CHAPTER 1

INTRODUCTION

1.1 SOME THEORIES OF SUPERCONDUCTIVITY IN THE CUPRATES

There are many theories of superconductivity in the cuprates. One class of theories tries to modify the theory of Bardeen, Cooper and Schrieffer (BCS) for superconductivity in normal metals and apply it to the cuprates. The basic interaction that pairs the electrons into Cooper pairs is still the electron-phonon interaction. Another class uses the typical two dimensional structure of the cuprates which allows them to be described by spin $1/2$ electrons on Cu-O plaquettes. Strong interactions between the electrons play a crucial role and the pairing interaction is based on an electron-electron mechanism. Here we give a short overview of the main theories (apart from BCS) that are relevant for the work in this thesis [1, 2, 3].

1.1.1 RVB

One of the first theories of superconductivity in the cuprates after its discovery came from Anderson [4, 5]. He proposed that pairs of spins on the copper atoms would form singlet pairs in a dynamic way [6], that is, by continuously changing partner, where double occupancy of the sites are not allowed. This results in a so called "resonating valence bond" state. The corresponding wave function is very similar to a BCS wave function and this forms Anderson's Ansatz for the wave function in the cuprates [7]. The Hamiltonian that works on this wave function is the $t - J$ Hamiltonian. The excitations of the RVB state are peculiar [8, 9]. When a singlet pair with total spin zero is broken (which costs an energy J) the system is left in an exited spin state. With respect to the ground state there

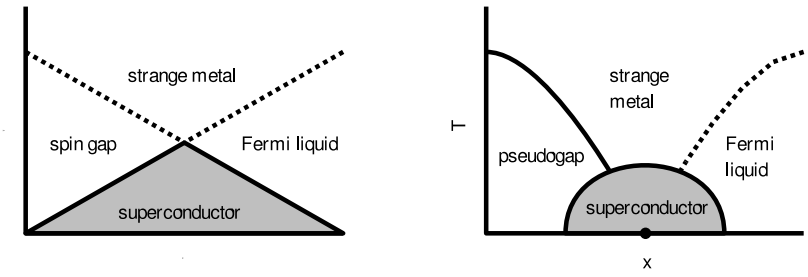

Figure 1.1: *Phase diagrams for the cuprates as obtained from the RVB picture (left) of from a quantum critcal picture (right).*

is no change in charge, but there is a change in the spin, giving one object with spin up and one with spin down. Another excitation can be made by taking out an electron which changes the total charge of the system and leaves one single spin from a broken pair. The quasiparticles are therefore objects with spin but no charge (spinons) and objects with charge but no spin (holons). For zero doping the mean field temperature T_{MF} at which the singlets form is highest, but the pairs are not mobile and superconductivity is suppressed. As the doping is increased T_{MF} lowers, but the phase coherence temperature of the doped holes increases because it is proportional to doping. This results in the phase diagram shown in figure 1.1. In the right quadrant the system is a normal metal. In the lower quadrant the system is a superconductor, where T_c is limited on the left side of optimal doping by the hole concentration and on the right side by T_{MF}. In the left quadrant the system has a spin gap caused by the antiferromagnetic superexchange. The extra kinetic energy required to open the spin gap is released at the superconducting temperature T_c by making the charge fluctuations coherent [10]. In the upper quadrant the system is a 'strange metal'.

For zero doping the groundstate of the $t - J$ Hamiltonian turns out to be not the RVB state, but the antiferromagnetic state, due to 3 dimensional antiferromagnetic coupling. At finite doping and finite (low) temperature it is possible [7] that the RVB state is indeed the ground state of the Hamiltonian, which results in superconductivity.

