THE INTERLAYER PAIR HOPPING MECHANISM OF HIGH TEMPERATURE SUPERCONDUCTIVITY

by

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CERTIFICATE

This is to certify that the Ph.D. thesis titled *The Interlayer Pair Hopping Mechanism of High Temperature Superconductivity* submitted by *V. N. Muthukumar* is a record of bonafide research work done under my supervision. The research work presented in this thesis has not formed the basis for the award to the candidate of any Degree, Diploma, Associateship, Fellowship or other similar titles. It is further certified that the thesis represents independent work by the candidate and collaboration was necessitated by the nature and scope of the problems dealt with.

G. Baskaran

April 1993

Thesis Supervisor

Abstract

In this thesis, we undertake a theoretical study of the interlayer pair hopping mechanism of high temperature superconductivity. Any theory claiming to explain high transition temperatures in the Cu-O based compounds has to account for the anomalous normal state observed experimentally in these materials. Accordingly, in chapter 1, we review a few well known experimental facts and argue these can be reconciled with the assumptions that (a) the low energy excitations in the normal state are spin-charge decoupled and (b) the conducting state above T_c is two dimensional. We then review observed T_c systematics in the Bi family of high T_c superconductors and show how interlayer hopping can account for this. In chapter 2, we review some basic notions of RVB theory. Our main results are presented in chapters 3, 4, 5 and 6. Chapter 3 concerns the origins of the pair hopping mechanism. In this chapter, we present a simple microscopic derivation of the effective hamiltonian describing pair hopping. We examine how a system of noninteracting spinons and holons responds to a weak interlayer coupling $t_\perp$ and show that physical processes involving holon pair hopping (between the coupled layers) are generated. In chapter 4, we discuss the limitations of working with the effective hamiltonian for the holons. We present a model hamiltonian for pair hopping and obtain a gap equation which is different from the BCS equation. We study the momentum and temperature dependence of the gap in detail. We see that the gap remains constant almost upto T_c and then falls steeply. To illustrate this peculiar behaviour, we calculate the Josephson current between two superconductors and obtain results in good agreement with experiment. Chapter 5 contains some exact results for finite size clusters.

We show that inplane superconducting correlations are established and enhanced by the interlayer coupling $t_\perp$. We also show that if the constraint on double occupancy (arising from the large U) is relaxed, these correlations decrease with $t_\perp$. These results demonstrate the importance of strong correlation *vis a vis* pair hopping. We address this issue again in chapter 6 where we show if single electron hopping between the layers were not blocked, T_c would actually decrease with $t_\perp$. Finally, we discuss how single electron hopping (between the coupled Cu-O layers) acts as a pair breaking mechanism and examine its effect on the superconducting gap.

To Podā - with fond remembrance

and

To Ramu, Kali - Adios, amigos !

Acknowledgements

This thesis is based on ideas developed by many people, particularly, P. W. Anderson, G. Baskaran, T. C. Hsu, J. M. Wheatley and Z. Zou.

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Finally, I wish to thank my friends Ananda, Rahul, Ramakrishnan, Subbudu, Sundar, Venkat and Vythee for hours of unadulterated fun at Matscience.

காண முயலெய்த அம்பினில் யாணை
பிழைத்தவே லேந்த லினிது

-குறள்

To hold a spear which hath missed a tusker is to fare
Much better than to hold a dart that's killed a forest hare.

-Kural

Contents

Chapter 1

Introduction

The phenomenon of high temperature superconductivity obseved in Cu-O based compounds continues to be one of the outstanding problems in condensed matter physics. The primary reason for this is that any candidate theory claiming to explain high transition temperatures has necessarily to account for the anomalous normal state of these compounds. Since the discovery of these compounds, a variety of experiments have been done to study the normal state. From these experimental results, it is becoming increasingly evident that the normal state of the ceramic superconductors is *not* a Fermi liquid and the physics can well be described by a one band large U Hubbard model [1]. This has been the mainstay of the Resonating Valence Bond (RVB) theory developed by Anderson and collaborators [2], [3]. Hence it is desirable to study the mechanism of high temperature superconductivity within the framework of the RVB theory. The first step in this direction was taken by Wheatley, Hsu and Anderson (WHA) [4] who proposed the interlayer pair hopping mechanism of high temperature superconductivity.

In this thesis, we study the origins and some consequences of this mechanism. Since the large U Hubbard model (in two dimensions) is yet to be solved, we cannot claim to have a complete theory of the superconducting state. Our aim is to show

that the WHA mechanism is *consistent*, both with our understanding of the large U Hubbard model as well as many experimental results, if not complete.

The WHA mechanism proposes that superconductivity in the cuprates is due to the coupling between Cu-O layers. The interlayer coupling causes pairs of electrons to hop between the coupled layers and this, in turn, causes three dimensional superconducting order. This mechanism is peculiar to the cuprate superconductors, i.e., it cannot be envisaged in materials that behave like conventional Fermi liquids. More precisely, the WHA mechanism is an extension of the physics of a large-U Hubbard model. Indeed, the most attractive feature of the RVB scenario is that the anomalous normal state, superconductivity and high transition temperatures are all intimately related to one another.

The idea of interlayer pair hopping as a mechanism of superconductivity is built on the following important notions:

- The normal state of the cuprate superconductors is a non Fermi Liquid.
- Single electron hopping between the Cu-O layers is suppressed.
- T_c is governed primarily, if not solely, by the interlayer coupling.

In this introductory chapter, we argue that most of the available experimental results can be reconciled with these notions.

1.1 The normal state

The very need to formulate a theory of superconductivity which is different from the conventional BCS theory arises from the experimentally observed *normal state*

properties of the cuprate superconductors. This is because the BCS theory of superconductivity presupposes that the normal state is a Fermi liquid, i.e., one in which the quasiparticles have the same quantum numbers as electrons. Therefore, the non-interacting Fermi system is a good zeroth order approximation of the normal state and interactions can be analysed by perturbation theory. The quasiparticle excitation is related to the bare electron by the wave function renormalization constant Z_k, which is defined by

$$Z_k \;=\; \mid 1 - \frac{\partial}{\partial \omega}\, \mathrm{Re}\Sigma(k,\omega) \mid^{-1}_{\omega = E_k - \mu} ,$$

where $\Sigma(k,\omega)$ is the self energy of the interacting system and E_k is the quasiparticle energy. Z_k is directly related to the strength of the quasiparticle peak as can be seen from the expression for the single particle Green's function

$$G(k,\omega) \;=\; \frac{Z_k}{\omega - (E_k - \mu)} + \text{ incoherent part.}$$

(Z_k is the fraction of amplitude in, say, photoemission spectroscopy that appears in the peak associated with the quasiparticle. Another measure of Z_k is the discontinuity observed in occupancy n_k at the Fermi level k_f. If Z_k is zero, the quasiparticle picture is inadequate to describe the physics and Fermi liquid theory fails.) Superconductivity is caused by some mechanism (not necessarily due to phonons) that causes an attractive force between these quasiparticles. This leads to pair condensation at low temperatures. However, in the cuprate superconductors, there is strong experimental evidence to suggest that the normal state is not a Fermi liquid. This then invalidates the basis of the standard BCS theory and necessitates a different formalism. So we now review some of the well established facts.

1.1.1 Planar resistivity

One of the most striking features of the normal state of the Cu-O superconductors is the inplane resistivity, ρ_{ab}. It is linearly dependent on temperature from fairly high temperatures (700 K) down to the superconducting transition temperature, T_c. This is so even when $T_c \sim 10$ K (in the Bi 2201 compound). This behavior is generic and material independent. (See [5] for a review.) This then implies that the transport relaxation rate (i.e., the lifetime of charge carriers), τ, is proportional to T^{-1}, T being the temperature. This fact is further confirmed by infrared conductivity [6] studies. Such a result is inconsistent with the normal state being a Fermi liquid for which $\tau \propto T^{-2}$ in three dimensions and $(T^2 \ln T)^{-1}$ in two dimensions. Recall that τ is the lifetime due to electron-electron scattering. Electron-phonon scattering does cause $\tau \propto T^{-1}$ but this happens only at temperatures $T \geq \frac{\theta_D}{4}$, where θ_D is the Debye temperature. There is no known mechanism by which, in a Fermi liquid, the lifetime can be $\propto T^{-1}$. In fact it can be shown theoretically [7] that if $\tau \propto T^{-1}$, then the system is not a Fermi liquid in the precise technical sense. The wave function renormalisation Z_k become zero at the Fermi surface. Planar resistivity therefore constitutes one of the strongest indications that the normal state is not a Fermi liquid. This was first noted by Anderson and Zou [8] who showed that the linear temperature dependence arises naturally if the low energy quasiparticles are spinons and holons rather than electrons. The electron (not being a stable quasiparticle) decays into a spinon and holon. This lifetime turns out to be inversely proportional to temperature giving rise to linear resistivity.

1.1.2 Hall effect

The Hall effect in the cuprate superconductors is another experiment which indicates the breakdown of conventional Fermi liquid theory. In these materials, the Hall coefficient R_H is strongly temperature dependent. R_H is observed to be inversely proportional to temperature while in a Fermi liquid it is independent of temperature. The non Fermi liquid aspect of this result is most clearly brought out by the experimental results on the Hall angle θ_H.

Let $\hat{z}$ be the direction of the applied magnetic field B and let $\hat{x}$ be the direction along which the current is passed. (The Hall field is then along the $\hat{y}$ direction.) We then have (Ohm's law)

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix}$$

where ρ_{ij} is measured directly and σ_{ij} calculated from the relation

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix}$$

. In the steady state, $J_y = 0$ (no Hall current) and $J_x \equiv J$. Then in the weak field limit $\frac{eB}{mc}\tau \ll 1$, it is easy to show that $\sigma_{xy} = \frac{\rho_{xy}}{\rho_{xx}\rho_{yy}}$ and $\sigma_{xx} = \sigma_{yy} = \frac{1}{\rho_{xx}} \equiv \sigma$ where $\sigma = \frac{ne^2}{m}\tau_{tr}$. As we saw earlier, $\tau_{tr} \propto T^{-1}$ (giving linear resistivity). The Hall angle θ_H is defined as $\tan\theta_H = \frac{\rho_{xy}}{\rho_{xx}}$. For reasons that will become obvious, we introduce, following Anderson, a second lifetime τ_H (in addition to τ_{tr}) and write the off-diagonal component σ_{xy} as $\sigma\omega_c\tau_H$ where $\omega_c = \frac{eB}{mc}$. From the definition of the Hall angle, it follows that the measurement of the Hall angle is actually a measurement of τ_H (the τ_{tr} dependence is lost because σ cancels out). Experimentally, it is found

that $\tan\theta_H \sim T^{-2}$ as shown in fig. (1.1). [9]. Therefore $\tau_H \sim T^{-2}$, i.e., the lifetime associated with the Hall effect τ_H is not the same as that associated with resistivity (τ_{tr}). In a Fermi liquid these two lifetimes have identical temperature dependences and there is only one transport lifetime τ. The emergence of two lifetimes is extremely suggestive of two types of quasiparticles—the spinons and holons. An external electric field causes transitions from momentum states $\vec{k}$ to $\vec{k'}$ where $\vec{k} \parallel \vec{k'}$ and the relevant lifetime is that of the decay time of the electron into a spinon and holon. On the other hand, an external magnetic field causes transitions from $\vec{k}$ to $\vec{k'}$ where $\vec{k} \perp \vec{k'}$. It has been argued that the lifetime associated with this scattering is just the spinon-spinon scattering rate [10] which gives rise to the observed temperature dependence of the Hall angle.

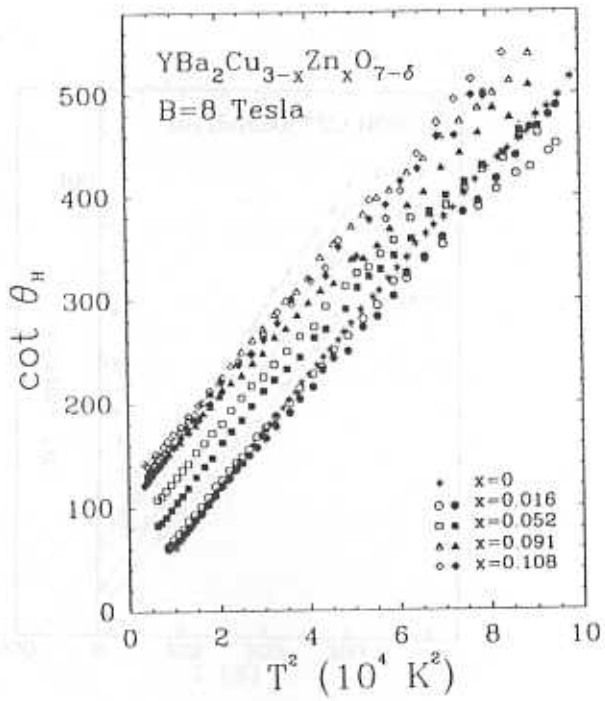

Fig. 1.1 Temperature dependence of the Hall angle.

1.1.3 NMR relaxation

This is yet another "anomalous" experiment. The relaxation time for the Cu nuclei T_1^{Cu} can be fitted well with the following expression : $\frac{1}{T_1^{Cu}} = a + bT^r$, as shown in fig. (1.2). This is quite remarkable because of the nonzero a. This implies that there is, in principle, a finite relaxation time even at zero temperature (assuming the normal state to persist till zero temperature). The quantity a is strongly dependent on the doping concentration. This behaviour of $\frac{1}{T_1^{Cu}}$ has been studied by Sardar and Baskaran [11]. Their idea is based on the fact that the spin flip operator acting on an RVB ground state produces a physical state whose overlap with a two-spinon state is nonzero. Thus, the nuclear spin can relax even at zero temperature. As we move away from half filling, the phase coherence between spinon pairs is lost due to the motion of the holons. This causes the constant a to vanish.

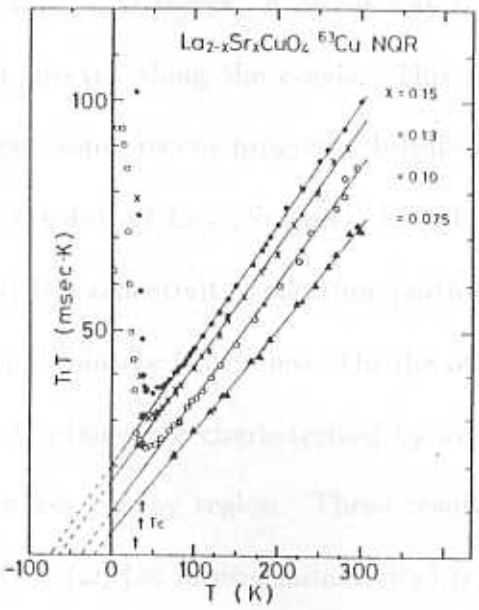

Fig. 1.2 Temperature dependence of the NMR relaxation time.

1.1.4 Conductivity in the c-direction

The phenomenon of spin-charge decoupling leads to the very interesting possibility that the coupling between Cu-O layers, $t_\perp$, becomes inoperative. This is because $t_\perp$ transports electrons across the layers and owing to spin-charge decoupling, there are no electron–like quasiparticles at the Fermi level . This effect has been dubbed "confinement". An obvious consequence is that the c-axis resistivity will be inordinately high. This is a fact which is well established experimentally [5]. The experimentally observed c-axis conductivity is very often proportional to temperature (when T is close to T_c) and is always much smaller than the in-plane conductivity. The anisotropy ratio $\frac{\sigma_{ab}}{\sigma_c} \sim 300$ to 1000. σ_c is much smaller than Mott's limit for minimum metallic conductivity, i.e., the mean free path of the electrons along the c-direction is much smaller than the dimensions of the unit cell. Hence, there is no dispersion in the c-direction which means there is no metallic conduction perpendicular to the Cu-O layers. A direct way of checking this is to obtain reflectivity/absorption spectra along the c-axis. This is a very difficult measurement but there has been some recent progress. Infrared reflectivity measurements on high quality single crystals of $La_{2-x}Sr_xCuO_4$ have been obtained by Tamasaku et al. [12]. They find the reflectivity spectrum (with the electric field polarized along the c-axis) to be absolutely featureless. On the other hand, reflectivity spectra parallel to the Cu-O planes are characterized by an edge at ~ 6000 cm^{-1} and high reflectivity in the low energy region. These results are shown in fig. (1.3). The c-axis conductivity $\sigma_c(\omega)$ (as in dc conductivity) is much smaller than Mott's minimum metallic conductivity. They also find that $\sigma_c(\omega)$ remains very small even for very high frequencies of the order of 150 cm^{-1}. These qualitative features of the

spectrum do not change appreciably when the sample is cooled from $\sim$ 300 K to temperatures just above T_c ($\sim$ 30 K). This rules out the possibility that the charge carriers in the planes are localized because of disorder, phonons etc., and provides direct evidence for the two dimensionality of the conducting state above T_c (viz., "confinement"). A dramatic change in the c-axis spectrum is seen when the sample becomes superconducting. A sharp reflectivity edge appears in the frequency range 20-50 cm^{-1}. The edge feature becomes sharper as the temperature is lowered and the edge frequency does not scale with T_c. (In fact, the edge energy ω_p is much smaller than the BCS weak coupling limit. Typically, $\frac{\hbar\omega_p}{k_B T_c} \sim 1$.) The energy of the reflectivity edge is not associated with the gap but is determined by the density of superconducting carriers. Below T_c, the conductivity is rapidly depressed and is dominated by thermally generated quasiparticles.

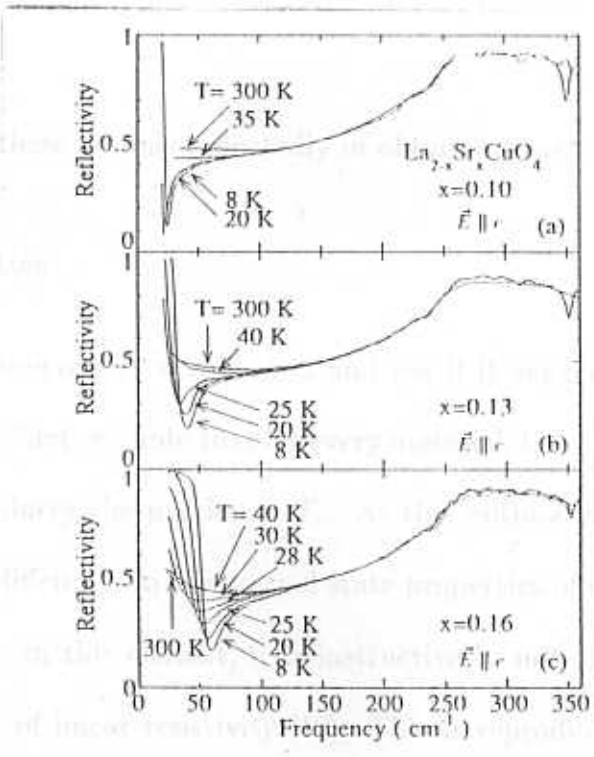

Fig. 1.3 IR Reflectivity in the 2-1-4 compound.

The observed temperature dependence of the quasiparticle scattering rate , $\gamma(T)$, is similar to that observed along the $a-b$ *plane* in the Bi 2212 and YBCO materials. A rapid decrease of γ below T_c is seen and this is a demonstration of the fact that coherent transport along the c-axis is restored below T_c. Hence, the superconducting transition restores three dimensionality.

A host of other experiments probing the normal state can be cited in addition to the ones we have discussed above. (For a comprehensive review, see [1]) All of them can be reconciled with the following assumptions:

- The normal state of the cuprate superconductors is not a Fermi liquid.
- The low lying excitations are spin-charge decoupled.
- Coherent transport of electrons across the Cu-O layers is possible only when $T \; ¡ \; T_c$.

We shall be using these notions repeatedly in obtaining our results.

1.2 T_c systematics

We now turn to observed T_c systematics and see if it suggests the mechanism of superconductivity. First, we note that for every material, there is an optimum degree of doping that produces the maximum T_c. At this optimal doping concentration, there is very little difference in the normal state properties of compounds belonging to diverse families. In this context, it is instructive to note Batlogg's observation on the universality of linear resistivity [13]. This is reproduced in fig. (1.4). We see that while T_c varies from ~ 5 K to ~ 100 K, there is not much difference in the

value of $\frac{d\rho_{ab}}{dT}$. It is natural to ask why there should be such a large variation in T_c.

