant times the density of states.

μ, the Coulomb potential, is given by

$$\mu = \frac{N}{\pi} \int_0^{2k_o} \frac{dq}{(4k_o^2 - q^2)} \; V(q, \omega = 0)$$

$q = (q_x, q_y)$, k_o is the Fermi wave vector, N the density of states near the Fermi energy in a 2D electronic system. $V(q, \omega = 0)$ is the Fourier transform of the potential V.

This relations shows that $T_c = T_c(\nu, d)$ represents a family of curves determined by "d" which are characteristic for each superconductor.

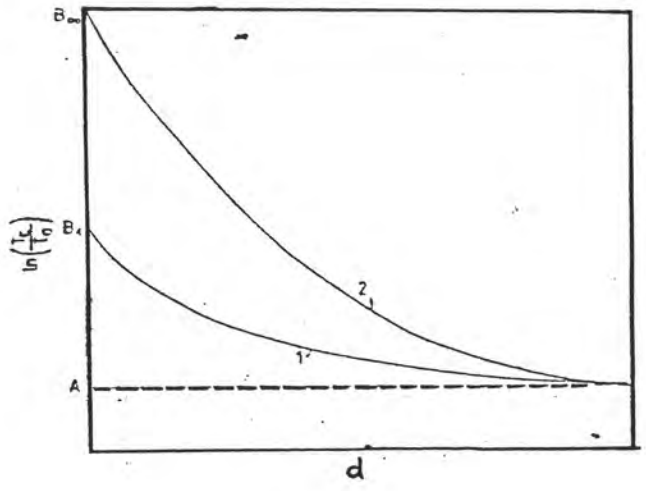

Fig. 2.3 The dependence of T_c on d, the interlayer spacing. The curve 1 corresponds to one set of layers and the curve 2 to infinite set of layers (48).

The most important result of this paper is the decreasing of the calculated critical temperature with the increasing of the interlayer spacing, and the increasing of the critical temperature with the number of layers per unit cell. Their conclusion is identical with that obtained by Schneider and Baeriswyl (49).

Wheatley, Hsu and Anderson's Model

To Wheatley et.al (50), superconductivity in the high-T_c materials is interpreted as the condensation of hole bosons. Coherent interlayer tunneling of boson pairs results in order -parameter equations which are quite different from those of the Bardeen-Cooper-Schrieffer theory.

By considering the free bosons with weak dispersion along the c axis, and the presence of Josephson-like coupling between the layers, they considered processes contributing to interlayer conductance which came from spinons and holons in the layers, and by allowing interlayer pair hopping to form a paired state from this holon gas, their model predicts that T_c is proportional to doping, and if the Josephson pair mechanism dominates, one would expect that T_c is an increasing function of the c-axis conductance and carrier concentration.

Schneider and Baeriswyle's Model

Schneider and Baeriswyle (49) suggested a model for layer superconductor with single electron interlayer tunneling. They investigated the model for layered superconductors with single-electron interlayer tunneling and a unit cell containing an

arbitary number of sheets. For an effective pairing of two-dimensional origin, T_c is found to be independent of the layer spacing. However, pairing of three-dimensional nature, allowing for spacing dependent coupling strength, fits remarkably well the observed climb in T_c for the Bi-O and Tl-O layered systems, as the number of CuO_2 planes in the unit cell is increased from two to four and six. This agreement points to a weak coupling pairing mechanism of three-dimensional origin.

They describe the electron band structure by the Hamiltonian

$$\mathcal{H}_o = \sum_{l,n,n',\sigma} E_{//}(R_n - R_{n'}) C^{+}_{nl\sigma} C_{n'l\sigma} - \sum_{l,n,\sigma} t_l (C_{nl\sigma} C_{nl+1\sigma} + h.c.) \qquad (2.37)$$

where l labels the layers, R_n the lattice sites within the sheets and energies are measured with respect to the chemical potential. They assumed a periodic sequence of layers with m sheets per period of length c, as depicted in Fig.(2.4), and a square lattice with lattice constant a within the sheets.