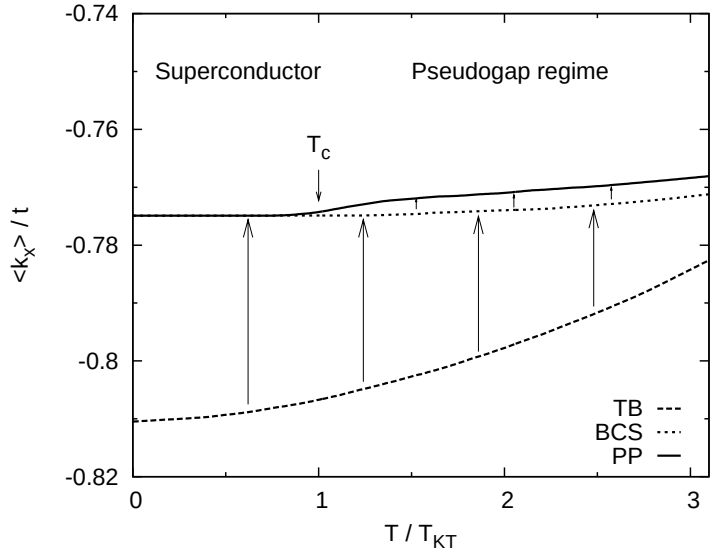

Figure 1.2: *Kinetic energy per bond, $< k_x >$, as a function of temperature for the noninteracting tight-binding electrons (TB), the BCS solution (BCS), and the phase-fluctuation (PP) model. The large vertical arrows indicate the increase in kinetic energy upon pairing, relative to the free tight-binding model, and the small arrows indicate the additional increase due to phase fluctuations. This additional phase-fluctuation energy rapidly vanishes near T_c. Figure from [11].*

1.1.2 PHASE FLUCTUATION SCENARIO

Cuprates should be thought of as doped Mott insulators, which means that, for low doping, the number of carriers is small. As the superconducting phase is conjugate to the number operator, this implies that phase fluctuations can play an important role on the underdoped side of the phase diagram, destroying superconductivity if they are too strong. The key idea of the phase fluctuation scenario in the high-T_c superconductors is the notion that the pseudogap arises from phase fluctuations of the superconducting order parameter [11]. In this scenario, below the mean-field temperature scale T_{MF}, a $d_{x^2-y^2}$-wave gap amplitude is assumed to develop. However, the superconducting transition is suppressed to a considerably lower transition temperature by phase fluctuations. In the intermediate temperature regime phase fluctuations of the superconducting order parameter give rise to the pseudogap phenomena. In order to have con-

densation into the superconducting state one needs, in addition to the binding of charge carriers into Cooper pairs, long-range phase coherence among the pairs. When coherence is lost due to thermal fluctuations of the phase at and above the transition temperature T_c, pairing remains, together with short-range phase correlations. Phase fluctuations contribute to a significant reduction of the in-plane kinetic energy upon entering the superconducting phase below T_c. The physical reason for this kinetic energy lowering is that due to phase fluctuations and the associated incoherent motion of the Cooper pairs, the pseudogap region has an higher kinetic energy (figure 1.2). When long range phase coherence finally develops at T_c, the Cooper-pair motion becomes phase coherent and the kinetic energy decreases. This effect is independent of the particular mechanism leading to pair formation [12].

1.1.3 HOLE SUPERCONDUCTIVITY

Also quite early after the discovery of superconductivity in the cuprates Hirsch proposed the theory of hole superconductivity [13, 14, 15, 16]. An important aspect of the model is a fundamental asymmetry between electrons and holes [17]. Hirsch proposes that holes are the key component of superconductivity, and in particular that in high-T_c oxides superconductivity originates from conduction of holes through O^{2-} anions. A hole causes a large disruption of its background, the filled shell anion. This deformation, which leads to considerable modification in outer-shell electron wave functions, facilitates hopping of a hole of spin σ to a neighboring site which has already been occupied by a hole of spin $-\sigma$ [18]. This results in a term in the Hamiltonian describing an enhanced hopping rate for a hole if other holes are in the vicinity. This term explicitly breaks electron-hole symmetry and, together with an attractive interaction between holes, causes considerable effective-mass enhancement for nearly filled electron bands.

