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EXPERIMENTAL WORKSHOP ON
HIGH TEMPERATURE SUPERCONDUCTORS AND RELATED MATERIALS
(BASIC ACTIVITIES)

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" Introduction to High T_c Theory "

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Introduction to High-Tc Theory

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Abstract

In these introductory lectures the basic experimental facts of high temperature superconductivity are briefly reviewed. The weak coupling approach based on Fermi liquid theory is then discussed versus the strong-coupling theory starting from the Mott-Hubbard insulating state. Finally, the working models in the strong coupling approach are considered.

1. Basic Experimental Facts

The revolutionizing discovery of high temperature superconductivity (SC) by Bednorz and Müller [1] has given rise to enormous efforts in experimental and theoretical studies of such a striking phenomenon. At the early stage of this endeavour the experimental results were diverging, mainly due to difficulties in preparing good quality samples. Recently, the situation has been improved significantly, and experiments of various groups seem to yield converging results, implying thus quite strict constraints on possible theoretical models.

Structures of so far discovered oxide superconductors are described in the lectures of Prof. Uchida and will not be repeated here. In what follows we briefly summarize the main experimental observations. More complete reviews can be found in recent conference proceedings [2 - 4] and the review series [5].

1.1 Superconducting Properties

First of all, these oxide superconductors share all basic properties of ordinary superconductors like Meissner effect, zero resistance and flux quantization in units hc/2e [6], i.e. the charge carriers are paired. The existence of an energy gap in the excitation spectrum was disputed at the beginning of the high T_c heat wave, but now it is more or less established by optical absorption [7], tunneling measurements [8] and high-resolution photoemission experiments [9]. The ratio $2\Delta/kT_c$ is within the range $2 \sim 8$ depending still on materials, samples and measuring techniques. There is a jump in the specific heat at the transition temperature in La- and Y- compounds and the ratio $\Delta C/\gamma T_c$ is more or less consistent with the BCS theory [10]. However, no such jump has been observed in Bi- compounds [11].

Moreover, the Ginzburg-Landau phenomenological theory discussed in Prof. Kumar's lectures is still a good description for this new type of superconductors [12]. In particular, the critical magnetic field H_c and the energy gap parameter Δ vanish continuously at T_c, while the coherence length ξ and the London penetration depth λ diverge at this point. The main modifications needed are connected with the short correlation length (only a few lattice constants in CuO_2 plane) and the strong anisotropy (difference in one order of magnitude). Because of the short correlation length all of them are extreme type II superconductors.

Furthermore, all manifestations of macroscopic coherence due to electron pairing, like Josephson effects (dc and ac) and Andreev

reflection do take place in oxide superconductors. As for more subtle effects due to microscopic coherence such as the difference between the absorption of acoustic waves and the nuclear relaxation rate near T_c (see Prof. Kumar's lecture), they are less pronounced in these superconductors, probably due to the smearing effect of pair breaking scattering.

1.2 Anomalous Properties of Normal State

There are some normal state properties of oxide superconductors which can be interpreted as doped semiconductors. For example, one can extract the effective mass from the measured Pauli magnetic susceptibility and the Drude component of the optical absorption [10,13]. These values are consistent with each other and they are about twice the free electron mass. However, the mere fact of the reference compound being an insulator cannot be explained within the single particle picture (See the next section). As a whole, the normal state properties of oxide superconductors are as perplexing as the high transition temperature itself.

1.2.1 Transport Properties

The transport properties are among the most puzzling ones. The resistivity in the CuO_2 plane is linear in temperature for almost all layered superconductors [14,15]. The possibility of interpreting this result as due to coupling to phonons (in which case a linear dependence is expected for $T > \theta/4$ with θ as the Debye temperature) is ruled out by very recent experiments on Bi-compounds with T_c down to 10K showing good linear behavior over two orders of temperature change (See Fig.1) [16]. Of course, from resistance measurements alone it is difficult to conclude whether the temperature dependence is due to the density of states, or due to the scattering rate τ^{-1}. The optical absorption consists of a Drude peak and a broad background [13]. The scattering rate can be

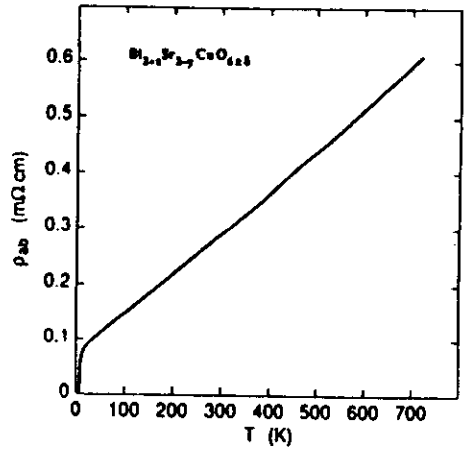

Fig. 1: Resistivity of the single layer Bi superconductor. From Ref. [16], S. Martin et al.

determined from the width of the Drude peak which turns out to be $\sim 2kT$. Hence this linear temperature dependence is not a density of states effect.