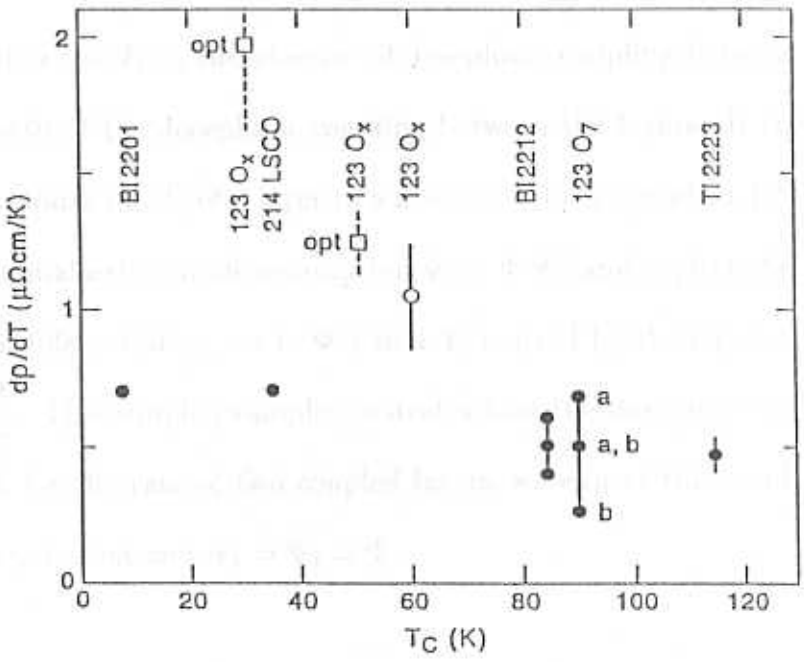

Fig. 1.4 Universality of linear resistivity.

This motivated WHA to postulate that the T_c variation is due to the difference in the number of coupled Cu-O layers in a unit cell of each compound. The Bi family $Bi_2Sr_2Ca_{n-1}Cu_nO_y$ provides the best example. The $n = 1$ compound has one Cu-O plane sandwiched by two BiO layers. The T_c of this compound is $\sim$ 10 K. The $n = 2$ compound has two Cu-O planes sandwiched by the BiO layers and its T_c is $\sim$ 80 K. (See fig.(1.5)) The $n = 3$ compound having three Cu-O closely coupled planes has a $T_c \sim 120$ K. Based on their idea that T_c is governed by the interlayer coupling, WHA calculated T_c as a function of n [14]. These results can be obtained most simply by constructing the following free energy functional

$$\mathcal{F} = \int d^2\vec{r} \left[a(T - T_c^{(0)}) \, |\Psi_j|^2 + \frac{\hbar^2}{2m} \, |\vec{\nabla}\Psi_j|^2 + \frac{b}{2} \, |\Psi_j|^4 - \Lambda(\Psi_j \Psi_{j+1}^* + h.c.) \right]. \tag{1.1}$$

Here Ψ_j is the macroscopic wave function in the layer j. $T_c^{(0)}$ is the T_c of an isolated layer, i.e., it is the T_c in the absence of Josephson coupling between the layers. Λ is the strength of the Josephson coupling between the layers. It is clear that this coupling can raise the T_c of a layer to a nonzero value even when $T_c^{(0)}$ is zero. If, for instance, we make the simple assumption $\Psi_j = \Psi \; \forall \; j$ and neglect the gradient term, we find (on differentiating w.r.t. Ψ^*) that T_c is fixed by the equation $aT_c - \Lambda = 0$, i.e., $T_c = \dfrac{\Lambda}{a}$. This simple example illustrates how the interlayer coupling enhances T_c. Indeed, for the case of two coupled layers, we expect this result since the two layers are equivalent and $\Psi_1 = \Psi_2 = \Psi$.

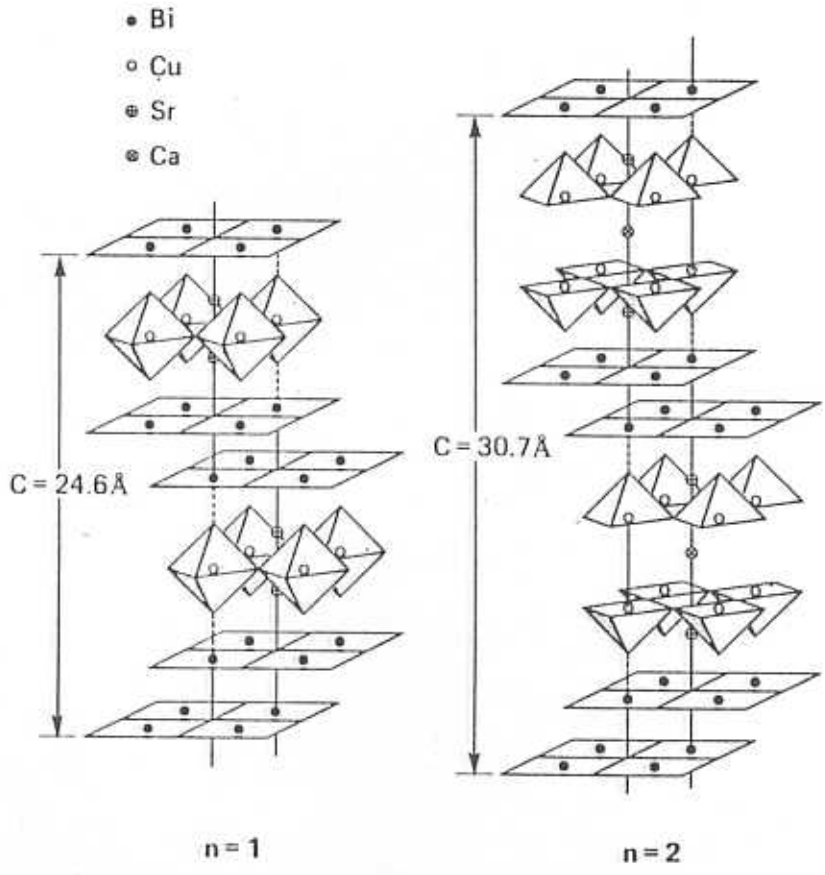

Fig. 1.5 BSCCO compounds with one and two Cu-O layers in a unit cell.

Here Ψ_j is the macroscopic wave function in the layer j. $T_c^{(0)}$ is the T_c of an isolated layer, i.e., it is the T_c in the absence of Josephson coupling between the layers. Λ is the strength of the Josephson coupling between the layers. It is clear that this coupling can raise the T_c of a layer to a nonzero value even when $T_c^{(0)}$ is zero. If, for instance, we make the simple assumption $\Psi_j = \Psi \; \forall \; j$ and neglect the gradient term, we find (on differentiating w.r.t. Ψ^*) that T_c is fixed by the equation $aT_c - \Lambda = 0$, i.e., $T_c = \dfrac{\Lambda}{a}$. This simple example illustrates how the interlayer coupling enhances T_c. Indeed, for the case of two coupled layers, we expect this result since the two layers are equivalent and $\Psi_1 = \Psi_2 = \Psi$.

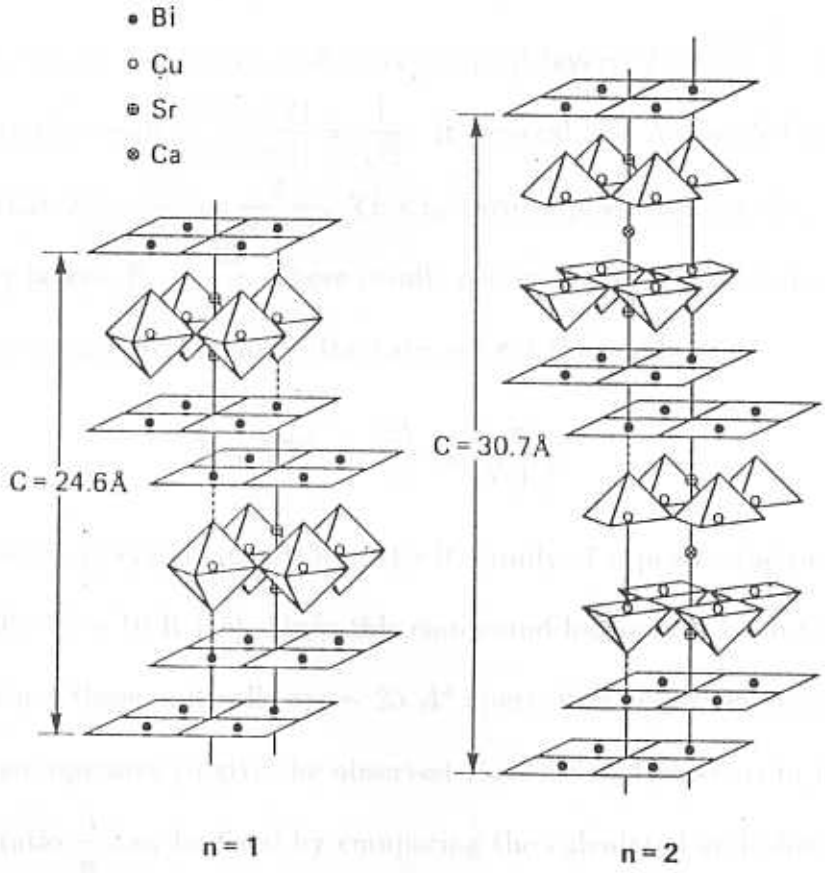

Fig. 1.5 BSCCO compounds with one and two Cu-O layers in a unit cell.

This can be seen easily on diagonalizing the free energy functional (at $T = T_c$)

$$\mathcal{F} = \int d^2\vec{r} \sum_{j=1,2} \left[aT \, |\Psi_j|^2 - \Lambda \, (\, \Psi_1^* \Psi_2 + h.c. \,) \right].$$

On the other hand, if there are three coupled layers, then the middle one is inequivalent. We have

$$\mathcal{F} = \int d^2\vec{r} \sum_{j=1}^{3} \left[aT \, |\Psi_j|^2 - \Lambda \, (\, \Psi_1^* \Psi_2 + \Psi_2^* \Psi_3 + h.c. \,) \right].$$

Obtaining T_c is tantamount to diagonalizing the matrix

$$\begin{pmatrix} aT & -\Lambda & 0 \\ -\Lambda & aT & -\Lambda \\ 0 & -\Lambda & aT \end{pmatrix}.$$

On doing this, we get for the case of three coupled layers, $T_c = \frac{\Lambda\sqrt{2}}{a}$. Therefore, we have the simple result $\frac{T_c(n=2)}{T_c(n=3)} = \frac{1}{\sqrt{2}}$. In general, for N coupled layers, it is easily shown that $T_c = \frac{2\Lambda}{a} \cos\frac{\pi}{N+1}$. This in turn implies that for a system with infinitely many layers, $T_c \to \frac{2\Lambda}{a}$. These results can easily be generalized to the case of $T_c^{(0)}$ being non zero. When this is the case, we get the result

$$T_c = T_c^{(0)} + \frac{2\Lambda}{a} \cos\frac{\pi}{N+1}. \tag{1.2}$$

Let us first discuss T_c systematics [15] in the Bi family of superconductors. For the compound 2201, $T_c \sim 10$ K [16]. Since this compound has only one Cu-O layer per unit cell and since these unit cells are ~ 25 A° apart, it is very likely that an intra layer mechanism operates to give the observed T_c. This motivates us in fixing $T_c^{(0)}$ = 10 K. The ratio $\frac{\Lambda}{a}$ can be fixed by comparing the calculated and observed T_c 's of the two-layer compound Bi 2212. The observed T_c of this compound [16] is 85 K.

So we get the result $T_c^{(0)} + \frac{\Lambda}{a} = 85$. This fixes $\frac{\Lambda}{a}$ to be 75 K. We can use this result to predict the T_c of the three layer compound Bi 2223. In this case, we have

$$T_c(n=3) \;=\; \sqrt{2}\,\frac{\Lambda}{a} \;+\; T_c^{(0)},$$

giving us a value of 116 K for the T_c. This is in good agreement with the observed T_c [16] of 110 K. A similar procedure can be adopted for the Tl family of superconductors. We show results for the Bi family in fig. (1.6). In the same figure, we also show how T_c saturates when n is increased. The Tl family of superconductors also shows a similar variation of T_c 's but the $n = 1$ compound has a $T_c \sim 75$ K. This may be construed as a direct piece of evidence against the idea that high T_c 's are because of interlayer interactions.

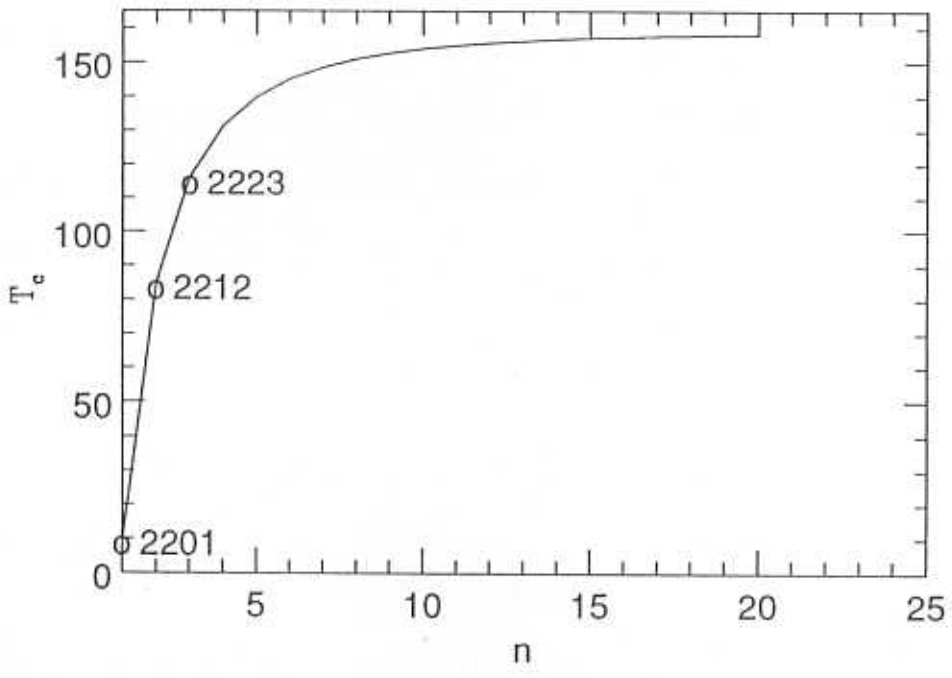

Fig. 1.6 T_c systematics for the BSCCO family from the WHA mechanism.

However, the following points are to be noted. (a) The T_c of the $n = 1$ compound can be made as small as 10 K [17]. (b) These compounds are not well characterized. The amount of oxygen concentration in the planes is still a mystery. It might be that the TlO and the CuO bands are strongly hybridized providing a large value of $t_\perp$, the one electron hopping matrix element between the Cu-O layers. More work needs to be done in this area. It would be especially interesting to see if the normal state properties of the n=1 compound with $T_c \sim 10$ K are the same as those with $T_c \sim 75$ K.

Chapter 2

Basic notions of RVB theory

In this chapter, we introduce some basic notions of RVB theory. This subject has been studied extensively ever since Anderson proposed it in the context of high temperature superconductivity [1]. We shall not attempt to review all the available results here. Instead, we focus on the central theme of RVB theory, viz., spin-charge decoupling and describe certain fundamental ideas. In section 2.1, we examine the nature of spin excitations in an RVB state and explain the concept of the pseudo Fermi surface. In section 2.2, we give a brief description of the slave boson approach to model charge and spin excitations in the large U Hubbard model and discuss the limitations of such an approach. In section 2.3, we discuss the nature of low energy excitations in the one dimensional Hubbard model for which an exact solution is available. Finally, in section 2.4, we introduce Anderson's two dimensional Luttinger liquid and describe the arguments he has advanced for spin-charge decoupling in two dimensions.

2.1 Spinons and the pseudo Fermi surface

In this section, we introduce the notion of spinon excitations and the pseudo Fermi surface [20]. Our starting point is the $S = 1/2$ Heisenberg antiferromagnet with

nearest neighbor interactions,

$$H = J \sum_{\langle ij \rangle} \vec{S}_i . \vec{S}_j \ . \tag{2.1}$$

It is well known that in one dimension, there can be no long range magnetic order arising from the Heisenberg interaction and the ground state is a coherent superposition of valence bond states. This valence bond character of the ground state suggests the possibility of novel spin excitations. In two dimensions, there is no conclusive theoretical result that the ground state is magnetically ordered. However, there seems to be a consensus amongst theorists that the ground state is magnetically ordered (Neel order) and low lying excitations can be well described by conventional spin wave theory. Experimental results obtained from neutron scattering in the insulating compounds, La_2CuO_4 and $YBa_2Cu_3O_{6.5}$ also favor this view point. But the long range order gets suppressed very quickly on doping the parent compounds and it is likely that the RVB or the quantum spin liquid state gets stabilized. So it is not entirely irrelevant to introduce the notion of spinons in the two dimensional Heisenberg antiferromagnet. In fact, it may be more meaningful to discuss the Neel state as a density wave state of an RVB spin liquid [21].

We begin by rewriting H in terms of electron operators. This is easily done by substituting

$$\vec{S}_i = c^{\dagger}_{i\alpha} \ \vec{\sigma}_{\alpha\beta} \ c_{i\beta},$$

where $\vec{\sigma}$ are the Pauli matrices. The fact that H describes an insulator is reflected in the constraint on double occupancy $n_{i\uparrow} + n_{i\downarrow} = 1$. We now define the creation operator of a valence bond between sites i and j,

$$b^{\dagger}_{ij} = \frac{1}{\sqrt{2}} \left(c^{\dagger}_{i\uparrow} \, c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow} \, c^{\dagger}_{j\uparrow} \right) .$$

It is easy to show that H can be written in terms of these operators as

$$H = -J \sum_{\langle ij \rangle} b_{ij}^{\dagger} \, b_{ij} \; .$$

We are thus liberated from using spin variables. The above hamiltonian is reminiscent of the pairing term in the BCS hamiltonian

$$-\sum_{kk'} V_{kk'} \, b_k \, b_{k'} \; ,$$

where $b_k = c_{-k\downarrow} \, c_{k\uparrow}$. However, there are two important differences between H and the BCS pairing term. The first is the absence of the kinetic energy term and the second is the local constraint $n_{i\uparrow} + n_{i\downarrow} = 1$. This local constraint is actually the result of a local $U(1)$ symmetry. Apart from this symmetry, H is also invariant under rotations in spin space. Since we are in search of a quantum spin liquid state, it is not desirable to break the rotational symmetry. On the other hand, it is quite tempting to break the local $U(1)$ symmetry and exploit the analogy between H and the BCS hamiltonian. Accordingly, we do a simple Hartree-Fock factorization

$$b_{ij}^{\dagger} \, b_{ij} = b_{ij}^{\dagger} \, \langle b_{ij} \rangle + \langle b_{ij}^{\dagger} \rangle \, b_{ij} - |\langle b_{ij} \rangle|^2 \; ,$$

and define the RVB order parameter $\langle b_{ij} \rangle = \triangle$, which will be obtained self consistently. The resulting mean field hamiltonian can be diagonalized in the usual way by defining appropriate Bogoliubov transforms and it is easy to see that the ground state wave function can be written as

$$|G\rangle_{MF} \; = \; \prod_{k} \left(u_k + v_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} \right) |0\rangle .$$

This mean field ground state has the same form as a BCS wave function. However, it should be noted that we started with an insulating magnet! The crucial ingredient

missing here is the constraint on occupancy which we sacrificed when we did the Hartree-Fock factorization. This local constraint can be recovered by making two modifications to the mean field ground state. As a first step, we put $N/2$ valence bond states in the zero momentum state. This is done by defining

$$P_N \, |G\rangle_{MF} \equiv \left(\sum_k a_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right)^{\frac{N}{2}} |0\rangle \; .$$

This can be rewritten in real space as

$$|G\rangle_N \equiv \left(\sum_{ij} a_{ij} \, b^\dagger_{ij} \right)^{\frac{N}{2}} |0\rangle \; .$$

The next step is to project out all double occupancies by Gutzwiller projection, viz.,

$$P_G \, |G\rangle_N \equiv \prod_i (1 - n_{i\uparrow} \, n_{i\downarrow}) \, |G\rangle_N \; .$$

This state has all the symmetries of the hamiltonian H and is the definition of the RVB state. The RVB state in real space can be written in terms of the valence bond operators as

$$|\mathrm{RVB}\rangle = P_G \left(\sum_{ij} a_{ij} \, b^\dagger_{ij} \right)^{\frac{N}{2}} |0\rangle \; ,$$

where a_{ij} is the valence bond wave function. Most of the well known RVB states like the extended-s, s+id, etc., can be characterized by various choices of a_{ij}.