The kinetic energy part of the Hamiltonian is given by:

$$T = -\sum_{<ij>\sigma} t_{ij\sigma}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.\right) \tag{1.1}$$

with

$$t_{ij\sigma} = t + \Delta t\left(n_{i,-\sigma} + n_{j,-\sigma}\right)$$

where i, j are nearest neighbor sites on a two dimensional square lattice and $c^{\dagger}_{i}$ creates a hole on site i. It describes the hopping of holes from an O^{2-} to the next O^{2-} anion in a CuO_2 plane. The hopping term for hopping from site i to j is

larger by Δt if a hole with opposite spin is already present on the oxygen atoms [19].

At low carrier density, carriers are heavily dressed in the normal state, due to coupling to a bosonic degree of freedom. When carriers pair and the system becomes superconducting, carriers partially undress. Similarly, when the system is doped in the normal state, carriers increasingly undress [20]. This will occur if the coupling to the boson degree of freedom is a function of the local carrier concentration, and becomes weaker as the local carrier concentration increases. This feature is what makes the material a high-temperature superconductor: carriers will pair in order to undress, i.e., in order to reduce the coupling to this bosonic degree of freedom. At high concentrations, carriers are already undressed in the normal state, and hence superconductivity does not occur. The undressing will result in a lowering of the system's free energy, and hence to the condensation energy of the superconductor. Because it is an undressing transition, the kinetic energy is lowered as the system becomes superconducting; as the carriers undress, their effective mass decreases, and this higher mobility in the superconducting state is what provides the "glue" for the collective order.

1.1.4 INTERLAYER TUNNELING THEORY

In the interlayer tunneling theory by Anderson [21, 22, 23] the interlayer pairing energy is the mechanism for superconductivity in the cuprates. The two-dimensional state of the electrons in the copper oxide planes has separation of charge and spin into excitations which are meaningful only within their two-dimensional substrate; to hop coherently as an electron to another plane is not possible, since the electron is a composite object, not an elementary excitation [24]. Absence of coherent c-axis electron motion in the cuprate layer compounds implies excess of kinetic energy in this direction. Josephson-type, two-electron transport is not blocked because the spinon fluid is a pair condensate, so that singlet pairs tunnel freely. This makes the superconducting transition a 2 to 3 dimensional crossover. The actual nature of the pairing wave function is determined not by the basic interlayer mechanism which raises T_c but by the "residual interactions", be they caused by phonons, spin-fluctuations or another source.

The pairing mechanism is thus amplified within a given layer by allowing the Cooper pairs to tunnel to an adjacent layer by the Josephson mechanism. The electrons are paired at a higher temperature because the interlayer mechanism allows them to lower their c-axis kinetic energy. The ILT model predicts that the superconducting condensation energy is approximately equal to the gain in kinetic energy of the electron pairs due to tunneling. Both these quantities can

be determined independently. In a series of papers by a team in Princeton and Groningen [25, 26, 27, 28, 29] it was shown that for $Tl_2Ba_2CuO_6$ the prediction based on the ILT model was two orders of magnitude different from the measured value. This ruled out ILT as a mechanism for superconductivity in the cuprates.

1.1.5 SO(5)

In the SO(5) theory of superconductivity the antiferromagnetic phase and the superconducting phase are two projections of one and the same 5-dimensional 'superspin' order parameter [30]. Three components of this order parameter are the three degrees of freedom of the Néel order and two components are the real and imaginary part of the superconducting order parameter. The superspin order parameter can, for example, point entirely in the 'antiferromagnetic' direction, giving antiferromagnetism, and then be rotated to the 'superconducting' direction. Such a rotation corresponds to applying a new operator, resulting from the SO(5) theory, to the state of the system. The order parameter of the antiferromagnetic state is the sublattice magnetization, a real 3D vector; if this vector is different from zero, there is antiferromagnetic order. Consider two fixed neighboring sites in the 2D antiferromagnet, for example in the $(\uparrow\downarrow)$ configuration. This fixed spin configuration may be viewed as a superposition of the singlet $(\uparrow\downarrow - \downarrow\uparrow)$ and the $(S_z = 0)$ triplet $(\uparrow\downarrow + \downarrow\uparrow)$. To create the macroscopic 2D antiferromagnet in the CuO_2 plane, therefore, we have to mix triplet excitations already at high temperatures into the possible singlet configurations of the spin liquid [31]. The antiferromagnetic state then results as a kind of 'condensation' of the triplet excitations into the lowest possible energy state. The density of the 'condensed triplets' corresponds to the magnitude of the sublattice magnetization. If, in the antiferromagnetic state the triplet excitation operator is replaced by a hole pair creation operator, we obtain a state which creates a macroscopic number of Cooper pairs, i.e., a superconducting state. The antiferromagnetic to superconductor 'rotation', therefore, is described by an operator, the π-operator, which replaces triplets by hole pairs.