The conductivity in the perpendicular direction is more controversial, but roughly speaking, it is proportional to T^{α} with α close to 1 [14-15]. Of course, one may still argue whether this is an intrinsic property. On the other hand, the thermal conductivity in the CuO_2 plane is almost temperature independent [17]. If one assumes that both electric and thermal conductivities are contributed by the same carriers (holes or electrons), the Wiedemann-Franz law $K(T)/\sigma(T)T$ = const is still valid, although its meaning is different from the case of ordinary metals.

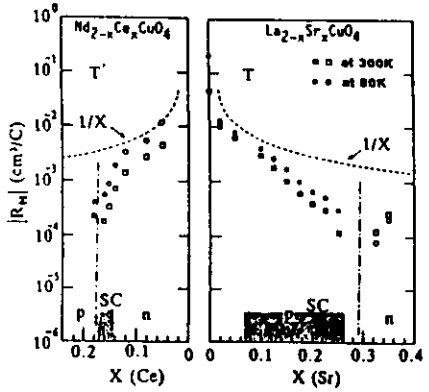

Fig. 2: The absolute value of the Hall coefficient as a function of Ce compostition for reduced $Nd_{2-x}Ce_xCuO_{4-y}$. The same plot for $La_{2-x}Sr_xCuO_4$ are shown for comparison. From Ref. (18), S. Uchida et al.

Among others, the behavior of Hall constant R_H as a function of charge carrier concentration is most striking. As shown in Fig.2 taken from Ref.18, the Hall constant is positive for doped La-compounds (the shaded range corresponds to superconductors), but R_H changes sign near $x = 0.3$ (please note, the absolute value $|R_H|$ is plotted in Fig.2). This means that some drastic change (metal-insulator transition?) is taking place there. On the other hand, R_H is negative for the newly discovered electron superconductors (See Prof. Uchida's lecture). Similarly, it changes sign at the boundary of normal metals and superconductors. In principle, the sign of R_H is very sensitive to the geometry of the iso-energy surface of charge carriers. However, such a pronounced regularity cannot be pure accident. As for the magnitude of R_H, it is proportional to $1/x$ for small concentration x, and it deviates from this rule for higher concentrations. As we will discuss in the next section, this anomalous behavior of R_H is consistent with the Mott-Hubbard model, but it is very difficult to fit the conventional Fermi liquid (FL) picture.

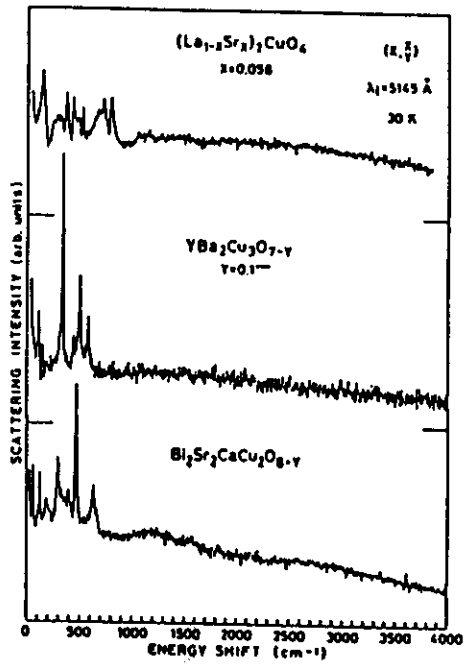

Fig. 3: Raman scattering intensity for various superconducting Cu-O compounds. From Ref. (19), Sugai et al.

1.2.2 Background Scattering

There are several experiments which show quite clearly strong scattering of charge carriers on background fluctuations.

First of all, it shows up in Raman experiments [19] where the background extends up to 0.5 eV or 4000 cm^{-1} (See Fig.3). In the ordinary metals, similar background due to electron-hole pair fluctuations is limited to a few tens of wave numbers (i.e. two orders of magnitude less).

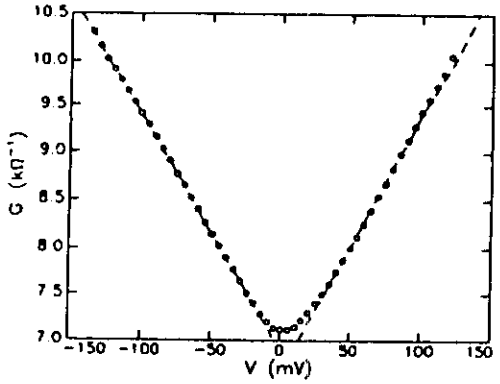

Fig. 4: Tunneling conductance of $YBa_2Cu_3O_{6.9}$, from Ref. (4), M. Gurvitch et al., and J. Valles (p. 364).