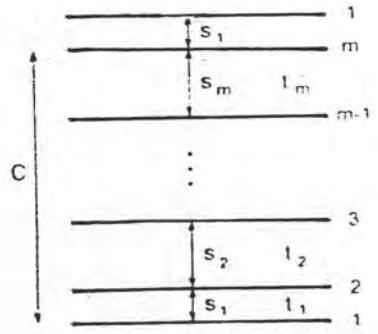

Fig. 2.4 Schematic sketch of the layered unit cell. s_n is the spacing between layer n and n+1 coupled by single-particle tunneling of strength t_l, $c = s_1 + s_2 + \ldots + s_m$ is the lattice constant in the z-direction (49).

By applying the de Gennes's mean-field treatment (51) for an inhomogeneous order parameter, they obtain a BCS-type equation for T_c,

$$T_c \approx 1.13\Theta\exp[-(1/N_{||}(0)a^2 g(s))], \qquad (2.38)$$

where N(0) denotes the density of states within a layer, g(s) is an attractive coupling strength, and a is a constant.

Current experimental values for two, four and six CuO_2 layers per unit cell in the Bi-O and Tl-O materials, are summarized in Table 2.2.

Tl-Cu-Ba-Cu oxides			
m	2	4	6
c(Å)	28	29.6	36.2
T_c(K)	20	105	125
Bi-Sr-Ca-Cu oxides			
m	2	4	6
c(Å)	24.5	31	37
T_c(K)	22	85	110

Table 2.2 Measured T_c values for compounds of the Tl-O and Bi-O family containing m=2,4 and 6 CuO_2 layers per unit cell, and values for the c lattice parameter (49).

To compare these data with the prediction of their model, they plotted $\ln(T_c/T_o)$ versus $s^{2/3}$.

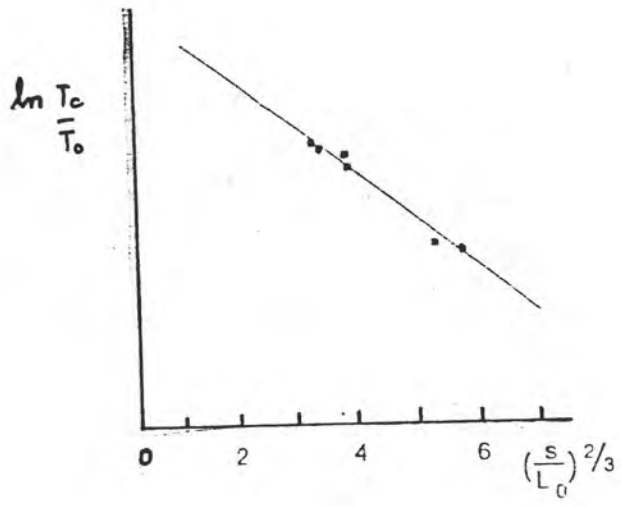

Fig. 2.5 $\ln(T_c/T_o)$ versus $s^{2/3}$. s denotes the mean layer spacing, T_o=1 K, L_o=1 °A. Squares correspond to experimental values taken from Table 2.2 for m=2,4 and 6 CuO_2 layers in the Bi-O and Tl-O family (49).

Birman and Lu's Model

Birman and Lu (52) used a phenomenological model with coupled parameters to study polytype multilayer systems, and demonstrated that polytypism can increase T_c. Explicit expressions and results are given for $T_c(N)$ where N is the polytype number ($N=2,3,\ldots,\infty$). Classes of structures investigated are monolayer polytypes such as $[-(CuO_2)_N-]$, bilayer TlO polytypes such as $[-TlOTlO(CuO_2)_N-]$, and monolayer TlO polytypes, and 1:2:3 polytypes such as $[-(CuO_2)(CuO-CuO)_n-]$. Two types of nearest-layer bilinear

coupling were studied: weak link (Josephson) and spin-spin. Polytypism is predicted to increase T_c in all classes. For the same N, monolayer TlO polytypes have lower T_c than the bilayer TlO analog. Using reasonable values of parameters they predicted a maximum T_c of 140 K in the monolayer and bilayer TlO series.