1.1.6 QUANTUM CRITICALITY

In three dimensions fluctuations are usually weak and in one dimension they are too strong for long range order. However, In two dimensions there is a delicate balance between order and fluctuations with many interesting properties. The phase diagram of the cuprates as a function of doping and temperature is

rich with all kinds of (competing) orders and transitions between these orders, even at zero temperature. Because the dominating physics of the cuprates is believed to be 2-dimensional, the theory of quantum criticality might give some insight in the phase diagram [32] (A somewhat longer introduction into quantum criticality is given in chapter 5). One phase diagram for the cuprates with a quantum critical point is shown in figure 1.1. The proposed theory is that on the right hand of the critical point there is normal superconductivity, while on the left hand side there is a coexistence of charge ordering and superconductivity [33, 34, 35, 36]. Above the critical temperature the charge ordering leads to the pseudogap phase. In another theory of quantum criticality in the cuprates the ordered phase consists of stripe ordering [37]. In fact, there are more critical points in the phase diagram: one where the Néel order vanishes, one where superconductivity emerges, and one where superconductivity vanishes, but the main focus is on the evasive and enigmatic critical point close to optimal doping.

1.1.7 Marginal Fermi Liquid

The temperature dependence of the in-plane normal state resistivity of the cuprates is surprisingly linear, unlike the T^2 temperature dependence expected for a Fermi-liquid. Varma and co-workers proposed a theory to explain this property [38, 39]. The momentum distribution function no longer has a jump at k_F, but the derivative does diverge at his point, like in a usual Fermi-liquid distribution function. Hence the name marginal Fermi-liquid.

Translated into a frequency dependent scattering rate this results in

$$1/\tau(\omega) \sim max(\omega, T) \tag{1.2}$$

In the marginal Fermi-liquid theory there is no energy scale other than temperature and therefore shows quantum critical scaling.

1.2 Outline

A general property many of the theories that use strong electron-electron interaction to form Cooper pairs is the lowering of kinetic energy when the system goes superconducting. In such theories, above T_c, the interaction keeps the electrons confined and in a higher kinetic energy state with less possibilities to move around. When the electrons are paired and condensed, this energy is released and the kinetic energy of the system is lowered. This is the main source for the internal energy to be lowered, which results in the transition to the superconducting state. This is to be contrasted with the usual BCS theory where the

kinetic energy is increased when the system becomes superconducting and the main internal energy lowering comes from the lowering of potential energy.

This is a clear difference between the two classes of theories about superconductivity in the cuprates and a measurement of the kinetic energy is needed. This turns out to be possible when the optical conductivity of the material is measured, since this is related to the kinetic energy in certain cases. Careful measurements of the temperature dependence of the optical conductivity can give insight into the changes in kinetic energy that occur as T_c is crossed.

Also the quantum critical scenario has clear consequences for the optical conductivity of the system, this time in the frequency dependence for the infrared region.

In chapter 2 we describe the characterization of a new infrared ellipsometer build in our group. In chapter 3 measurements of spectral weight changes in several cuprate superconductors are presented and carefully analyzed. In chapter 4 ellipsometry measurements of conventional superconductors are presented. In chapter 5 the phase of the optical conductivity in the normal state of $Bi_2Sr_2Ca_{0.92}Y_{0.08}Cu_2O_{8+\delta}$ is shown to be consistent with a quantum critical scenario for the cuprates around optimal doping.