Having defined the RVB state, we now examine the nature of low lying excitations. To do this, we first note that the quasiparticle energy (obtained from the mean field theory we outlined) is given by

$$E_k = J \, \triangle \, (\cos k_x + \cos k_y) \; .$$

So we see that there is a surface of zero energy defined by

$$\cos k_x + \cos k_y = 0 \; .$$

This is called the pseudo Fermi surface and should not be mistaken for the Fermi surface of electrons. As we shall see, the low lying excitations are not the usual particle-hole excitations and hence the prefix "pseudo".

We now write the ground state in momentum space as

$$|G\rangle_N = \prod_{|k|<k_F\sigma} c^\dagger_{k\sigma} |0\rangle ,$$

where k_F is the Fermi wave vector. Our first guess for an excited state would be $c^\dagger_{k\sigma} |G\rangle$ or $c_{k\sigma} |G\rangle$. But this takes us away from the reduced Hilbert space (corresponding to no double occupancies). Obviously, these are high energy charge excitations. Therefore, we are led to consider the choice $c^\dagger_{k\sigma} c_{k'\sigma'} |G\rangle_N$, where $k' < k_F$ and $k > k_F$. This is a particle-hole excitation but again, it disturbs the spin and charge distributions in the ground state. The single occupancy constraint does not favor any local charge fluctuations. Therefore, we Gutzwiller project our trial state and remove local charge fluctuations. The resulting state is

$$P_G\, c^\dagger_{k\sigma}\, c_{k'\sigma'}\, |G\rangle_N = P_G\, c^\dagger_{k\sigma}\, c_{k'\sigma'} \left(\sum_{ij} a_{ij}\, b^\dagger_{ij} \right)^{\frac{N}{2}} |0\rangle ,$$

which describes only local spin fluctuations. It is instructive to write this in real space. Let us consider

$$P_G\, c^\dagger_{l\sigma}\, c_{m\sigma'} \left(\sum_{ij} a_{ij}\, b^\dagger_{ij} \right)^{\frac{N}{2}} |0\rangle .$$

Clearly, we are left with two unpaired spins σ and $-\sigma'$ at sites l and m respectively. These are defined as the spinon excitations in an RVB state, viz.,

$$\xi^\dagger_{l\sigma}\, \xi^\dagger_{m-\sigma'} |\mathrm{RVB}\rangle \equiv P_G\, c^\dagger_{l\sigma}\, c_{m\sigma'} |G\rangle_N$$

where $\xi^\dagger$ are the spinon creation operators. The analogous definition in momentum

space is given by

$$\xi^{\dagger}_{k\sigma}\ \xi^{\dagger}_{k'-\sigma'}\ |\mathrm{RVB}\rangle\ \equiv\ P_G\ c^{\dagger}_{k\sigma}\ c_{k'\sigma'}\ |G\rangle_N\ .$$

It is obvious that spinons cannot be created singly, but two of them can be created and well separated in space like a pair of domain walls.

Thus we see that the local constraint on double occupancy plays a crucial role in determining the nature of the low lying excitations. It is clear that this will persist when we work with a large U Hubbard model instead of the Heisenberg hamiltonian. In this case, it would be natural to look for novel charge excitations in addition to the spinon excitations we discussed so far. We now review a formalism that illustrates these ideas to a certain extent.

2.2 The slave boson formalism and its limitations

In this section, we give a brief description of the slave boson formalism which is used to model spin-charge decoupling in the large U Hubbard model. We begin by writing the Hubbard hamiltonian

$$H = -t \sum_{\langle ij\rangle\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}\ , \tag{2.2}$$

where the chemical potential μ determines the carrier concentration. At any site i, there are four possible physical states, $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$ and $|\uparrow\downarrow\rangle$. Therefore we have the following completeness relation [22]

$$|0\rangle\langle 0| + |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| = 1.$$

Since these four states form a complete set, any local operator can be written in terms of projection operators formed out of these states. The algebra of the projection

operators can be mimicked by a combined boson-fermion theory. Thus the electron operator is expressed as

$$c_{i\sigma}^{\dagger} = e_i s_{i\sigma}^{\dagger} \pm d_i s_{i-\sigma}^{\dagger} \ , \tag{2.3}$$

where e_i 's and d_i 's are boson operators and s_i 's are fermions. The $\pm$ sign corresponds to σ being an up or a down spin label. It is easily checked that $c_{i\sigma}^{\dagger}$ as defined above satisfies the usual anticommutation relations provided

$$e_i^{\dagger} e_i + d_i^{\dagger} d_i + \sum_{\sigma} s_{i\sigma}^{\dagger} s_{i\sigma} = 1 \ .$$

This constraint corresponds to the completeness relation we wrote down earlier. Physically, $e_i^{\dagger}$ corresponds to creating an empty site and $d_i^{\dagger}$ corresponds to creating a doubly occupied site. Therefore, $e^{\dagger}$ and $d^{\dagger}$ have opposite charges ($+e$ and $-e$ respectively). Clearly, we can then treat $s_{i\sigma}^{\dagger}$ as creating a neutral particle. It is easy to check that this choice is consistent by a direct calculation of the current. However, it should be noted that this choice is not unique. We have only made a choice that is physically more plausible and the final physical results should be independent of this assignment.

Since we are interested in the hamiltonian (2.2) in the limit of large U, we use equation (2.3) in (2.2) and do a canonical transformation to eliminate terms of the order of $\frac{t}{U}$. We also set $d = 0$ since double occupancies cost an energy U. (Any self consistent theory would always give $d = 0$) On doing this we get the effective hamiltonian [23]

$$H_{eff} = -t \sum_{\langle ij \rangle \sigma} e_i e_j^{\dagger} s_{i\sigma}^{\dagger} s_{j\sigma} - J \sum_{\langle ij \rangle} b_{ij}^{\dagger} b_{ij} + \mu \sum_i \left(e_i^{\dagger} e_i - 1 \right) \ , \tag{2.4}$$

where $J = \frac{4t^2}{U}$ and b_{ij} are the valence bond operators defined in the previous section.

The constraint on double occupancy now becomes

$$e_i^\dagger e_i + \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} = 1 \ . \tag{2.5}$$

The major difficulty in the study of H_{eff} is in satisfying the constraint (2.5). Explicit calculations can be done only by making mean field approximations that violate the constraint. The mean field theories have two order parameters, $\triangle = \langle b_{ij} \rangle$ and $\chi = \langle s_{i\sigma}^\dagger s_{j\sigma} \rangle$ that are obtained self consistently. In the simplest mean field theory, the local constraint is replaced by a global constraint and the mean field hamiltonian is given by

$$H_{eff}^{MF} = -\tilde{t} \sum_{(ij)} c_i c_j^\dagger - \tilde{J} \sum_{(ij)\sigma} s_{i\sigma}^\dagger s_{j\sigma} + h.c. \ .$$

This mean field hamiltonian implies condensation of holes in the ground state which violates the local $U(1)$ symmetry [18]. Nevertheless, it is still possible to enforce the constraint by appropriately modifying the mean field ground state as we did in the case of the Heisenberg model. The mean field ground state is given by

$$|\Psi_0\rangle \ = P_G \left(e_0^\dagger \right)^{N_h} \prod_{k<k_F\sigma} s_{k\sigma}^\dagger \ |0\rangle \ ,$$

where N_h is the number of holes. This is analogous to the RVB state defined in the previous section. It is clear that we can create two types of excitations [19]. One corresponds to creating a pair of spinons leaving the hole condensate untouched, viz.,

$$|q^s; q'^s\rangle \ = P_G \left(c_0^\dagger \right)^{N_h} s_{q\sigma}^\dagger \ s_{q'\sigma'} \prod_{k<k_F\sigma} s_{k\sigma}^\dagger \ |0\rangle \ ,$$

and the other type of excitation involves creation of a holon-antiholon pair, viz.,

$$|0; q\rangle \ = P_G \ e_q^\dagger \ c_0 \ \left(e_0^\dagger \right)^{N_h} \prod_{k<k_F\sigma} s_{k\sigma}^\dagger \ |0\rangle \ .$$

These two states can be construed to be variational ground states for spinon and holon excitations as the constraint on double occupancy has been taken care of by Gutzwiller projection. However, this is easier said than done since calculations involving Gutzwiller projected wave functions are seldom tractable. Consequently most calculations with slave bosons do away with the local constraint and are therefore unreliable. The classic difficulty with this approach arises when we try to calculate electron occupancy n_k. A discontinuity in n_k at k_F would signal the presence of a Fermi surface. The presence of a Fermi surface in the high temperature superconductors has been conclusively demonstrated by ARPES and positron annihilation experiments but calculations using slave boson mean field theories do not reproduce this feature [24]. This is because of the following reason. In the slave boson approach, the electron Green's function is obtained by convoluting the spinon and holon components. Thus the single electron Green's function $G^e(k,\omega)$ is given by

$$G^e(k,\omega) = \sum_q G^s(q,\epsilon^s_q)\; G^h(k+q,\epsilon^h_{k+q})\;,$$

where ϵ^s and ϵ^h are spinon and holon energies respectively. Though there is a Fermi surface corresponding to the spinons, the convolution with the holon part wipes this feature out and as a result no discontinuity is seen in n_k at k_F. (However, it is quite surprising that many normal state transport properties can be explained qualitatively by the convolution given above. We have not understood why this is so.)

Therefore, it is clear that we have to go beyond the slave boson mean field theory to give a satisfactory description of spin-charge decoupling. We are forced to do a mean field theory only because an exact solution is not available. But in one

dimension, the Hubbard model has been solved exactly by Lieb and Wu. It would therefore be more appropriate to first study the nature of low lying excitations in the one dimensional Hubbard model and then come back to the two dimensional case.

2.3 The one dimensional Hubbard model

In this section, we discuss spin-charge decoupling in the one dimensional Hubbard model. Though the exact solution of this model was written down 20 years ago by Lieb and Wu [25], it is only now that the nature of low lying excitations, correlation functions, etc., are being understood [26]. We first write down the Lieb-Wu solution and follow Ogata and Shiba [27] to illustrate spin-charge separation in the $U \rightarrow \infty$ limit. We then summarize Anderson's results obtained from an analysis of the Lieb-Wu solution showing the failure of Fermi liquid theory. This analysis also illustrates the shortcomings of the slave boson formalism. Finally, we also mention some results obtained from bosonization methods.

The Lieb-Wu solution has the Bethe ansatz form

$$\Psi(x_1, ..., x_N) = \sum_P (Q, P) \exp i \sum_{j=1}^{N} k_{P_j} x_{Q_j} \quad ,$$

where $P_j = (P_1, ..., P_N)$ and $Q_j = (Q_1, ..., Q_N)$ are permutation labels of momenta and coordinates respectively. Here, N is the number of electrons of which M are electrons with up spin. It is understood that $N \leq N_a$ and $2M \leq N$, where N_a is the number of lattice sites. The solution to the problem is contained in the equations determining the $N! \times N!$ coefficients (Q, P). These coefficients are obtained by

solving the following set of coupled equations for the quantum numbers k_j and Λ_α,

$$\begin{aligned} N_a k_j &= 2\pi I_j + \theta(2\sin k_j - \Lambda_\alpha) \\ \sum_{j=1}^{N} \theta(2\Lambda_\alpha - 2\sin k_j) &= 2\pi J_\alpha - \sum_{\beta=1}^{N} \theta(\Lambda_\alpha - \Lambda_\beta) \ , \end{aligned} \tag{2.6}$$

where $\alpha = 1, ..., M$ and $j = 1, ..., N$. I_j 's are integers (half integers) for $N - M$ odd (even). $\theta(x)$ is defined by the following relation,

$$\theta(x) = -2 \tan^{-1}\left(\frac{2x}{U}\right) \ .$$

The total momentum and energy of the system are given by

$$\begin{aligned} P &= \sum_{j=1}^{N} k_j \\ E &= -2t \sum_{j=1}^{N} \cos k_j \ . \end{aligned} \tag{2.7}$$

It is very instructive to study the ground state wave function in the limit of $U \to \infty$ as was first done by Ogata and Shiba [27]. (There is no loss of generality in doing this as the one dimensional Hubbard model has only two fixed points, $U = 0$ and $U = \infty$. Therefore, the results for $U \to \infty$ will be connected smoothly to those for small U.) In this limit, the ground state wave function can be written as [27]

$$\Psi(x_1, ..., x_N; y_1, ..., y_M) = \det[\exp ik_j x_j] \ \phi(y_1, ..., y_M) \ ,$$

where y_i 's label the positions of electrons with down spin. The wave function is a product of a Slater determinant of noninteracting spinless fermions (describing charge degrees of freedom) and a Bethe solution of an one dimensional Heisenberg antiferromagnet with reduced number of spins (describing the spin degrees of freedom). As far as the spin degrees of freedom are concerned, we see that their dynamics is still governed by the Heisenberg hamiltonian, albeit on a "squeezed"

lattice, i.e., a lattice in which the hole degrees of freedom are squeezed out. Based on the discussion of the Heisenberg hamiltonian in section 2.1, we anticipate neutral spinon excitations at k_F (the pseudo Fermi "surface"). The charge degrees of freedom are described by a Slater determinant of spinless fermions. Hence we expect charge excitations at $2k_F$, rather than at k_F. These features can be seen on writing equation (2.6) in the $U \to \infty$ limit. We now have

$$\begin{aligned} N_a k_j &= 2\pi I_j + \frac{2\pi}{N}\sum_\alpha J_\alpha \\ \frac{2\pi}{N}\sum_\alpha J_\alpha &= -\sum_\beta \theta(2\Lambda_\beta) \quad . \end{aligned} \tag{2.8}$$

The creation of a spinon excitation (called type I excitation in the Lieb-Wu scheme) corresponds to adding or removing one J_α value. On the other hand, when we add one I_j value, the Λ_α 's do not change. We simply add one more k_j to the Slater determinant. This corresponds to an antiholon excitation at $2k_F$ (called type II excitations in the Lieb-Wu scheme). From this, we might be tempted to conclude that an electron excitation is a simple product of a spinon and an antiholon excitation as in the slave boson scheme. However, as pointed out by Anderson [26] there is a subtlety which cannot be ignored. While the Λ_α 's are determined by the corresponding J_α 's, the k_j 's are determined by *all* the J_α 's through a sum. The addition of an electron with momentum k_F corresponds to adding one I_j and one J_α value. From equation (2.8), it is clear that this will shift all the k_j 's. The shift in k_j will be

$$\delta = N_a\, \delta k_j = \frac{2\pi M}{2N} = \frac{M\pi}{N} \quad .$$

This phase shift leads to the following orthogonality relation [26].

$$|\ \langle \Psi_{N+1,k} | c_k^\dagger | \Psi_{N,K} \rangle\ |^2 \sim \exp \frac{-\delta^2 \log N}{4\pi^2} \quad .$$

This result implies the failure of Fermi liquid theory, for the overlap calculated above is nothing but the wave function renormalization constant Z_k defined in the previous chapter. That the ground state is not a Fermi liquid can also be seen on writing the electron Green's function which is given by [26]

$$G_e(x,t) \sim \frac{\exp(ik_F x)}{(x-v_s t)^{\frac{1}{2}}(x-v_c t)^{\frac{9}{16}}(x+v_c t)^{\frac{1}{16}}} ,$$

where v_s and v_c are the group velocities of the spin and charge excitations respectively. Written in momentum space, the Green's function would have a branch cut (indicating multiparticle excitations) instead of a quasiparticle pole. This is a generic behaviour seen in interacting one dimensional systems that have been characterized by Haldane [28] as Luttinger liquids.

The expressions for one electron Green's function, correlation functions etc., can also be derived without taking recourse to the Lieb-Wu solution. Weng and coworkers have used bosonization methods to study the one dimensional Hubbard model [29]. In this method, the spin quantization axis is defined along the spin direction at each site. In the new reference frame, each spin will be polarized along the z-axis by a fictitious magnetic field. Such a "symmetry broken" fictitious field plays the same role as in the SDW theories. The SDW gap here is nothing but the Mott-Hubbard gap U. The local spin direction is determined self consistently through its coupling with the charge carriers in the lower Hubbard band only, to a certain order in $\frac{t}{U}$ so that the resulting effective hamiltonian retains only terms of the order of $\frac{t^2}{U}$. The end result is that one can write down a hamiltonian for the spin and charge degrees of freedom separately without having to remember the all important constraint in the slave boson formalism. The hamiltonian for the holons

is given by

$$H_h \;=\; -t \sum_i \left(\tilde{h}^\dagger \; \tilde{h}_{i+1} \; + h.c. \right) \;,$$

where $\tilde{h}_i = \exp\left(\frac{i\pi x_i}{2a}\right) h_i$. The holons behave like free spinless fermions with the dispersion $\epsilon_k^h = -2t\cos ka$. The Fermi velocity is given by $v_h = 2ta\sin\pi\delta$ at the holon Fermi momentum $\tilde{k}_F = \frac{\pi\delta}{a}$. (Here, δ is the doping concentration.) The effective hamiltonian for the spinons is given by

$$H_s \;=\; \sum_k \epsilon_k^s \left(d_{kA}^\dagger \; d_{kA} \; + h.c. \right) \;,$$

where the summation is over the reduced Brillouin zone correponding to a sublattice A. The spinon dispersion is given by $\epsilon_k^s \propto \tilde{J}\sin ka$, where

$$\tilde{J} = J(1-\delta)\left[1 - \frac{\sin 2\pi\,(1-\delta)}{2\pi\,(1-\delta)}\right] \;,$$

is the effective superexchange coupling. The bare electron operator $c_{i\sigma}$ is then given by

$$c_{i\sigma} \;\sim\; h_i^\dagger \; s_{i\sigma} \; \exp i\frac{\pi}{2} \sum_{l<i} h_l^\dagger h_l \;.$$

So we see that unlike in slave boson theories where the electron is just a product of holon and spinon operators, there is an additional nonlocal string field. This string field is related to the nonlocal phase shift of the quantum numbers k_j that we saw in the Lieb-Wu solution.

To conclude this section, we see that spin-charge separation in the one dimensional Hubbard model is a subtle feature and the slave boson approach cannot give an adequate description of this phenomenon. We now move on to the more interesting case of the two dimensional Hubbard model. Though an exact solution is not available, there has been some progress in recent times and we review these developments now.

2.4 Anderson's two dimensional Luttinger liquid

In the previous section, we discussed the physics of the one dimensional Hubbard model. We discussed the nature of spinon and holon excitations and showed how the electron can be thought of as a composite object made out of these two excitations. In this section, we are concerned with the two dimensional Hubbard model which is of immediate relevance to the high temperature superconductors. We ask, in particular, if these nontrivial features of the one dimensional Hubbard model carry over to two dimensions. In a series of remarkable papers, Anderson has argued that they do [30]. The central theme in Anderson's arguments is that in two dimensions, as in one, forward scattering of electrons with opposite spin is singular and hence Fermi liquid theory fails. The fixed point of the doped Hubbard model in two dimensions is a Luttinger liquid. The chain of reasoning behind this assertion can be broken into three essential steps. The first step is to calculate the phase shift due to forward scattering in two dimensions and show this is finite. The next step is to establish the connection between this phase shift and the Landau parameter for forward scattering in a Fermi liquid. The final step is to argue for the failure of Fermi liquid theory from the singular nature of forward scattering. We now summarize these results.