Secondly, as mentioned earlier, there is a strong background scattering up to about 1eV in optical absorption [7,20]. This part of absorption decays roughly like ω^{-1}.

Thirdly, the tunneling conductance in the normal state G shows a linear dependence on voltage (See Fig.4)

$$G = g_0 + g_1 |V| \qquad (1)$$

over a wide range (up to 150 meV). Apparently, this is a density of states effect because the conductance is a constant for normal metals. It is, of course, not excluded that this is again due to an anomalously strong background scattering.

Finally, the NMR and NQR relaxation behavior in the normal state is very peculiar [21]. The relaxation of Y and in-plane O nuclei obeys the Korringa law, i.e. the relaxation rate $T^{-1} \sim T$, while the relaxation rate for Cu in the same plane is much higher and deviates from the Korringa behavior (See Fig.5).

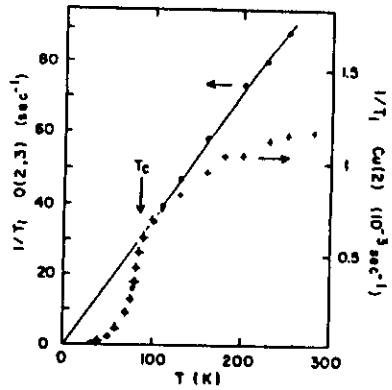

Fig. 5: Temperature dependence of $1/T_1$ at the O(2,3) (solid dots) and the Cu(2) (crosses) sites. From Ref. (2), M. Takigawa et al., p.856

1.2.3 Angle-Resolved Photoemission

The above described experiments indicate that the normal state properties of oxide superconductors deviate significantly from ordinary metals. However, the angle resolved photoemission measurements [22] seem to show the existence of a well-defined Fermi-surface which is more or less consistent with the single-particle band calculations [23]. As shown in Fig.6, the spectral density of states measured from photoemission is getting much sharper while approaching the Fermi surface. Of course, how does the imaginary part of the self-energy vary with frequency is a much more subtle question, but qualitatively it looks like an ordinary metal.

To summarize, the situation is rather controversial. On the one hand, the superconducting properties of these oxide superconductors are rather similar to what is described by the BCS

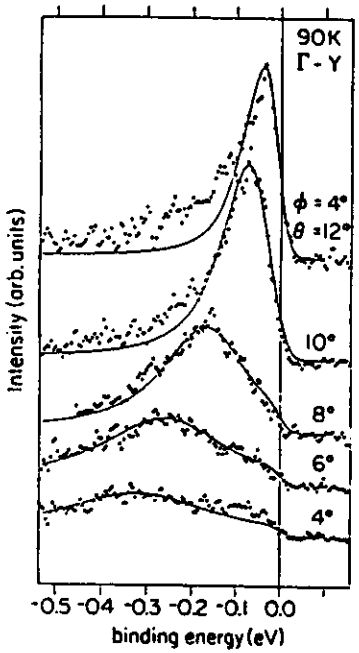

Fig. 6: Angle-resolved energy distribution curves for several angles above the Γ - Y direction in the Brillouin zone using photons of energy 22eV after removing the background. The lines are fits using a linear energy dependent broadening. From Ref. (22), C.G. Olson et al.

theory which is based on the Landau FL picture. On the other hand, the major properties in the normal state are quite abnormal, very different from ordinary metals with the exception of photoemission experiments. How to construct a theoretical model which can explain these two apparently conflicting aspects, is a great challenge to the condensed matter theory.

2. Weak vs Strong Coupling Approaches

2.1 Main Questions to be Answered

As discussed in Prof. Kumar's lectures, there are two aspects of SC theory: One is more phenomenological like the Ginzburg-Landau theory, for describing the macroscopic quantum effect while the other is more microscopic to explain the origin of this striking phenomenon. Here one should be able to answer several basic questions, namely: (1) What is the scenario for macroscopic quantum effect? Is it Bose-condensation, bipolaron effect, Cooper pairing, or something entirely new? (2) What is the interaction responsible for this macroscopic condensation? Is it electron-phonon interaction, or Coulomb interaction in terms of magnetic or charge fluctuations? (3) What is the appropriate model? And finally, (4) What is the theoretical basis for describing this phenomenon?