Birman and Lu introduced a simple model for the copper oxide high-T_c superconductors based on Ginzburg-Landau theory in the homogeneous Landau approximation. The model utilized the assumption that in each of the classes of materials considered there are active entities to which an ordered parameter should be assigned. A common active entity in the systems considered is the CuO_2 plane. The transition temperature T^* is obtained by extremizing the free energy, and is the maximum eigenvalue of a certain determinant for that structure.

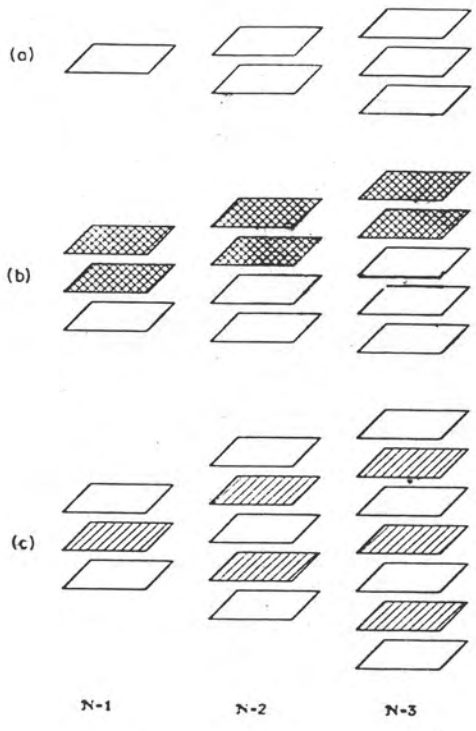

Fig. 2.6 Model for polytypes of different classes.

Polytypes N=1,2,3 are illustrated (52).

(a) Monolayer polytypes, the basic layer in taken as a CuO_2 layer.

(b) Polytypes of the bilayer TlO types in the TlBa class.

(c) Polytypes of 1:2:3 class.

The layers with filament are the layers of CuO chains, the open squares are CuO_2 layers.

$T^*(N)$ for TlBa class						
Number N	1	2	3	4	5	..... ∞
Experiment	80 K	110 K	125 K			
Theory			123 K	129 K	133 K	..... 141 K

Table 2.3 Transition temperature for monolayer polytypes $-(CuO_2)_N-$ (52).

Number	$-[TT(C)_N]$-class $T^*(N)$		$-[T(C)_N]$-class $T^*(N)$	
N	Experiment	Theory	Experiment	Theory
1	85 K	88 K	not available	56 K
2	110 K	112 K	85 K	96 K
3	125 K	121 K	110 K	112 K
4		124 K	122 K	120 K
.				
.				
∞		136 K		136 K

Table 2.4 Transition temperature for polytypes of the TlBa class. The table gives predicted transition temperatures $T^*(N)$ for polytypes of bilayer TlO (TT) and monolayer TlO members (T) of the TlBa class, with N sheets of CuO_2 ($(C)_N$) (52).

Their major results and predictions in the framework of the coupled order parameter model are as follows:

(1) In the TlBa classes, for reasonable values of parameters, the model accounts for experimental T_c, and 95 % of the maximum possible T^* is reached for polytype N=5.

(2) The monolayer Tl0 compounds $[T(c)_N]$ have lower T^* than corresponding bilayer Tl0 $[T(c)_N]$.

(3) The maximum possible T^* for the monolayer Tl0 and bilayer Tl0 classes is $T^*(\infty) \approx 140$ K.

It is to be noted that in almost all of the papers, the influence of the insulating layers was completely neglected. In view of the fact that excitation from the neighbour layers should have a strong influence on the interactions in a Cu-O layer and vice versa, the role of "insulating" layer in high-T_c compound when it posseses a nonzero superconductivity should be investigated. It is therefore interesting to study the role of intermediary layer in high-T_c oxide superconductors by using a simple model of inter- and intra-layer coupling based on the BCS theory of layered superconductors to calculate the transition temperature of a number of layered systems.

Both the mechanisms of direct hopping and pair tunneling between active layers will be incorporated in the model. The dependence of superconducting transition temperature upon the layer parameters will be investigated in the next chapter.