The importance of scattering between electrons carrying opposite spin in a Hubbard model can be seen even at the level of the two particle problem [31]. Let us consider only the spin singlet state since this is the state that is affected by the on site repulsion term. The eigen function for the orbital part can be written as

$$\psi(n_1, n_2) \;=\; \exp\left(\frac{iK}{2}(n_1 + n_2)\right) \;\; \phi(n_1 - n_2) \;\; ,$$

where K is the center of mass momentum of the pair and $\phi(n_1 - n_2)$ is.the relative coordinate wave function. The Schrodinger equation for $\phi(n_1 - n_2)$ is given by

$$-t\ [\ \phi(n-1) + \phi(n+1)\ ]\ +\ U\ \delta_{n,0}\ \phi(n)\ =\ E\ \phi(n)\ \ ,$$

where $n \equiv n_1 - n_2$. When U=0, the spectrum is continuous and extends from $-t+\epsilon_k$ to $t + \epsilon_k$ where ϵ_k is the center of mass energy. However when $U > 0$, a single state splits off at the top of this continuum. This state has no overlap with the continuum of scattering states and is called an "antibound" state. The most important feature here is that even an infinitesimal U causes this orthogonality, i.e.,

$$\sum_n\ \phi_E^*(n, U=0)\ \phi_E(n, U>0)\ =\ 0\ \ ,$$

for $E = -t + \epsilon_k$ and any $U > 0$. The above result tells us that the two particle state is made orthogonal even by an infinitesimal U. It is reasonable to expect this phenomenon to manifest in the case of finitely many particles. For instance, let us imagine adding an extra particle to a free Fermi gas and switching on the Hubbard U only between this test particle and the rest of the electrons. The analysis of the two particle problem suggests that the scattering experienced by the test particle would lead to an orthogonality of the many body wave function. This is the crux of Anderson's arguments.

To demonstrate the failure of Fermi liquid theory in two dimensions, Anderson has used a very unconventional approach based on scattering theory. He has calculated the phase shift δ arising from scattering of electrons carrying opposite spins and shown that

$$\delta\ \propto\ \frac{1}{\pi \log k_F a + [N(0)U]^{-1}}\ \ , \tag{2.9}$$

where $N(0)$ is the density of states at the Fermi level and a is the lattice spacing. It should be noted that δ vanishes for U=0. The above result for δ is important because of its relation to the scattering length α. Perturbation theory presupposes a finite scattering length α which is related to δ by

$$\delta = Q\,\alpha\ .$$

Now from equation (2.9), it is clear that for large U and high densities, δ will be a finite fraction of π. Therefore, for low energy processes, i.e., $Q \to 0$, $\alpha \to \infty$ to ensure finiteness of δ, thus signalling a breakdown of perturbation theory. This result has very interesting consequences for the Landau parameter $f_{kk'}$ in Fermi liquid theory. Recall that in Fermi liquid theory, the excitation energy E of a quasiparticle can be expanded as

$$E - E_0 = \sum_{k\sigma} \epsilon_k\, n_{k\sigma} + \sum_{kk'\sigma\sigma'} f_{kk'\sigma\sigma'}\, n_{k\sigma}\, n_{k'\sigma'}\ ,$$

where $n_{k\sigma}$ is the quasiparticle density and $f_{kk'\sigma\sigma'}$ are the Landau parameters that are proportional to the forward scattering amplitudes. Using equation (2.9), Anderson has obtained the following form for $f_{kk'}$.

$$f_{kk'} \propto \frac{\vec{k}'\ .\ \left(\vec{k}-\vec{k}'\right)}{|\vec{k}-\vec{k}'|^2}\ . \tag{2.10}$$

Clearly, $f_{kk'}$ is singular for $\vec{k} = \vec{k}'$. This tells us that no two electrons carrying opposite spins like to occupy the same momentum state. Thus, the effect of the Hubbard U is to enforce a "fractional exclusion principle" for particles carrying opposite spins.

The breakdown of Fermi liquid theory in the presence of a singular interaction (2.10) has been established by Stamp [32] who has shown that a hierarchy of singular

terms arise in the one particle self energy and on summing these selfconsistently, the quasiparticle pole vanishes. i.e., the wave function renormalization $Z_k(\omega) \rightarrow 0$ when $\omega \rightarrow 0$ as

$$Z_k(\omega) \propto \left(\frac{\omega}{\omega_0}\right)^{\frac{\rho\delta^2}{N(0)\omega_0}} ,$$

where ρ is the density of electrons and ω_0 is an upper cutoff in energy.

These results then indicate the breakdown of conventional Fermi liquid theory for the large U Hubbard model in two dimensions. The natural question that arises is, what is the alternative? The analysis of Stamp [32] only establishes the failure of Fermi liquid theory but does not specify the alternative. But in order to calculate physical quantities, we need a zeroth order Hamiltonian that captures the essential features we discussed so far. To see what this could be, let us look at the interaction $f_{kk'}$ as given by equation (2.10) near the singular point $\vec{k} = \vec{k}'$ by putting $\vec{k} = \vec{k}' + \vec{q}$ where $|\vec{q}| << |\vec{k}|, |\vec{k}'|$. We then have

$$f_{kk'} \propto \frac{\cos\theta_{kk'}}{|\vec{q}|} ,$$

where $\theta_{kk'}$ is the angle between $\vec{k}$ and $\vec{k}'$. Thus, the singularity is strongest when $\vec{k}$ is parallel to $\vec{k}'$. This motivated Anderson to postulate that the appropriate zeroth order hamiltonian should be a sum of decoupled one dimensional Hubbard hamiltonians, the decoupling being done in *momentum* space. The effective hamiltonian H_0 would be written as

$$H_0 = \sum_{\Omega} H_k(\Omega) , \qquad (2.11)$$

where k, Ω are the polar coordinates of $\vec{k}$ and $H_k(\Omega)$ is the one dimensional Hubbard model with $\vec{k}$ being the momentum. Thus, in contrast with Fermi liquid theory where the zeroth order hamiltonian is the noninteracting system with all

the $\vec{k}$- modes decoupled, the interactions between $\vec{k}$-modes in the same direction cannot be ignored even in the lowest order now. The hamiltonian (2.11) is called a "Tomographic Luttinger liquid" for obvious reasons. This hamiltonian exhibits spin-charge decoupling since in each direction Ω, the physics is governed by the one dimensional Hubbard model which, as we saw in the previous section has spinon and holon excitations. This is the way spin-charge separation has been envisaged in the cuprate superconductors. This is only a hypothesis and more work is needed to prove it. However, this model has been used with success by Anderson and Ren [33] to explain the Fermi surface seen in photoemission spectra. Thus this model can explain both the anomalous transport properties *and* the existence of a Fermi surface. This model has also been used by Anderson [10] to explain the anomalous temperature dependence of the Hall angle and by Baskaran and Sardar [11] to explain the temperature dependence of the NMR relaxation time in the normal state of the high temperature superconductors.

2.5 Summary

To summarize, we have reviewed some basic ideas of RVB theory in this chapter. We have introduced the concept of a spin liquid state and neutral spinon excitations. We then reviewed the slave boson formalism and its limitations. The main difficulty with this approach is its failure to reconcile the existence of a Fermi surface with the anomalous normal state transport properties. Our search for acceptable holons then led us to the one dimensional Hubbard model, where we examined the nature of spinon and holon excitations with the help of the exact solution available. Finally, we summarized Anderson's arguments for the failure of Fermi liquid theory in two

dimensions and introduced his concept of the Tomographic Luttinger liquid. Clearly, the RVB theory has come a long way since its beginnings and there is very little technical resemblance between the early results and the present ones. However, the central ideas have remained very much the same. The last word in the theory of high temperature superconductivity is yet to be said, but we believe there is enough experimental evidence to justify the RVB point of view.

Chapter 3

The Mechanism : Microscopic derivation of the effective hamiltonian

In the introductory chapter we saw that the anomalous normal state properties of the cuprate superconductors can be reconciled with the assumption that the low energy excitations in the Cu-O planes are spin-charge decoupled. In this chapter, we examine how such a normal state responds to a weak interlayer coupling. In particular, we show that if two systems that exhibit spin-charge separation are weakly coupled, then superconductivity is an inevitable consequence. The central result in this chapter is the derivation of the WHA hamiltonian for holons which is presented in section 3.1 where we show explicitly how the interlayer coupling leads to processes that involve hopping of pairs of holons between two coupled Cu-O layers [34]. This leads to a superconducting instability in the system. In section 3.2, we give a simple quantum mechanical picture of holon pair hopping between the layers.

3.1 Derivation of the WHA hamiltonian

We use the slave boson decomposition which we discussed in the previous section to model spin-charge decoupling. The bare electron operators are expressed as

$$c^{\dagger}_{i\sigma} = e_i s^{\dagger}_{i\sigma},$$

with the constraint that there are no doubly occupied sites, viz.,

$$e_i^\dagger e_i \; + \; \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} \; = \; 1.$$

Physically, $e_i^\dagger$ corresponds to the creation of an empty site i (the holon excitation) and $s_{i\sigma}^\dagger$ creates a neutral spin half particle (the spinon). We use a simple effective hamiltonian for the normal state

$$H_0 = \sum_q \; \omega_q \; e_q^\dagger \; e_q + \sum_{k\sigma} \; (\epsilon_k - \mu) \; s_{k\sigma}^\dagger \; s_{k\sigma} - J \sum_k \; (b_k \; s_{k\uparrow}^\dagger \; s_{-k\downarrow}^\dagger \; + \; h.c.).$$

H_0 is nothing but the mean field t-J hamiltonian written in the slave boson scheme. The holon dispersion is given by $\omega_q = tq^2$ and $\epsilon_k = \tilde{t}(\cos k_x + \cos k_y)$ is the spinon dispersion. $\tilde{t}$ is the effective bandwidth of the spinons and b_k is the BZA[3] order parameter $\langle s_{k\uparrow}^\dagger s_{-k\downarrow}^\dagger \rangle$ for spinon pairing. H_0 is the simplest hamiltonian which can be used to describe the physics of spin-charge decoupling. The following comments are in order. First note that we assume the spinons are paired. This is characteristic of an RVB ground state. In fact, it will become clear that in the absence of spinon pairing, the pair hopping mechanism cannot operate. The holons are assumed to be free bosons. This is, of course, unrealistic. Therefore, the above modelling would be inadequate to obtain physical quantities like the superconducting gap, T_c, etc. Nevertheless, it is still possible to illustrate the origins of the pair hopping mechanism with this simplistic approach.

Let us now introduce a coupling between 2 adjacent Cu–O layers l and m

$$H_{int} \; = \; t_\perp \sum_{i\sigma} \; c_{i\sigma}^{l\dagger} \; c_{i\sigma}^m \; + \; \; h.c.$$

as a perturbation. H_{int} can be rewritten in the slave boson scheme as

$$t_\perp \sum_{i\sigma} \; e_i^l \; e_i^{m\dagger} \; s_{i\sigma}^{l\dagger} \; s_{i\sigma}^m \; + \; h.c.$$

We go over to momentum space and write

$$H' = \frac{1}{N}\sum_{q\sigma}\sum_{kk'} e^{l}_{q}\, e^{m\dagger}_{k-k'+q}\, s^{l\dagger}_{k'\sigma}\, s^{m}_{k\sigma} \;+\; h.c.$$

The full hamiltonian is given by

$$\begin{aligned} H &= H_0 + t_\perp H' \\ &= \sum_q \omega_q\, e^{l\dagger}_q\, e^{l}_q + \sum_{k\sigma}(\epsilon_k - \mu) s^{l\dagger}_{k\sigma}\, s^{l}_{k\sigma} - J\sum_k (b_k\, s^{l\dagger}_{k\uparrow}\, s^{l\dagger}_{-k\downarrow} \;+\; h.c.) \\ &\quad + l \rightarrow m \\ &\quad + \frac{t_\perp}{N}\sum_{q\sigma}\sum_{kk'} c^{l}_{q}\, c^{m\dagger}_{k-k'+q}\, s^{l\dagger}_{k'\sigma}\, s^{m}_{k\sigma} \;+\; h.c. \end{aligned} \tag{3.1}$$

As mentioned in the introductory chapter, we assume that the first order process caused by the interlayer coupling, viz., one electron hopping between the layers, is suppressed ("confinement"). We now show that the second order processes are "deconfining" and cause superconductivity. To see this, we treat the interlayer coupling as a perturbation and obtain an effective hamiltonian to order $t_\perp^2$. Before proceeding to do this, let us examine the various energy scales involved. Since the spinon dispersion is related to the time scale of singlet fluctuations, it will be governed by an energy scale $\sim J$. On the other hand, the holon dispersion will be related to t. $t_\perp$ can be estimated from c-axis superexchange integrals or from band structure calculations. These estimates suggest $t_\perp \sim 0.1t$. So, the three relevant energy scales in the Cu-O superconductors are $t \sim 0.4$ eV, $J \sim 0.13$ eV and $t_\perp \sim 0.05$ eV. In the parameter range $t_\perp < J < t$, therefore, we are justified in treating $t_\perp$ as a small parameter and using perturbation theory.

We now have

$$\widetilde{H}_I(0) \simeq H_0 + \frac{i}{2}t_\perp^2 \int_{-\infty}^{0} dt[H'_I(t), H'_I(0)]. \tag{3.2}$$

(The H's are now written in the Interaction picture).

The commutator in the above equation would involve spinon and holon operators in our case. After evaluating the commutator, we trace over the spinons and obtain an effective hamiltonian for the holons. The procedure we adopt is not unlike the BCS case where one derives the reduced BCS hamiltonian from an electron-phonon interaction by taking the trace over the ground state of the phonons. We could, in principle, trace over the holon ground state and obtain an effective hamiltonian for the spinons. However, since we are interested in describing superconductivity and it is the holon part of the hamiltonian that carries the appropriate quantum numbers, we derive an effective hamiltonian for the holons.

We proceed to evaluate the commutator $[H_J'(t), H_J'(0)]$ with

$$H_J'(t) = \frac{1}{N} \sum_{kk'q} e_q^l(t)\ e_{k-k'+q}^{m\dagger}(t)\ \{s_{k'\uparrow}^{l\dagger}(t)\ s_{k\uparrow}^m(t)\ +\ s_{k'\downarrow}^{l\dagger}(t)\ s_{k\downarrow}^m(t)\}\ + h.c.$$

Let us first consider only a part of the full commutator viz.

$$\sum_{kk'q}\sum_{pp'r}[e_q^l(t)\ e_{k-k'+q}^{m\dagger}(t)\ \{s_{k'\uparrow}^{l\dagger}(t)\ s_{k\uparrow}^m(t) + s_{k'\downarrow}^{l\dagger}(t)\ s_{k\downarrow}^m(t)\}, e_r^l\ e_{p-p'+r}^{m\dagger}\ \{s_{p'\uparrow}^{l\dagger}\ s_{p\uparrow}^m + s_{p'\downarrow}^{l\dagger}\ s_{p\downarrow}^m\}]$$

The holons are assumed to be free and the spinons are BZA paired. So, we have the following expressions for the time evolution of the spinon and holon operators.

$e_q(t) = e^{-i\omega_q t} e_q$ etc.; $\quad s_{k\uparrow}(t) = z_{1k}(t) s_{k\uparrow} + z_{2k}(t) s_{-k\downarrow}^\dagger$ and

$s_{-k\downarrow}^\dagger(t) = z_{1k}^*(t) s_{-k\downarrow}^\dagger - z_{2k}^*(t) s_{k\uparrow}$;

where $z_{1k}(t) = e^{-iE_k t} u_k^2 + e^{iE_k t} v_k^2$; $z_{2k}(t) = 2iu_k v_k \sin E_k t$;

and u_k^2 , $v_k^2 = \frac{1}{2}(1 \pm \frac{(\epsilon_k - \mu)}{E_k})$ with $E_k = \sqrt{(\epsilon_k - \mu)^2 + J^2 \triangle_k^{s2}}$.

Here, $\triangle_k^s$ denotes the spinon gap.

Substituting the above in the commutator to be evaluated we get

$$\sum_{kk'qr} \exp i(\omega_{k-k'+q} - \omega_q)t e^l_q \; e^{m\dagger}_{k-k'+q} \; e^l_r \; e^{m\dagger}_{k'-k+r}$$
$$\times[s^\dagger_{k\uparrow} \; s^\dagger_{-k\downarrow} \; z^*_{2k'}(t) \; z_{1k}(t) \; - \; s^\dagger_{k'\uparrow} \; s^\dagger_{-k'\downarrow} \; z^*_{1k'}(t) \; z_{2k}(t) \;] \; .$$

Since we have assumed the spinons to be paired, both terms in the above expression will be non-zero on tracing over the spinon ground state. (It should be noted that we are actually tracing over the spinon-paired or the singlet ground state.) This gives us the following expression:

$$\sum_{kk'qr} \exp i(\omega_{k-k'+q} - \omega_q)t \; e^l_q \; e^{m\dagger}_{k-k'+q} \; e^l_r \; e^{m\dagger}_{k'-k+r}$$
$$\times[\; z^*_{2k'}(t) \; z_{1k}(t) \; u_k \; v_k \; - \; z^*_{1k'}(t) \; z_{2k}(t) \; u_{k'} \; v_{k'} \;]$$

Substituting for the commutator in equation (3.2) and doing the integral over t,we get the following effective interaction for the holons.

$$2\frac{{t_\perp}^2}{N} \sum_{kk'qr} u_k v_k u_{k'} v_{k'} \frac{(E_k \; + \; E_{k'})}{(\omega_{k-k'+q} \; - \; \omega_q)^2 \; - \; (E_k + E_{k'})^2} \; e^l_q \; e^{m\dagger}_{k-k'+q} \; e^l_r \; e^{m\dagger}_{k'-k+r} \qquad (3.3)$$

So, what we have generated as the effective hamiltonian for holons involves annihilation of two holons in one layer and their creation in the other layer. Since the quantum numbers of a pair of holons are the same as those of a Cooper pair (in a spin singlet state), we see that the interlayer coupling generates superconducting fluctuations. The expression (3.3) is the holon pair hopping hamiltonian which was postulated by WHA.

3.2 Quantum mechanical picture

We now give a simple quantum mechanical picture of the pair tunneling process (See fig. 3.1). We wish to know the matrix element $V_{qq'}$ of the holon–holon interaction

between an initial state $|I\rangle$ where two holons are in the plane wave states q and $-q$ and a final state $|F\rangle$ where the holons are in states q' and $-q'$. The energy of the initial state $E_I = 2\omega_q$ and that of the final state $E_F = 2\omega_{q'}$. There are two intermediate states $|\nu\rangle$ allowed by momentum conservation:

(i) The interlayer coupling term $t_\perp\ c_i^{l\dagger}\ c_i^m$ causes a transition to an intermediate state where the holon in layer l with momentum q is annihilated and a spinon $(k\uparrow)$ is created in layer l. The matrix element $t_\perp$ transports this object (now an electron!) to layer m where a holon with momentum $q-k+k'$ is created together with annihilation of a spinon $(k'\uparrow)$. Since the layers can support spinon pair fluctuations, the layer m has an unpaired spinon $(-k'\downarrow)$. (At a later instant of time, the holon in layer l with momentum $-q$ gets across to layer m by creating and annihilating, respectively, the partners of the unpaired spinons in each layer.) The intermediate state $|\nu_1\rangle$ then describes a holon in layer m with momentum $q' = q - k + k'$, a holon in layer l with momentum $-q$, a spinon $(k\uparrow)$ in layer l and a spinon $(-k'\downarrow)$ in layer m. The energy associated with this intermediate state is $E_{\nu_1} = \omega_{q'} + \omega_q + E_k + E_{k'}$.

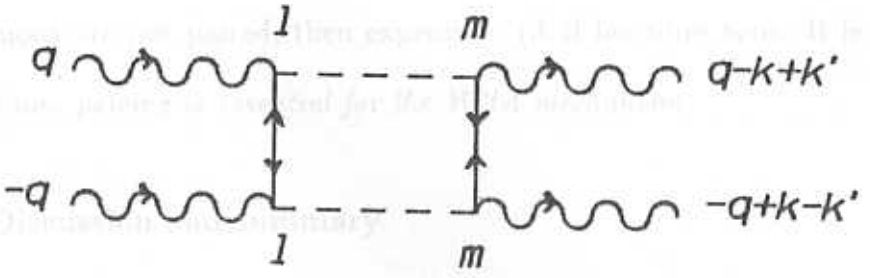

Fig. 3.1 Holon pair hopping between layers l and m

(ii) Similarly the second intermediate state is given by $|\nu_2\rangle$: a holon in layer m with momentum $-q'$, a holon in layer l with momentum q, a spinon $(k' \uparrow)$ in layer m and a spinon $(-k \downarrow)$ in layer l. The energy associated with this intermediate state $E_{\nu_2} = E_{\nu_1}$.

The second order matrix element coupling the states $|I\rangle$ and $|F\rangle$ is given by

$$\frac{1}{2} \sum_{|\nu\rangle} \langle F|H_{int}|\nu\rangle \left(\frac{1}{E_F - E_\nu} + \frac{1}{E_I - E_\nu}\right) \langle \nu|H_{int}|F\rangle$$

Since we assume that spinon pairs can be created or annihilated spontaneously in the layers, we have to introduce the spinon pair condensation amplitudes $u_k v_k u_{k'} v_{k'}$ in the above expression. On doing this and after some simplification, we get

$$t_\perp^2 \frac{2}{N} \sum_{kk'q} u_k v_k u_{k'} v_{k'} \frac{(E_k + E_{k'})}{(\omega_{q'} - \omega_q)^2 - (E_k + E_{k'})^2} e_q^l e_{q'}^{m\dagger} e_{-q}^l e_{-q'}^{m\dagger}.$$

This is precisely the reduced WHA hamiltonian as given by (3.3). Note the analogy with the reduced BCS hamiltonian. Instead of phonons mediating the interaction between electrons, we have spinon pairs mediating the interaction between the holons. What makes it all the more interesting is the fact that the perturbation actually acts as a source (sink) of *electrons* rather than that of holons or spinons. The factor $u_k v_k u_{k'} v_{k'}$ is the condensation amplitude for spinon pairs. When this is zero, i.e. if the spinons are not paired, then expression (3.3) becomes zero. It is obvious now that *spinon pairing is essential for the WHA mechanism.*

3.3 Discussion and summary

To estimate the energy denominator in expression (3.3), note that the energy of the spinons $E_k \sim J$. The relevant wave vectors for the holons (being modelled as free bosons) is temperature dependent and $\sim \frac{T}{t}$, T being the temperature. Therefore, if

we consider scattering between holons whose momenta are cutoff by $\sqrt{\frac{J}{t}}$, the pairing vertex $\sim -\frac{t_\perp^2}{J}$. The spinon condensation amplitudes are numbers of the order of unity. So if we neglect their k-dependence, we recover the WHA hamiltonian as originally proposed.

The pair hopping mechanism has several unique features that we mention below. First it is easy to check that the sign of the holon pairing vertex need not necessarily be negative to obtain superconductivity. i.e., self consistent solutions can be obtained even if the vertex has a positive sign since this sign can be absorbed by suitably altering the relative phase between the order parameter in the different layers. Next, we discuss the issue of Coulomb repulsion. Pair hopping of holons will be suppressed by the Coulomb repulsion to the extent that two holons cannot come arbitrarily close to each other. However, it is well known from BCS theory that a pairing interaction which is retarded in time can overcome a stronger repulsive interaction which is instantaneous. Similar results have been derived for the case of paired holons [36]. In this case, the effective pairing vertex Λ^{eff} is given by

$$\Lambda^{eff} = \Lambda - \frac{u}{1 + u \ln \frac{t}{J}},$$

where u is the instantaneous Coulomb repulsion and J is the characteristic spinon energy scale. This result is analogous to the BCS case where J is replaced by the phonon energy scale, $\hbar\omega_D$.

In this model for superconductivity, the inplane coherence length ξ_{ab} is actually the distance between the two holons that hop between layers and, because of the very nature of the process, is also the size of the spinon pair. Hence, it is clear that a gap in the spinon spectrum would suppress pair hopping. With our model hamiltonian

for the spinons, it is easy to check that ξ_{ab} would be of the order of a lattice spacing because of the gap in the spinon spectrum which is of the order of J. Experiments indicate $\xi_{ab} \sim 20$ A°. We believe that this discrepancy is more an artifact of our mean field treatment since a large spinon gap would also be inconsistent with other experiments like NMR and neutron scattering. Since holon pairing necessitates spinon pairing, what we need is the non-vanishing of the spinon pair order parameter *without* a spinon gap. One possibility is that the spinon gap vanishes at the Fermi surface. This can happen if the spinon pair wave function changes sign across the Fermi surface as it does in the half filled limit. From our derivation of the WHA hamiltonian, it is also clear that the symmetry of the holon pairing (or the superconducting) order parameter will be the same as that of the spinon pair order parameter. This is analogous to the BCS case where the symmetry of the electron–phonon interaction decides that of the superconducting order parameter. However, as we shall see in the next chapter, any *inplane* interaction acting in addition to the pair hopping mechanism will also play a role in deciding the symmetry of the superconducting order parameter.

Finally, we consider the part of the commutator $[H_1'(t), H_1'(0)]$ which we have neglected so far viz.

$$\sum_{kk'q} \sum_{pp'r} [e_q^l(t)\, e_{k-k'+q}^{m\dagger}(t)\, \{s_{k'\uparrow}^{l\dagger}(t)\, s_{k\uparrow}^m(t) + s_{k'\downarrow}^{l\dagger}(t)\, s_{k\downarrow}^m(t)\},$$
$$e_{p-p'+r}^m\, e_r^{l\dagger}\, \{s_{p\uparrow}^{m\dagger}\, s_{p'\uparrow}^l + s_{p\downarrow}^{m\dagger}\, s_{p'\downarrow}^l\}].$$

A similar procedure as used before leads to a pairing between holons in *different* layers. We obtain a non-pair hopping term of the form

$$\frac{2\, t_\perp^2}{N} \sum_{kk'qr} \left[\frac{(E_k + E_{k'})}{(\omega_{k-k'+q} - \omega_q)^2 - (E_k + E_{k'})^2} - \frac{(E_k - E_{k'})}{(\omega_{k-k'+q} - \omega_q)^2 - (E_k - E_{k'})^2} \right]$$
$$\times\, u_{k'}^2\, v_{k'}^2\, e_{q+k-k'}^{m\dagger} e_r^{l\dagger} e_q^l e_{k-k'+r}^m. \qquad (3.4)$$

This term correlates two holons in different layers. Using similar arguments as before, this interaction can also be shown to be attractive with the pairing vertex of the same order of magnitude as in the pair hopping case. However we believe this would no longer be true if one takes into account the Coulomb repulsion between holons in different layers. As pointed out earlier, the pair hopping processes do not compete with Coulomb repulsion whereas from the operator structure in expression (3.4), it is seen that the non pair hopping terms would have to overcome Coulomb scattering. Owing to this reason, we suggest that the non-pair hopping processes would be suppressed. An obvious consequence is that the holon pair size would be much smaller in the c-direction than in the ab-plane. i.e. $\xi_{ab} \gg \xi_c$. Experiments show that $\xi_c \sim$ 2-5 A°, a length much smaller than the interlayer separation.

To conclude this chapter, we have presented a simple microscopic derivation of the pair hopping mechanism assuming spin-charge decoupling in the normal state. The interlayer coupling causes coherent transport of pairs of holons between the layers. It is clear that this mechanism *has* to operate in the quasi one-dimensional (organic) superconductors, where it is known that there is spin-charge separation [37]. As pointed out in the beginning, our approach is rather simplistic since the single occupancy constraint has not been enforced exactly. But this derivation clarifies the nature of the pairing mechanism which operates when there is spin-charge decoupling. To go beyond these limitations and obtain expressions for physical quantities will be our next task. Accordingly, in the next chapter, we shall discuss gap equations for holon pairing, superconducting T_c, etc.

Chapter 4

A Model : Gap Equation, T_c and calculation of Josephson current

In the previous chapter, we obtained the response of a system of noninteracting spinons and holons to the interlayer coupling , $t_\perp$. We saw that $t_\perp$ generates processes that involve pair hopping of holons between layers. Since this process carries the right quantum numbers required to describe superconducting fluctuations, we identified the basic mechanism of superconductivity with the WHA hamiltonian for holons. In this chapter, we describe some attempts at obtaining gap equations for superconductivity. In section 4.1, we discuss briefly the early attempts of WHA. We then show that a pairing interaction for holons which is nonlocal in k-space (like in the BCS case, for instance) can only give low T_c 's. We argue, following Anderson that interlayer pair hopping leads to an interaction that is local in k-space, the consequences of which are studied in sections 4.2 and 4.3, where we present our main results. In section 4.2, we set up a model hamiltonian describing interlayer pair tunneling and obtain the gap equation. We analyse the momentum and temperature dependences of the gap in detail and compare them with experimental results. In section 4.3, we use the gap equation to calculate the Josephson current between two superconductors. Our calculation is in good agreement with experimental results available for the Bi 2212 compound. Finally, we study how the presence of an

additional intralayer interaction modifies the gap equation.

4.1 The WHA gap equation

Motivated by the results in section 3.1, we begin our discussion of the gap equations by considering the pair hopping term given in equation (3.3). This term causes holon pair condensation. The hamiltonian is given by

$$H = \sum_k (\epsilon_k - \mu)\ e_k^{l\dagger}\ e_k^l - \frac{\Lambda}{2} \sum_{kq} e_k^{l\dagger}\ e_{-k}^{l\dagger}\ e_{-q}^m\ e_q^m + l \leftrightarrow m$$

Here, k labels the momenta parallel to the layers. l and m are layer indices. We first consider the case of holons being free bosons. In this case, the holon dispersion ϵ_k is given by $\epsilon_k = tk^2$ and $\Lambda = \frac{t_\perp^2}{J}$. μ is the chemical potential that has to be solved for. Note the following two assumptions: (i) the holons are noninteracting and (ii) we have ignored any momentum dependence of the holon-holon vertex. For this system, WHA obtained expressions for T_c, $\triangle_k$ and μ. They found that though the free holons bose condense at $T = 0$ (i.e., $\langle e \rangle \neq 0$ at $T = 0$), there is a finite T_c below which temperature $< ee > \neq 0$. This corresponds to a holon pair condensate. To model the interactions between the holons, WHA postulated a large density of states at the bottom of the holon band. This automatically ensures that there is no macroscopic occupation of the $k = 0$ state. The large density of states is obtained by postulating a k-space pseudopotential of the form

$$V_k = \begin{cases} A - \frac{t}{\delta}|k|^2 & k < 2k_0 \\ 0 & \text{otherwise} \end{cases}$$

where $k_0 = \frac{4\pi\delta^{\frac{1}{2}}}{n_0}$ and n_0 is the occupation number of the $k = 0$ state. δ is the doping concentration. With this pseudopotential, the mean field T_c turns out to

be of the order of $\Lambda\delta$. The introduction of the holon pseudopotential is only a phenomenological attempt to mimic the long range forces between holons (arising from the single occupancy constraint). The difficulty with this approach is that it is not clear if the above assumption is consistent with the physics of the normal state. As we have emphasized in the introductory chapter, this consistency is required in any meaningful attempt. So we now turn our attention to the Tomographic Luttinger Liquid picture of the normal state developed by Anderson and Ren (cf. Section 2.4) [33] and see if it can be extended to the superconducting state by invoking the idea of interlayer pair hopping. In this picture, it is assumed that the zeroth order hamiltonian for the two dimensional Hubbard model is a collection of decoupled one dimensional Hubbard chains (the decoupling being in momentum space). The results in one dimension are used for each direction in k-space direction in two dimensions; hence the two dimensional model is reduced to a sum of decoupled one dimensional models. The spinon dispersion is given by

$$\epsilon^s_{k(\hat{\theta})} = v_s|k(\hat{\theta}) - k_F(\hat{\theta})|,$$

where $v_s = J(1-\delta)\left(1 - \dfrac{\sin 2\pi(1-\delta)}{2\pi(1-\delta)}\right)$ is the spinon velocity. Similarly, the holon dispersion relation is given by

$$\epsilon^h_{k(\hat{\theta})} = v_h|k(\hat{\theta}) - 2k_F(\hat{\theta})|,$$

where $v_h = 2t\sin\pi\delta$ is the holon velocity. Here $\hat{\theta}$ is the unit vector tangential to $\hat{k}$. Let us now assume there is a pairing interaction V between holons in a shell in momentum space about $2k_F$. The interaction V is taken to be a constant in the shell. The gap equations are obtained in the usual manner by linearizing the

following hamiltonian

$$H = \sum_k \epsilon_k^h \, (e_k^{l\dagger} e_k^l + e_k^{m\dagger} e_k^m) - V \sum_{kq} c_k^{l\dagger} e_{-k}^{l\dagger} e_{-q}^m e_q^m + h.c..$$

Since the layers are inside a bulk superconductor, we can assume

$$\langle e_{-k}^l e_k^l \rangle = \langle e_{-k}^m e_k^m \rangle.$$

The holon gap parameter δ is defined by the relation $\triangle = V \sum \langle e_{-q} e_q \rangle$ and is determined self consistently.

We get the familiar expression for the gap

$$1 = \frac{V}{2} \sum_k \frac{\tanh \frac{\beta E_k}{2}}{E_k} \quad \text{where } E_k = \sqrt{\epsilon_k^{h2} + \triangle^2}$$

It is easily verified that $T_c \approx \exp \frac{-v_h}{V}$. In particular, if the pairing interaction is identified with the pair tunneling process and we put $V = \Lambda$, then we find the T_c to be exponentially small. Clearly, any pairing interaction which is nonlocal in k-space will give the same result. It is here that interlayer hopping plays an important role. The interaction caused by pair hopping is actually local in k-space and this changes the form of the gap equation. We lost this feature in deriving expression (3.3) because of the following reason. In Chapter 2, we advocated a very naive decoupling of an electron into holon and spinon excitations, We then did a perturbative calculation (treating the interlayer coupling as the perturbation) and traced over the ground state of the spinons. However, the effective hamiltonian for the holons misses a very crucial aspect of the interlayer coupling, viz., single electron hopping between the layers conserves momentum. This becomes clear when we compare the interlayer coupling term for electrons with the same term for spinons and holons. While for

electrons we have $-t_\perp \sum_{k\sigma} c^{l\dagger}_{k\sigma} c^m_{k\sigma} + h.c.$, in terms of the spinons and holons we have

$$-t_\perp \frac{1}{N} \sum_{q\sigma} \sum_{kk'} e^l_q \; e^{m\dagger}_{k-k'+q} \; s^{l\dagger}_{k'\sigma} \; s^m_{k\sigma} + h.c.$$

Note that as far as the electrons are concerned, the in-plane momentum k is conserved by the hopping process. But this is not so for the holons. If we were to work with an effective hamiltonian for holons, we must ensure this aspect is not lost. This would in turn imply that in expression (3.3) for the holon pairing term we retain only those terms with $k = k'$. The effective hamiltonian for the holons is then

$$H_{eff} \sim \frac{t_\perp^2}{J} \frac{1}{N} \sum_{kq} \left(\; e^l_q \; e^l_r \; e^{m\dagger}_r \; e^{m\dagger}_q + h.c. \; \right)$$

This feature went unnoticed by WHA in their original work. This is one of the disadvantages of working with slave boson theories. Therefore, it might be better to work in terms of electrons though it is easier to visualize the mechanism of pair hopping in terms of spin-charge decoupling. It has also been pointed out [38] that though spin-charge decoupling may exist above T_c, there is a restoration of quasiparticle (electron like) character in the superconducting state. This is another reason why we prefer to work with electrons. Therefore, we write down the following hamiltonian

$$H \; = \; \sum_{k\sigma} \xi_k \left(\; c^{l\dagger}_{k\sigma} \; c^l_{k\sigma} + l \leftrightarrow m \; \right) \; - \; \Lambda \sum_{kq} c^{l\dagger}_{k\uparrow} \; c^{l\dagger}_{q\downarrow} \; c^m_{q\downarrow} \; c^m_{k\uparrow} + h.c. \qquad (4.1)$$

where $\Lambda \sim \frac{t_\perp^2}{J}$ and we assume $\xi_k = v|k - k_F|$ anticipating quasiparticle excitations below T_c. At first glance, it might seem that the above hamiltonian H is inconsistent with our assertions that the normal state is not a Fermi liquid. For in the limit of $\Lambda \to 0$, the hamiltonian H describes a Fermi liquid in the layers l and m. This is a valid objection and we now give two reasons why working with H is not meaningless.

The first is to note that though we have a Fermi liquid in each layer, there is no term that transports a single electron between the layers, i.e., we have suppressed single electron hopping between the layers by hand. There is no reason why this term should be absent in the case of Fermi liquids. It is not as though the matrix element for c-axis hopping, $t_\perp$, is very small. $t_\perp$ as was mentioned in the previous chapter has been estimated to be $\leq 0.15t$. (In Chapter 6, we show that the presence of the single electron hopping term actually inhibits superconductivity.) Therefore, the suppression of c-axis hopping is a nontrivial feature. The second reason for working with H is the unique form of the pairing term. Note the difference between the pairing term in H and the BCS pairing term which would be of the form

$$\sum_{kk'q} c^{l\dagger}_{k\uparrow} c^{l\dagger}_{q\downarrow} c^{m}_{q-q'\downarrow} c^{m}_{k+q'\uparrow} + h.c.$$

This difference, as we pointed out is because of the momentum conserving nature of the pairing interaction. It is brought out clearly in fig.(4.1) where we have shown the difference between the elementary vertex of electron-phonon scattering and interlayer tunneling.

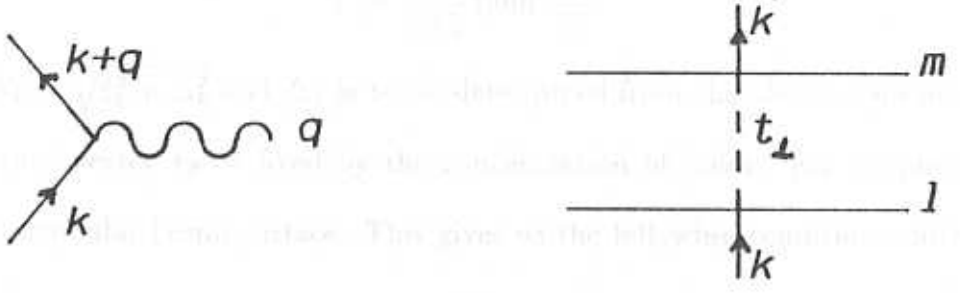

Fig. 4.1 Electron-Phonon scattering and interlayer tunneling.

Owing to this difference, the individual momenta of a pair of electrons being scattered are conserved, whereas in the electron-phonon case, only the center of mass momentum is conserved.

The results we present in the next section show that these two features, viz., suppression of c-axis hopping and the novel pairing term in the hamiltonian occuring because of interlayer tunneling are enough to obtain high T_c 's, i.e., high T_c 's do not arise because of any enhanced pairing susceptibility latent in the anomalous normal state but is the result of these two features. In this sense, we believe that if somehow a Fermi liquid could be made to exhibit "confinement", high T_c 's should result.

4.2 Gap equation for high T_c 's

We now diagonalize the hamiltonian (4.1) in the usual way. The pairing term of the mean field hamiltonian is of the form

$$-\Lambda \sum_k c^{l\dagger}_{k\uparrow}\, c^{l\dagger}_{-k\downarrow}\, \langle c^m_{-k\downarrow} c^m_{k\uparrow} \rangle + h.c.$$

where it should be noted, only one k value is being summed. The gap equation in this case becomes

$$1 \;=\; \frac{\Lambda}{2E_k} \tanh \frac{\beta E_k}{2} \tag{4.2}$$

where $E_k = \sqrt{\xi_k^2 + \triangle_k^2}$ and $\triangle_k$ is to be determined from the above equation. The Fermi wave vector k_F is fixed by the concentration of holes. For simplicity, we assume a circular Fermi surface. This gives us the following condition which fixes k_F.

$$\frac{1}{2\pi} \int_{k_F}^{\frac{\pi}{2}} k\, dk \;=\; \delta.$$

We have, for purposes of illustration, chosen $\Lambda = 0.05$ eV, $v = 0.7$ eV and $\delta = 0.25$ (which fixes k_F=1.296).

Let us first consider the gap at zero temperature. In this limit, the gap $\triangle_k$ is given by the simple expression

$$\triangle_k = \sqrt{\frac{\Lambda^2}{4} - {\xi_k}^2}. \tag{4.3}$$

The gap is isotropic but depends strongly on $|k - k_F|$. It becomes smaller as $|k - k_F|$ increases. The cutoff momentum k_c is fixed by the condition $\xi_{k_c} = \frac{\Lambda}{2}$. The maximum value of the gap at zero temperature is also the same as the cutoff energy. So, only those states that have energies less than the superconducting gap are involved in pairing. This feature persists at finite temperatures and is in contrast with the BCS case where all electron states having energies less than the Debye temperature are paired up at all temperatures less than T_c.

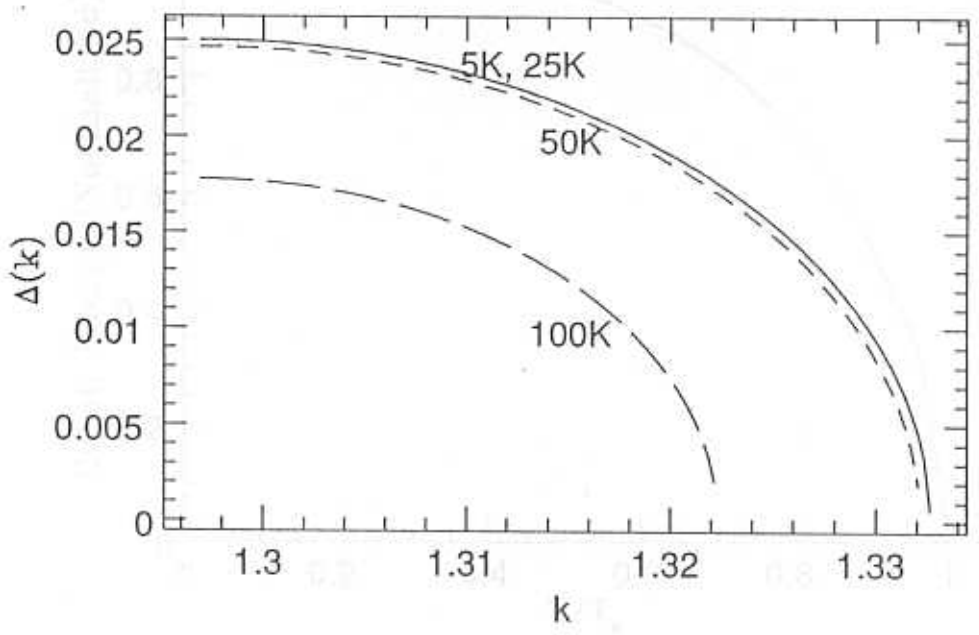

Fig. 4.2 Temperature dependence of the WHA gap.

We have solved the gap equation (4.2) numerically at finite temperatures. We obtain $T_c = 120$ K. with our choice of parameters. The temperature dependence of the gap is shown in fig.(4.2). Note that there is no difference between the magnitude of gaps at 5 and 25 K and very little difference between those at 5 and 50 K. This is a peculiar feature of the gap arising from (4.2). One reason for this is the temperature dependence of the cutoff energy ξ_{k_c}. We have shown this temperature dependence of the cutoff energy (normalized to its zero temperature value) in fig.(4.3). It is seen that the cutoff falls very steeply at $T \sim T_c$. The resulting anomalous temperature dependence of the gap is seen clearly if we plot the k-averaged gap as a function of temperature. This is shown in fig.(4.4). The gap remains constant almost upto T_c. This anomalous temperature dependence has been observed in many experiments.

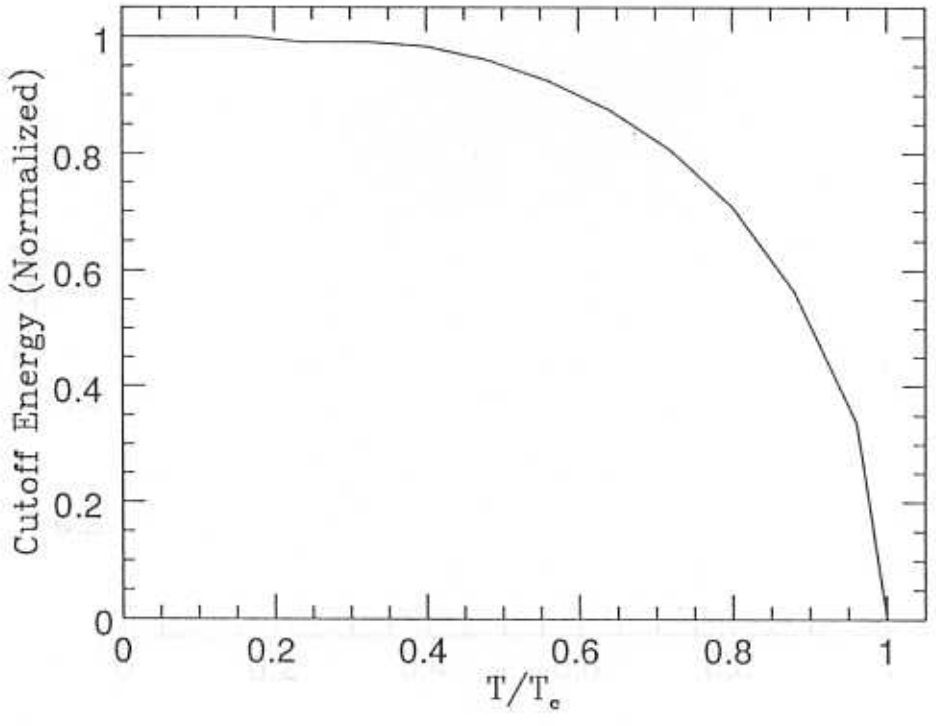

Fig. 4.3 Temperature dependence of the cutoff.

For instance, tunneling experiments [39] on YBCO show that the position of the density of states peak (corresponding to the position of maximum gap) remains almost unchanged as temperature increases. Similar results have also been reported for the Bi 2212 material. High resolution electron energy resolution spectroscopy [40] and Raman spectroscopy [41] have been used to determine the temperature dependence of the superconducting gap in Bi 2212. These results again show that the gap develops sharply for $T < T_c$. There have been attempts to fit the anomalous temperature dependence of the gap to BCS theory in the strong coupling regime. There has also been a suggestion that this peculiar temperature dependence is due to dynamical pair breaking [42]. The pair breaking is assumed due to single magnon scattering and this causes the gap to vanish at temperatures lower than the actual T_c.

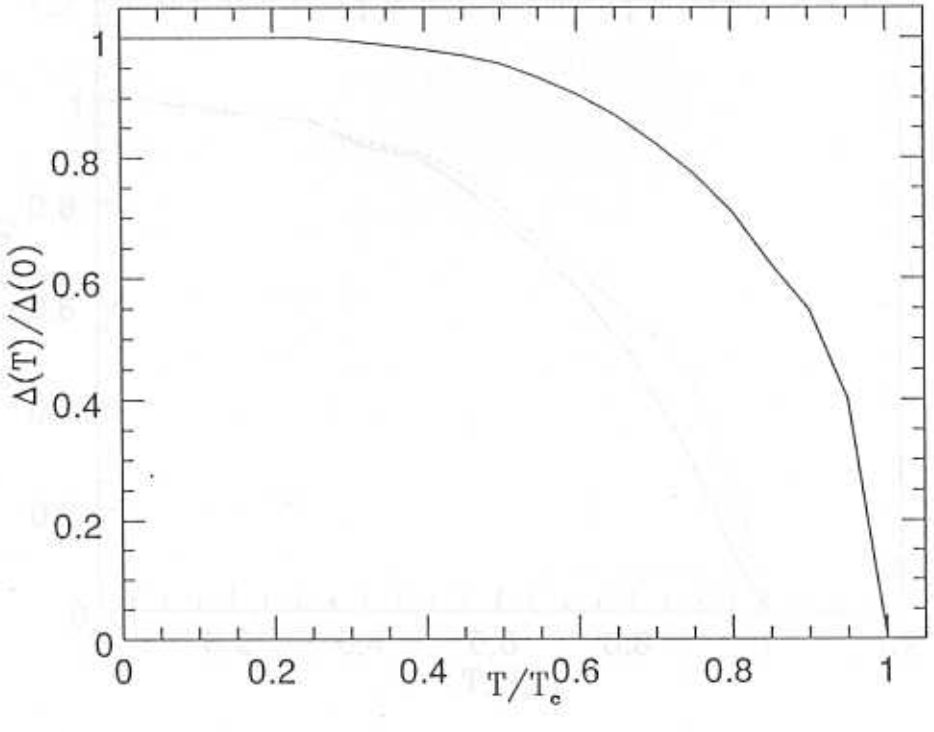

Fig. 4.4 Temperature dependence of the k-averaged gap.

However, in our approach this temperature dependence follows quite naturally from equation (4.2). i.e. we have not used any parameter fit to obtain the observed temperature dependence of the gap.

4.3 Josephson current

The results in the previous section indicate that the gap equation (4.2) captures many features of the gap observed in the cuprate superconductors. We now use equation (4.2) to calculate the Josephson current between two superconductors described by the hamiltonian H (4.1). The motivation for doing this is as follows. Josephson current between the Cu-O bilayers in Bi 2212 has been observed experimentally [43].

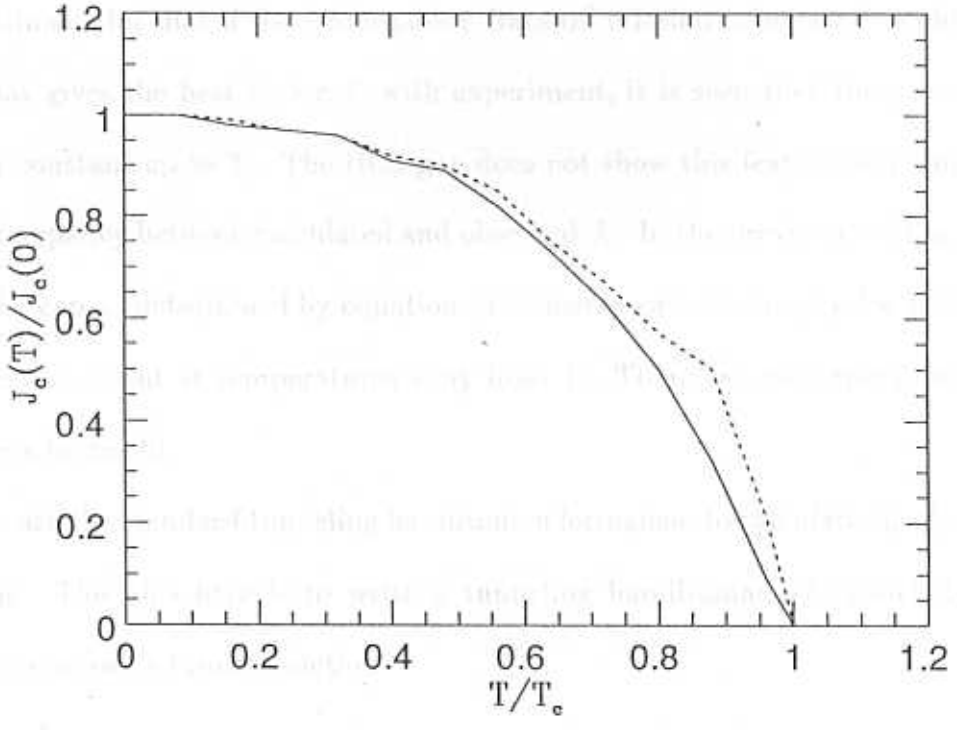

Fig. 4.5 Josephson current between Cu-O bilayers in Bi 2212. Solid line is the BCS prediction.

If the pair hopping mechanism operates between the Cu-O planes forming a bilayer, then Bi 2212 itself can be thought of as an array of Josephson junctions with each Cu-O bilayer forming a WHA superconductor. If this is true, we would expect the Josephson current $J_c(T)$ as calculated using equation (4.2) to agree with experimental results. Experimental results for $J_c(T)$ show that if a BCS-like temperature dependence for the gap is assumed, then the calculated and observed results agree only at low temperatures. There is a significant discrepancy at temperatures close to T_c as shown in fig.(4.5). To compare the experimental results with theory, the Ambegaokar-Baratoff relation [44]

$$J_c R_n \;=\; \frac{\pi}{2\triangle(T)}\;\tanh\frac{\triangle(T)}{2k_BT}$$

is used. (Here, R_n is the junction resistance in the normal state.) Furthermore, it is also claimed [43] that if the Ambegaokar-Baratoff relation is inverted to obtain the gap that gives the best fit for J_c with experiment, it is seen that the gap remains almost constant up to T_c. The BCS gap does not show this feature and this causes the discrepancy between calculated and observed J_c. In the previous section, we saw that the gap as determined by equation (4.2) increases very sharply for $T \simeq T_c$ and is almost constant at temperatures away from T_c. Therefore, we expect our results to give a better fit.

We use the standard tunneling hamiltonian formalism to calculate the Josephson current. The idea here is to write a tunneling hamiltonian H_T which transfers electrons across a tunnel junction

$$H_T \;=\; \sum_{kp} T_{kp}\;(\;c^{\dagger}_{Lk}\;c_{Rp} + h.c.\;),$$

where L and R denote the left and right sides of the junction. This tunneling

hamiltonian is used to derive a correlation function for electron tunneling currents. This correlation function gives the tunneling current as a function of voltage [45]. The tunneling current has two components–one coming from single particle tunneling and the other from pair (Josephson) tunneling. The Josephson current can be calculated by evaluating the correlation function

$$\Phi(i\omega) = -\sum_{kp\sigma}\sum_{k'p'\sigma'} T_{kp}T_{k'p'}\int_0^\beta d\tau\ \exp i\omega t\ \langle T_\tau c^\dagger_{k\sigma}(\tau)c_{p\sigma}(\tau)c^\dagger_{k'\sigma'}c_{p'\sigma'}\rangle,$$

and making the analytical continuation $i\omega \rightarrow eV + i\delta$. The final result for the Josephson current $J(eV)$ is

$$\begin{aligned} J(eV) &= 4e|T|^2\sum_{kp}\frac{\triangle_k\triangle_p}{E_kE_p}\Big\{[n_F(E_p)-n_F(E_k)](\frac{1}{eV+E_p-E_k}-\frac{1}{eV-E_p+E_k}) \\ &\quad +[1-n_F(E_p)-n_F(E_k)](\frac{1}{eV+E_p+E_k}-\frac{1}{eV-E_p-E_k})\Big\}, \end{aligned} \tag{4.4}$$

where $E_k = \sqrt{\xi_k^2+\triangle_k^2}$ etc., and n_F is the Fermi function. The matrix elements T_{kp} are assumed to be independent of momentum. $\triangle_k$ is obtained from the gap equation (4.2) and substituted in the above expression for Josephson current. Our results (normalized to the value at T=0) are shown in fig. (4.6). There is a good agreement between the theoretical and experimental results at temperatures close to T_c. Again it should be noted that we have not used any parameter fit to produce this result.

Thus we see that the gap resulting from interlayer tunneling has very unusual features. We now examine how the gap parameter as given by equation (4.2) changes in the presence of an additional intralayer interaction. These results may be relevant for the Bi 2201 material. This compound has only one Cu-O layer in each unit cell. The Cu-O layers in different unit cells are ~ 25 A° apart. Hence, it is quite likely that an intralayer mechanism operates in conjunction with a weak interlayer mechanism

to give observed T_c 's $\sim$ 10 K. The results we mention below also indicate that the strong k dependence of the gap we obtained from equation (4.3) gets modified and it becomes closer to the conventional k independent gap if there is an additional BCS like interaction.

We add to the hamiltonian H given by equation (4.1), a BCS like term

$$-V \sum_{kq} c^{l\dagger}_{k\uparrow}\ c^{l\dagger}_{-k\downarrow}\ c^{l}_{-q\downarrow}\ c^{l}_{q\uparrow}\ +\ l \rightarrow m$$

For purposes of illustration, we choose $N(0)V = 0.3$ (a typical BCS value) and $\hbar\omega_D \sim 250$ K. This gives us an intralayer $T_c \sim 10$ K.

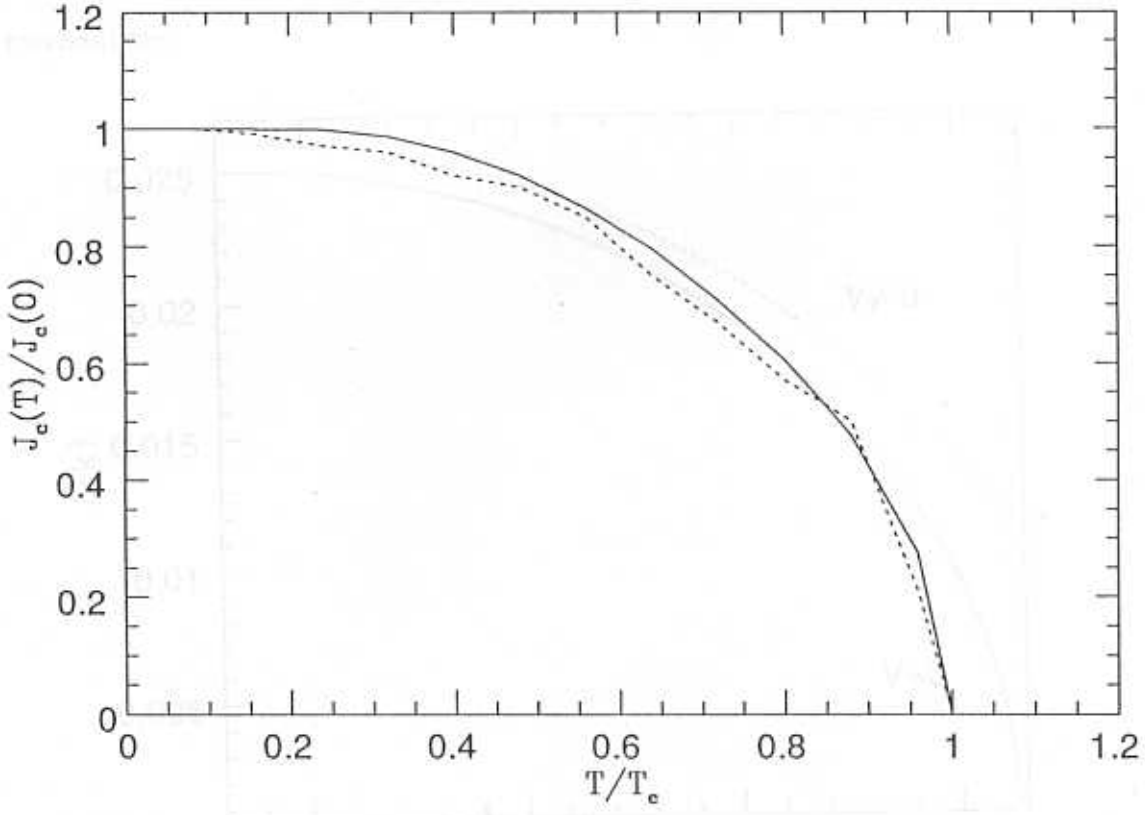

Fig. 4.6 Josephson current between Cu-O bilayers in Bi 2212. Solid line is as calculated from gap equation (4.2).

The gap equation (4.3) at zero temperature now becomes

$$\triangle_k = \frac{\Lambda \triangle_k}{2E_k} + V \sum_q \frac{\triangle_q}{2E_q} \tag{4.5}$$

We solve this equation self consistently. The results are shown in fig.(4.7). In contrast to the case when there is no BCS like mechanism operating in the layers, the zero temperature gap does not vanish anywhere in the region of interest. Also, since the cutoff in the BCS mechanism is temperature independent, the steep fall of the gap we saw earlier in fig.(4.4) is no longer likely. So we see that the unique features of the WHA gap get "blurred" by the presence of an additional intralayer mechanism. This effect will, of course, depend on the relative strengths of the two mechanisms.

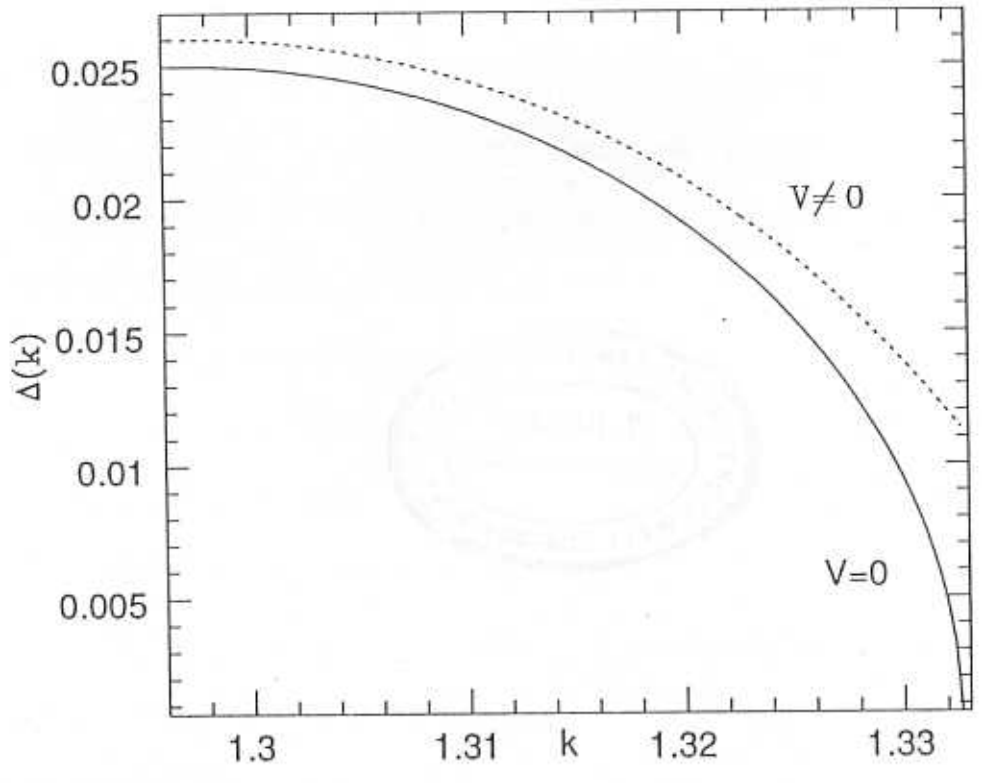

Fig. 4.7 Effect of a BCS-like intralayer interaction on the WHA gap at T=0.

For instance, with our choice of parameters, we see that the zero temperature gap at the cutoff value of k is 0.01 eV in the presence of V while it was zero when $V = 0$. The remnant gap is entirely due to the intralayer interaction. So, the gap resorts to more conventional behaviour when V is switched on. We believe that a similar analysis will go through if we add an intralayer interaction with d-wave symmetry and the resulting gap will show d-wave like features also as suggested by Anderson [46].

Chapter 5

Exact diagonalization

In obtaining the results we presented in the last two chapters, we made several assumptions whose validity may be questioned. In particular, we argued that pair tunneling is inevitable in the presence of spin-charge decoupling and "confinement" of electrons within the Cu-O plane. Despite the enormous amount of work done on this subject, these two issues remain contentious, at best. Therefore, there are only two ways to check if the WHA mechanism operates in the presence of strong correlations. One way is to formulate a macroscopic (Ginzburg-Landau) theory based on the ideas of WHA and see if the results so obtained are consistent with experiment. The other way is to obtain exact results for finite size systems. Of the two approaches, the former is too general for our purpose. Indeed, the macroscopic theory corresponding to the WHA mechanism would be akin to the usual Lawrence-Doniach theory [47] for layered superconductors. As we mentioned in chapter 1, the results for T_c systematics derived by WHA can be got from a Lawrence-Doniach theory for coupled Cu-O planes. Results for the orbital upper critical fields, the anisotropy ratio in the superconducting state etc., for the YBCO, 2-1-4 and BSCCO compounds have been obtained [48] using the free energy functional (1.1). However, these results are not unique to the assumption that the hamiltonian describing the

normal state is the large U Hubbard model. Therefore, we take recourse to the second approach [1] we mentioned, viz., a study of finite size clusters.

Ever since Anderson's proposal that the physics of the high T_c superconductors is contained in the one band Hubbard hamiltonian, the large U Hubbard model and its derivative, the t-J model have been the subject of several numerical studies. Finite size clusters of these models have also been analyzed extensively [49] by exact diagonalization and Variational Monte Carlo techniques. These studies indicate that several of the anomalous normal state properties of the Cu-O superconductors could be accounted for by the t-J hamiltonian. However in these numerical studies, there are no robust signals of a superconducting phase in either the Hubbard or the t-J model [50]. Given the results we have presented so far, this is hardly surprising.

5.1 Coupled t-J planes

If superconductivity in the cuprate materials is a result of strong correlation, then it is the interlayer coupling $t_\perp$ which drives the transition to the superconducting state. With this in mind, we have performed exact diagonalization [51] studies on $4+4$, $5+5$ and $6+6$ site clusters. 4+4, for instance, denotes two t-J planes having 4 sites each. The two planes are coupled by the $t_\perp$ term

$$-t_\perp \sum_{i\sigma} c_{i\sigma}^{l\dagger}\, c_{i\sigma}^{m} \;+\; h.c.$$

The in-plane hamiltonian is the t-J hamiltonian with the constraint on double occupancy being enforced *exactly*. We use periodic boundary conditions. In addition we use two different geometries for the $6+6$ case:(a) for a closed chain and (b) a grid.

[1] The results presented in this chapter were obtained in collaboration with M. Arjunwadkar, G. Baskaran and R. Basu.

We have presented results only for the grid geometry since the results for the closed chain are qualitatively similar. We have chosen, on a scale of $|t| = 1$, $J = 0.31$, and varied $|t_\perp|$ from 0 to 0.9. Our results are therefore of direct relevance to the Cu-O compounds in the region of small $t_\perp$. To illustrate the effect of $t_\perp$ in the absence of U, we have also diagonalized a $4 + 4$ cluster with two holes after relaxing the constraint on double occupancy.

To look for superconductivity we compute the extended-singlet correlation function as defined by Hirsch [50] which we explain below.

Let

$$b_{ij} = \frac{1}{\sqrt{2}}[c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}],$$

where (i, j) are nearest neighbor sites in a plane. Then the extended-singlet pairing correlation (SPX) is defined as

$$\chi = \frac{1}{N} \sum_{<i,j><k,l>} \langle b_{ij} b_{kl}^\dagger \rangle \tag{5.1}$$

where $\langle \cdots \rangle$ represents the expectation value in the ground state. Here N is the number of sites in the plane. If χ scales as N, then the result suggests a superconducting instability in the thermodynamic limit. This criterion is a special case of the usual requirement of ODLRO. i.e., if there is superconducting order in a system, we expect

$$\lim_{n\to\infty} \frac{1}{N^2} \sum_{ij} \langle c_{i\uparrow}^\dagger \; c_{j\downarrow}^\dagger \; c_{j+n\downarrow} \; c_{i+n\uparrow} \rangle \; = \; \text{const},$$

N being the number of sites. In our case, we have restricted ourselves to electron pairs of the size of a lattice spacing. We also look only for s-wave pairing. It should be noted that we are studying *inplane* superconducting correlations as a function of the *interplane* coupling $t_\perp$.

5.2 Results

The results of the above computation show several interesting features that are size–independent (see fig. 5.1, 5.2 and 5.3). First, we note that for the case of two holes, the SPX always increases with $t_\perp$. For cluster sizes $4+4$, $5+5$ and $6+6$, this corresponds to a doping of $\sim 25\%$, 20% and 16% respectively. As soon as we add two more holes, we enter a region of large doping. The results with four holes therefore show a qualitatively different behavior. The SPX in this case is not affected much by $t_\perp$ and the results resemble those of the unconstrained t-J model.

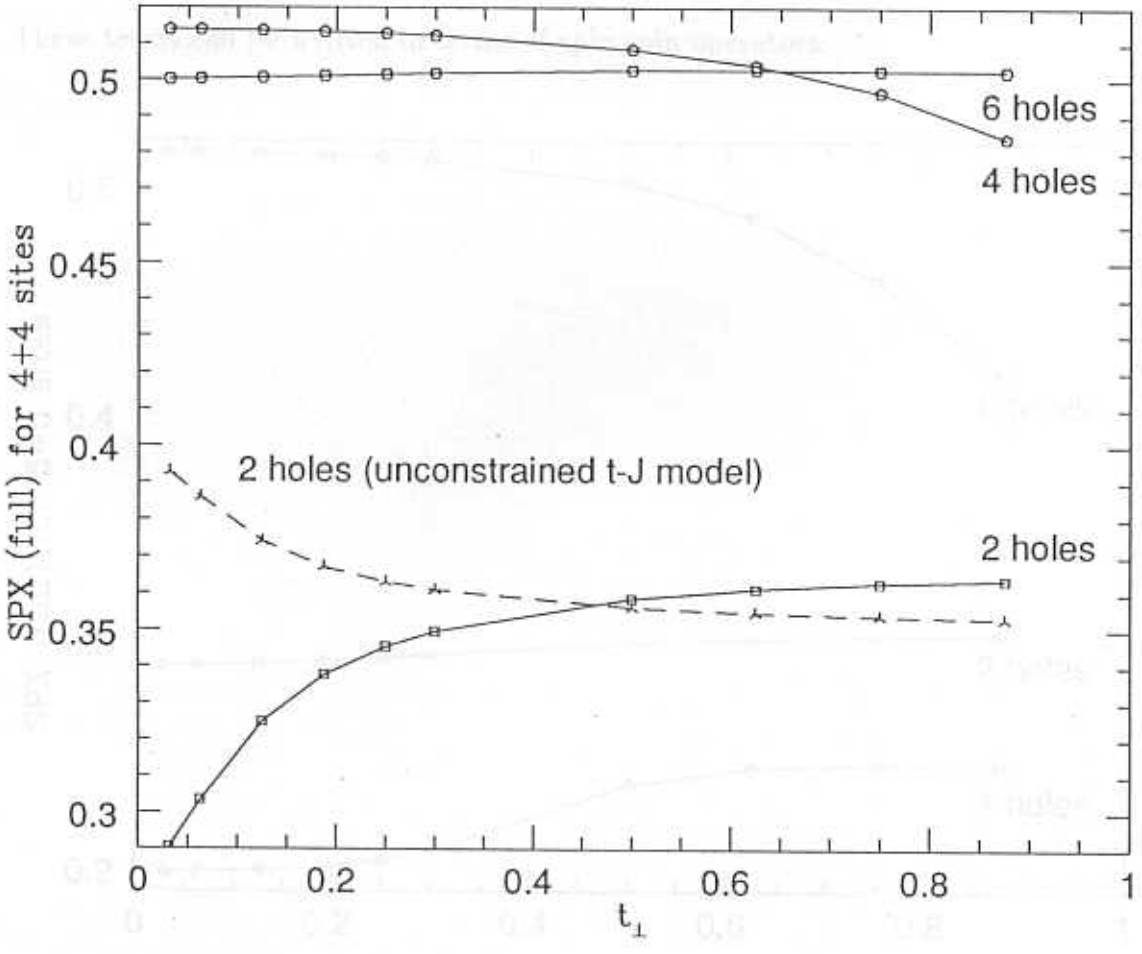

Fig. 5.1 SPX for the 4+4 cluster. The dashed line represents the behaviour of SPX when the constraint on double occupancy is relaxed.

The same behavior persists for larger hole concentrations. In this sense, we suggest that we have crossed over from a non–Fermi liquid phase (which is sensitive to $t_\perp$) to a phase which is less of a non–Fermi liquid.

Next we consider the limit $t_\perp \to 0$. In this limit with two holes in the system, the ground state has one hole in each layer on an average. Therefore the contribution to SPX is dominated by terms of the form $\langle O_{12} O_{12}^\dagger \rangle$, $\langle O_{12} O_{23}^\dagger \rangle$. Such essentially on–site correlations are not related to superconducting order in the thermodynamic limit. This can be seen easily from the definition of χ in equation (5.1). The summation in (5.1) consists of N^2 terms, of which terms of the form $\langle O_{12} O_{12}^\dagger \rangle$ are N in number. These terms can be written in terms of spin-spin operators.

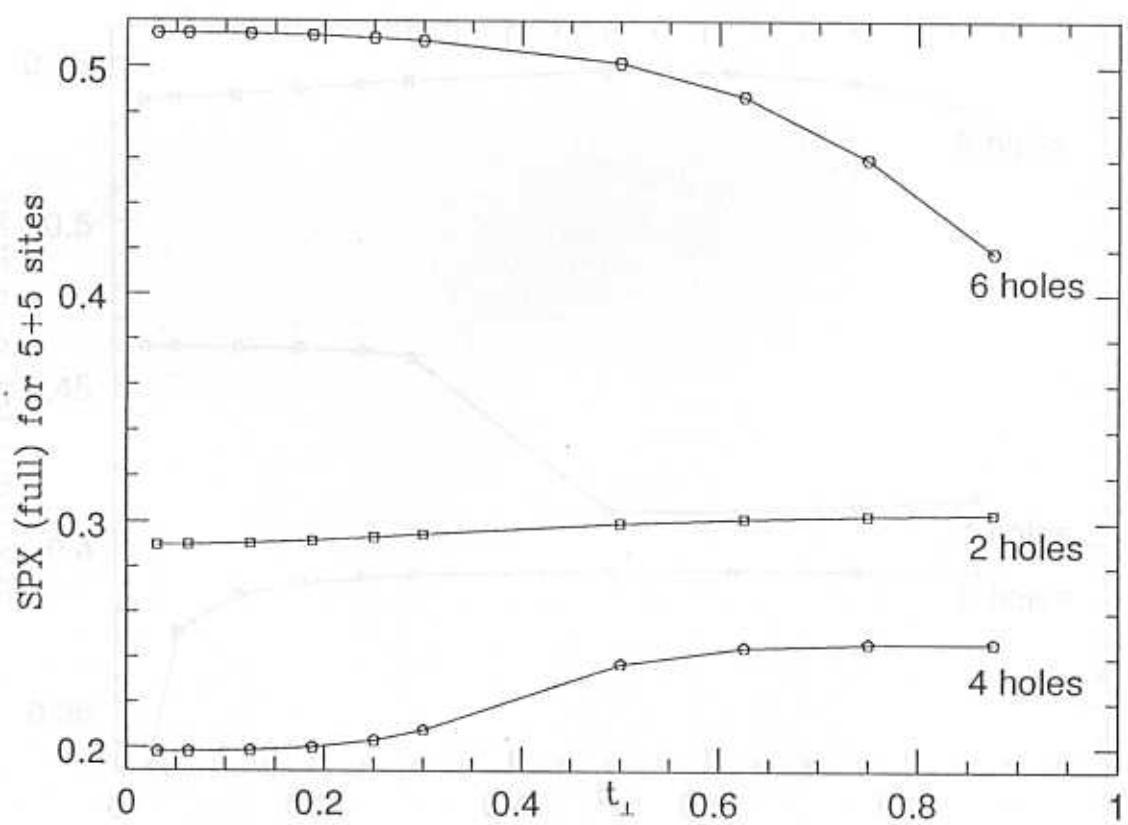

Fig. 5.2 SPX for the 5+5 cluster.

There are $2N$ terms of the form $\langle O_{12}O_{23}^{\dagger}\rangle$ and these terms can be written in terms of spin-hole operators. Clearly, if χ has to scale as N, it must be terms of the form $\langle O_{12}O_{34}^{\dagger}\rangle$ that contribute to the sum in (5.1). Such terms are the long range correlations. In previous studies [49] of the t-J model, it was noticed that these terms do not contribute to the SPX. This led to the conclusion there are no incipient long range (superconducting) correlations in the t-J model. Our results for $t_\perp = 0$ also reflect this.

However as $t_\perp$ increases, the long range correlations increase rapidly. In fact, it is this behavior of the long range correlations that causes the enhancement of the total SPX with $t_\perp$.

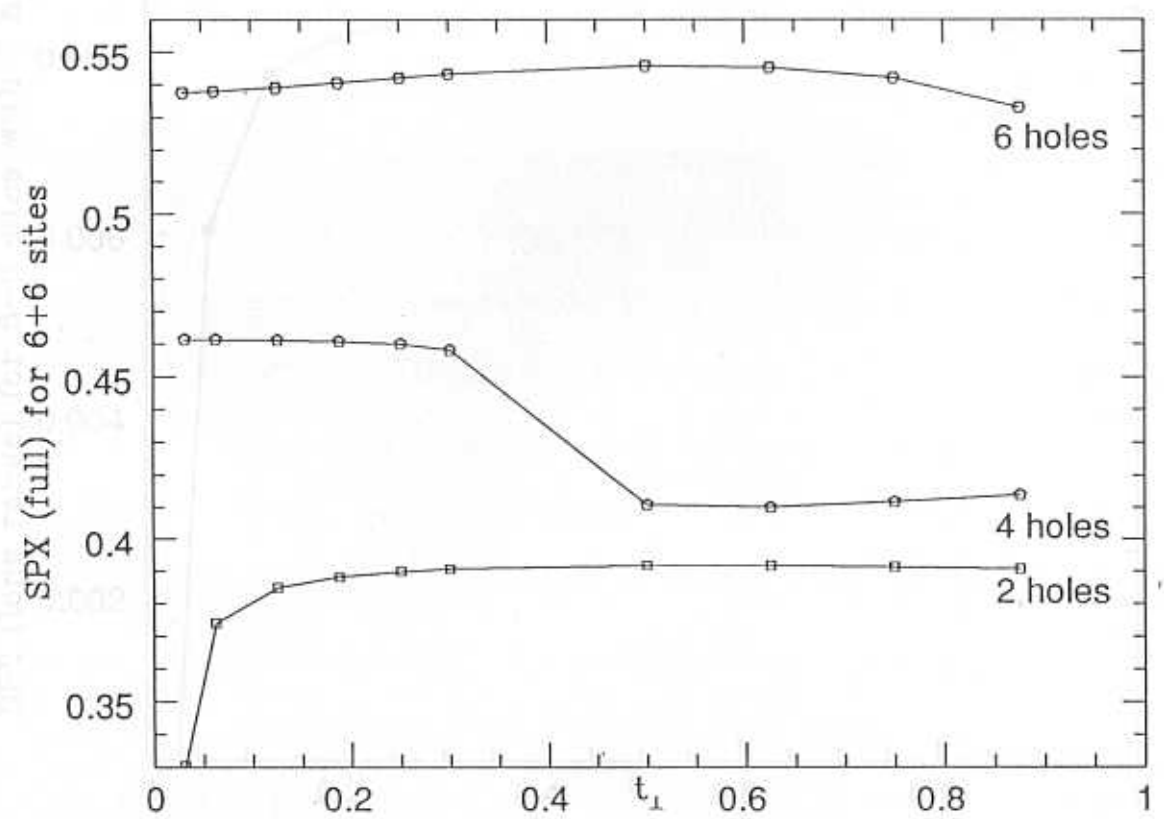

Fig. 5.3 SPX for the 6+6 cluster.

To show this, we have subtracted in the expression for SPX, those terms with none of the indices $< i,j >, < k,l >$ in equation (5.1) equal i.e. terms wherein bonds $< i,j >$ and $< k,l >$ neither overlap nor touch, and examined the resulting behavior of SPX with $t_\perp$ for 6+6 with two holes. The results are shown in fig. (5.4). The figure demonstrates the dramatic increase of the "long range" part of the pair susceptibility by a factor of 30. A similar increase is noticed for the $4+4$ and $5+5$ cases. We have also observed similar results for a large U Hubbard model where the enhancement of pair susceptibility due to interlayer tunneling is clearly visible.

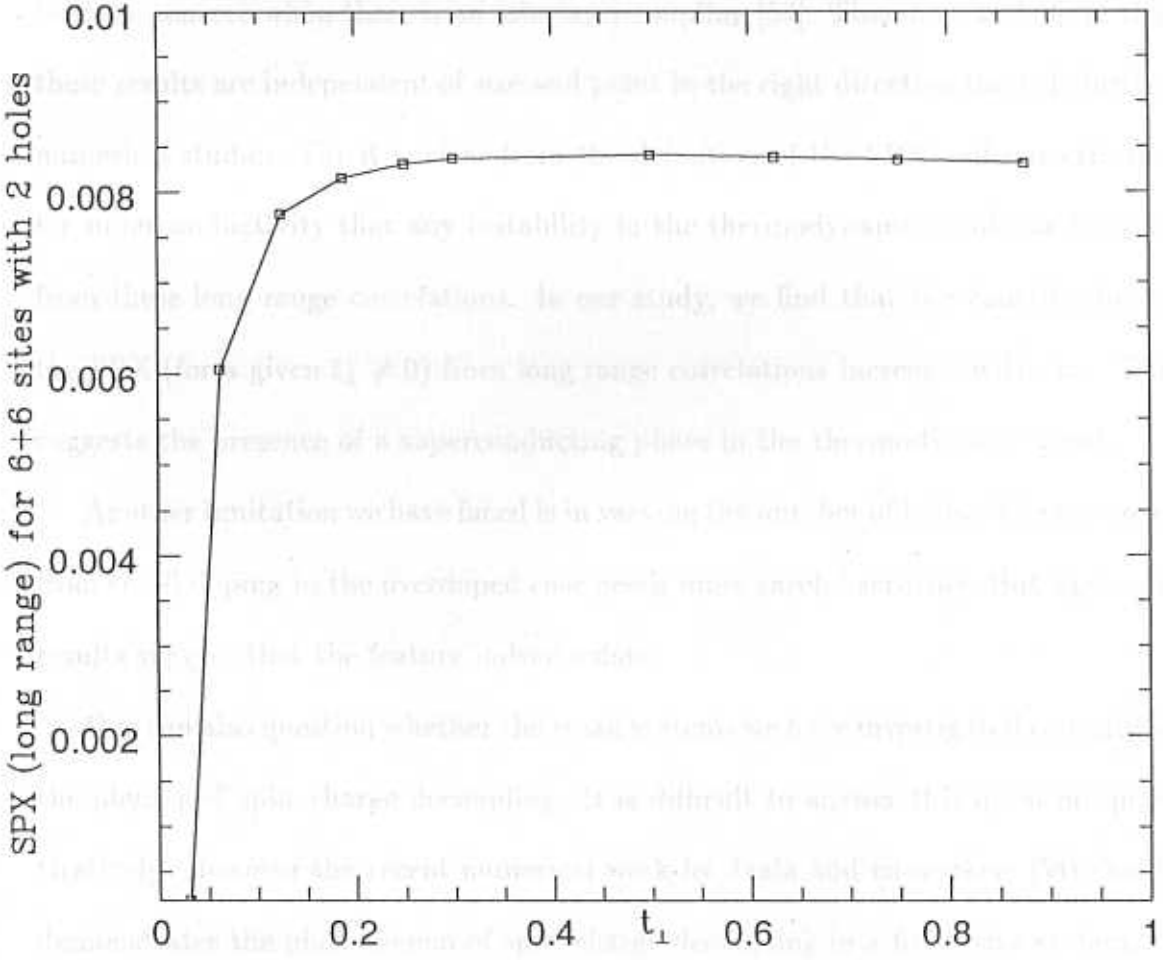

Fig. 5.4 Long range correlations in the 6+6 cluster.

5.3 Discussion and summary

First, we address the question of finite size scaling. Comparison of our data for the $4+4$ and $6+6$ cases shows a scaling which is slightly smaller than N. From our results it is also clear that $5+5$ is quantitatively different. This we believe to be an even–odd feature. Since we have not diagonalized larger clusters, we are aware that these results are not conclusive with regard to scaling. However, recent work on $8+8$ clusters show similar results [52]. There has also been a report that Monte Carlo studies of coupled Hubbard clusters show that inplane superconducting correlations become nonzero when there is an interlayer coupling [53]. Therefore we believe that these results are independent of size and point in the right direction towards further numerical studies. For it is clear from the definition of the SPX and our criterion for superconductivity that any instability in the thermodynamic limit has to come from these long range correlations. In our study, we find that the contribution to the SPX (for a given $t_\perp \neq 0$) from long range correlations increases with size. This suggests the presence of a superconducting phase in the thermodynamic limit.

Another limitation we have faced is in varying the number of holes. The crossover from small doping to the overdoped case needs more careful scrutiny. But again our results suggest that the feature indeed exists.

One can also question whether the small systems we have investigated can exhibit the physics of spin–charge decoupling. It is difficult to answer this question quantitatively. However the recent numerical work by Jagla and co-workers [54] clearly demonstrates the phenomenon of spin–charge decoupling in a finite size system.

Before we conclude, we note that for the case of $4+4$ sites with two holes, the SPX *decreases* with $t_\perp$ if the single occupancy constraint is not enforced. This result

Chapter 6

Single electron tunneling

In this last chapter, we describe two important results concerning single electron tunneling between the Cu-O planes. In section 6.1, we demonstrate why "confinement" is a *sine qua non* for pair tunneling to operate. In section 6.2, we use a toy model to analyse the effect of single particle tunneling on the WHA gap equation.

6.1 Importance of "confinement"

In chapter 4, we saw how the pair tunneling mechanism leads to high T_c 's. Interlayer hopping conserves the individual momenta of electrons that tunnel between coupled layers. This leads to a pairing term in the hamiltonian which is different from the usual BCS pairing term in that only one k-value is summed. The gap equation which results is different from the BCS gap equation and gives rise to high T_c 's. Since pair tunneling is nothing but Josephson coupling between the Cu-O layers, it is natural to ask why this mechanism cannot operate in conventional materials giving rise to high T_c 's. It is here that the role of "confinement" of electrons in a plane becomes crucial. To see this, let us consider the following hamiltonian H_0.

$$H_0 = \sum_{k\sigma} \xi_k (c^{l\dagger}_{k\sigma} c^{l}_{k\sigma} + c^{m\dagger}_{k\sigma} c^{m}_{k\sigma}) + \sum_{kq} V_{kq} (c^{l\dagger}_{k\uparrow} c^{l\dagger}_{-k\downarrow} c^{m}_{-q\downarrow} c^{m}_{q\uparrow} + h.c.). \qquad (6.1)$$

H_0 is a toy model describing a two layer (l and m are layer indices) system where superconductivity arises from a pair hopping term. V_{kq} is assumed to have the usual BCS form,

$$V_{kq} = \begin{cases} -V < 0 & \epsilon_F - \hbar\omega_c < |\xi_k|, |\xi_q| < \epsilon_F + \hbar\omega_c \\ 0 & \text{otherwise} \end{cases}$$

(All energies ξ_k are measured relative to the Fermi energy.)

If the electrons are not confined to the plane, viz., single electron tunneling between layers l and m is not blocked, then there is another term that has to be added to H_0. This term is of the form $-t_\perp \sum_{k\sigma}(c^{l\dagger}_{k\sigma}c^m_{k\sigma} + h.c.)$. (It might be pointed out that the pairing term in the hamiltonian H_0 is not the WHA term. Recall that in the WHA term, only one k-value is summed. The effect of single electron hopping between layers on the WHA gap equation is discussed in the next section. Here, we only want to demonstrate that the presence of single electron hopping inhibits superconductivity. This is a result that is independent of the actual mechanism of superconductivity.) With this extra term, we rediagonalize H_0 and obtain the following gap equation

$$\frac{1}{V} = \frac{1}{2}\sum_k \frac{\tanh\frac{\beta E^+_k}{2}}{2E^+_k} + \frac{1}{2}\sum_k \frac{\tanh\frac{\beta E^-_k}{2}}{2E^-_k} \tag{6.2}$$

where $E^\pm_k = \sqrt{(\epsilon_k \pm t_\perp)^2 + \triangle^2_k}$.

It is easy to see that T_c is given by

$$k_B T_C \propto \sqrt{\hbar^2\omega_c^2 - t_\perp^2}\ \exp -(\frac{1}{N(0)V}).$$

$N(0)$ is the density of states at the Fermi level. In fig. (6.1), we have plotted $\frac{k_B T_c(t_\perp)}{k_B T_c(0)}$ with $\hbar\omega_c$ chosen to be 0.1 eV (keeping in mind typical phonon energies). It is clear that T_c *decreases* with $t_\perp$ or is insensitive to it depending on the magnitude

of $\hbar\omega_c$ (the cutoff). This behaviour is in complete contrast with the WHA mechanism where T_c *increases* with $t_\perp$. The reason behind this becomes clear when we look at the zero temperature gap equation

$$\frac{2}{N(0)V} = \sinh^{-1}\left(\frac{\hbar\omega_c - t_\perp}{\triangle(0)}\right) + \sinh^{-1}\left(\frac{\hbar\omega_c + t_\perp}{\triangle(0)}\right)$$

The single electron tunneling term acts as a pair breaking mechanism and destroys superconductivity. i.e., the condensation energy gained can be compensated by the kinetic energy associated with c-axis tunneling. For purposes of illustration, we choose $N(0)V = 0.3$ and $\hbar\omega_c = 0.025$eV. The results for $\triangle(0)$ as a function of $t_\perp$ are plotted in fig. (6.2). These results show how single electron hopping between layers inhibit superconductivity.

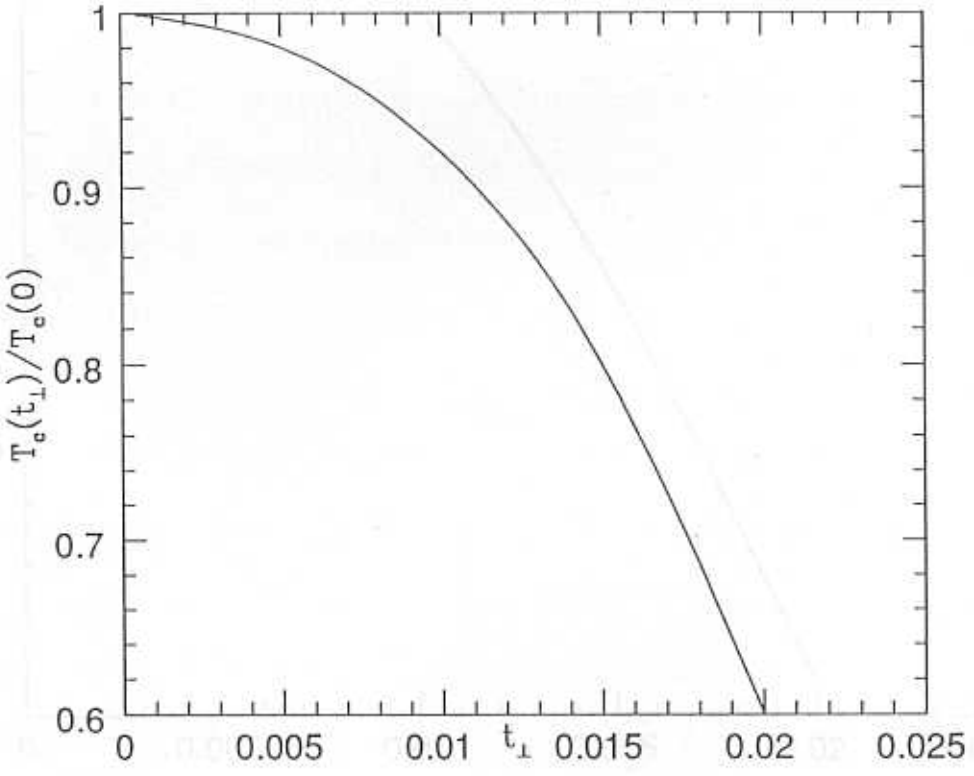

Fig. 6.1 T_c as a function of $t_\perp$ in the absence of "confinement".

They are especially important in the context of the cuprate superconductors, where $t_\perp \leq 0.15t$ and $t \sim 0.3$ eV. So, if the notion of confinement is not invoked, there is no reason why T_c should be enhanced by $t_\perp$. This means the notion of pair hopping without confinement is inconsistent, which is why mean field theories of the t-J model (where the notion of confinement is absent) show a decrease of T_c with $t_\perp$[55]. It is for the same reason that the inplane superconducting correlations were found to decrease with $t_\perp$ in our finite size study when the constraint on double occupancy was removed (cf. fig. 5.1).

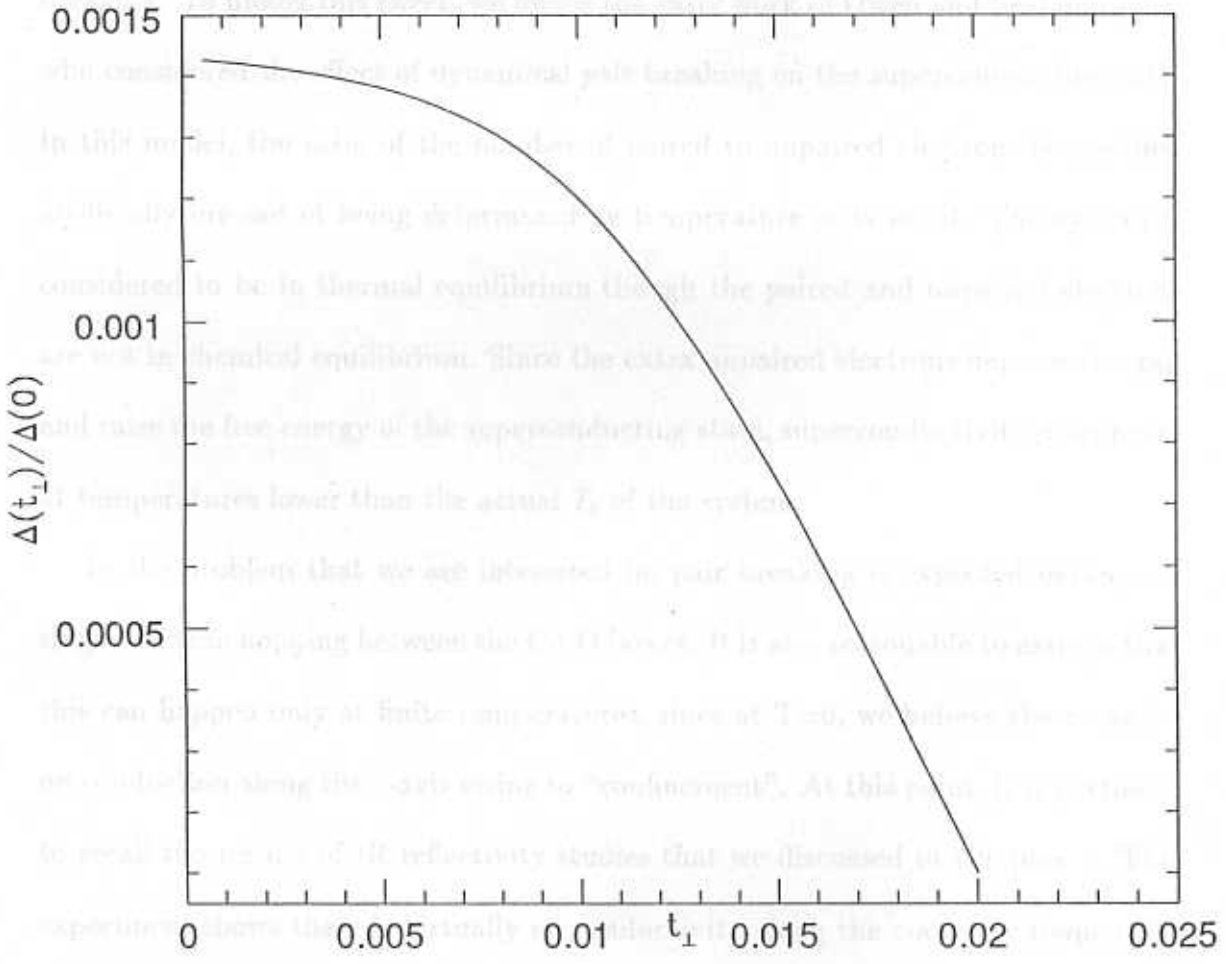

Fig. 6.2 Zero temperature gap

6.2 Dynamical pair breaking

In this section, we examine the effect of single electron hopping (between layers) on the gap equation (4.2). The correct way to do this is to write down the Hubbard hamiltonian for the layers with a c-axis hopping term coupling the layers and treat the latter perturbatively. This is a difficult problem and we do not know how to solve it. Instead, we adopt the following approach.

In the previous section, we saw that single electron hopping acts as a pair breaking mechanism. So we analyze how the WHA gap changes in the presence of pair breaking. To model this effect, we follow the early work of Owen and Scalapino [57] who considered the effect of dynamical pair breaking on the superconducting state. In this model, the ratio of the number of paired to unpaired electrons is specified artificially instead of being determined by temperature as is usual. The system is considered to be in thermal equilibrium though the paired and unpaired electrons are not in chemical equilibrium. Since the extra unpaired electrons depress the gap and raise the free energy of the superconducting state, superconductivity disappears at temperatures lower than the actual T_c of the system.

In the problem that we are interested in, pair breaking is expected because of single electron hopping between the Cu-O layers. It is also reasonable to assume that this can happen only at finite temperatures, since at T=0, we believe there can be no conduction along the c-axis owing to "confinement". At this point, it is pertinent to recall the results of IR reflectivity studies that we discussed in Chapter 1. This experiment shows there is virtually no conductivity along the c-axis for frequencies $\omega \sim$100 cm^{-1}. This suggests that c-axis hopping can operate at temperatures $\sim$ 100 K. This causes the number of unpaired electrons to increase and the gap decreases.

Once the gap decreases it becomes easier to break pairs and the mechanism feeds on itself. This causes the gap to fall steeply [56]. (As mentioned in Chapter 4 , the gap in the cuprate superconductors does fall steeply at the observed T_c and there has been some speculation that this is because of pair breaking.)

We now calculate the gap Δ_k as a function of temperature and the excess number of unpaired electrons N_q. N_q is fixed by the condition $\sum_{k\sigma}\langle\gamma^\dagger_{k\sigma}\gamma_{k\sigma}\rangle = N_q$ where γ_k are the usual quasiparticle operators. The effect of the additional constraint is to introduce another chemical potential μ^* in the gap equation (4.2) and the modified gap equation is

$$1 = \frac{\Lambda}{2E_k}\tanh\frac{\beta(E_k-\mu^*)}{2}, \tag{6.3}$$

where μ^* is fixed by the condition

$$\sum_k \frac{1}{\exp(\beta(E_k-\mu^*))+1} = \frac{N_q}{2}.$$

The above equation can be rewritten as

$$1 = \frac{\Lambda}{2E_k}[1-2n_k(\mu^*)], \tag{6.4}$$

where $n_k(\mu^*) = \dfrac{1}{\exp(\beta(E_k-\mu^*))+1}$.

When $\mu^* = 0$, we have the original gap equation which we write as

$$1 = \frac{\Lambda}{2E_k^0}\tanh\frac{\beta E_k^0}{2} \tag{6.5}$$

(where E_k^0 correponds to the case $\mu^* = 0$).

From equation (6.4), we obtain the expression for the excess quasiparticle number $\bar{n}_k$

$$\bar{n}_k = n_k(\mu^*) - n_k(0) = \frac{E_k^0 - E_k}{\Lambda}$$

The gap at any temperature, $\triangle_k(T)$ can now be expressed in terms of $\bar{n}_k$ as

$$\triangle_k^2 = \triangle_k^{02} + \Lambda^2 \bar{n}_k \left(\bar{n}_k - \tanh \frac{\beta E_k^0}{2} \right)$$

For small n_k, we have the general result

$$\triangle_k^2 = \triangle_k^{02} - \alpha(T),$$

where the temperature dependence of α will also be governed by that of n_k. Note that α will also depend on $t_\perp$. The addition of the temperature dependent term $\alpha(T)$ to the gap will cause disappearance of superconductivity at temperatures below the "real" T_c of the material. At any given temperature, it is also clear that an increase in $\bar{n}_k$ will lead to a decrease in $\triangle_k$ until it falls to zero. This result should be compared with Anderson's arguments [46] based on entropy considerations that $\triangle_k \rightarrow \triangle_k - \gamma_k T^2$. It should also be recalled that the gap equation (4.2) by itself leads to an anomalous temperature dependence of the gap which we discussed in Chapter 4. A more comprehensive theory is needed to discern which of these effects is the most important.

To summarize the results in this chapter, we discussed the role of single electron hopping in the context of the pair tunneling mechanism. We showed that if c-axis hopping is not blocked, then T_c is a decreasing function of the hopping matrix element, $t_\perp$. We also showed how single electron hopping at finite temperatures can act as a dynamical pair breaking mechanism and argued this might make the WHA gap fall steeply near T_c.

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