In the BCS case the answers to these questions are very clear. (1) The scenario is Cooper pairing, which is very different from bipolaron scenario in the sense that pairs overlap each other significantly. (2) The electron-phonon interaction is responsible for such pairing but one should also take into account the screened Coulomb interaction. (3) The Fröhlich Hamiltonian is the starting point, but one can use the simple truncated BCS Hamiltonian as a working model. (4) The theoretical basis is the Landau FL theory. Although FL is discussed in Prof. Anderson's and Prof. Kumar's lectures, I would like still to emphasize a few points.

The concept "FL behavior" would mainly mean the following:

(a) In spite of strong interaction between structure particles (like electrons, ions), quasiparticles are well-defined, i.e., their real part (usually proportional to ω, energy counted from the Fermi level) is much greater than the imaginary part ($\sim\omega^2$).

(b) The quasiparticles in conductors have charge e and spin 1/2 which cannot be separated from each other.

(c) There is a well-defined Fermi surface where the single particle distribution function $n(k)$ has a finite jump equal to the residue Z in the single particle propagator $G(k,\omega)$, where

$$G(k,\omega) = \frac{Z}{\omega - E(k) + i\delta\mathrm{sgn}(\omega)} + G_{inc} \qquad (2)$$

with G_{inc} as the incoherent part. The Fermi surface contains $N/2$ k-states (Luttinger theorem). It turns out that this is a much more subtle criterion, because it is very difficult to distinguish a jump from a power-law singularity in real or computer experiments.

2.2 Basic Electronic Structure

2.2.1 CuO_2 Plane

As discussed in Prof. Uchida's lecture, the presence of CuO_2 plane is the common feature of most classes of oxide superconductors and we will concentrate on them. There are several experimental facts indicating that precisely this plane is responsible for SC in these compounds. First of all, there are pronounced characteristic features of two-dimensionality ($2D$): Strong anisotropy in the normal state with resistance ratio $\rho_{\parallel}/\rho_{\perp} \sim 10^{-2}$-$10^{-5}$ [14], strong $2D$ antiferromagnetic fluctuations even above the Neél temperature [24]. Moreover, the earlier speculation of Cu-O chains in Y-compounds being responsible for SC has been given up after the discovery of Tl and Bi superconductors with higher T_c while not having any Cu-O chains. Finally, there is a strong correlation between T_c and the number of CuO_2 layers on top of each other in the unit cell (See Prof. Uchida's lecture). Therefore, we

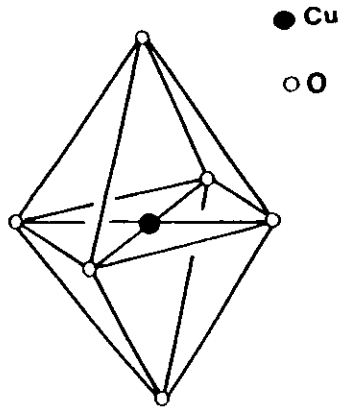

Fig. 7: The CuO_6 octahedron

limit ourselves to the discussion of physics in this plane. On the other hand, a weak but finite coupling between these planes is instrumental in bringing about the $3D$ SC.

2.2.2 Single-Particle Spectrum

We consider La_2CuO_4 as a typical reference compound and take the CuO_6 octahedron as the basic unit (Fig.7). Since copper is divalent Cu^{2+}, the electron configuration is $3d^9$. In the zeroth approximation the crystalline field is cubic, so the d-level is split into T_2g (with xy, xz, yz symmetry) and Eg (with x^2-y^2, $3z^2$-r^2 symmetry levels). Moreover, the cubic symmetry is distorted and the Cu-O distance is about 1.9Å in plane and 2.4Å in the perpendicular direction. Hence the Eg level is further split (so called Jahn-Teller effect). On the other hand, the chemical bonds here are partly ionic, partly covalent, and the hybridization with O_2p

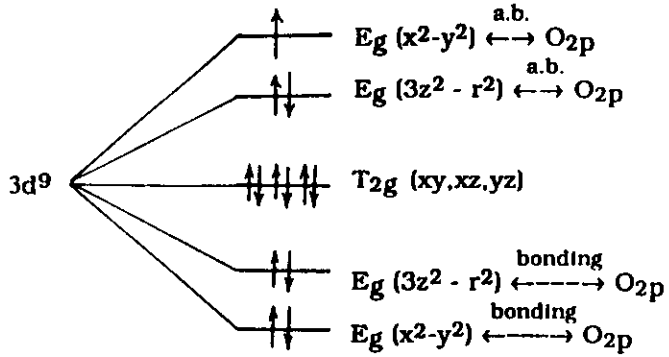

Fig. 8: Energy levels in CuO_2 plane

orbits leads to the energy diagram shown in Fig.8, where the top level is only half-filled. This means that the reference compound should be a metal, whereas in reality it is an insulator. This is also confirmed by the band structure calculation. One of the early results is shown in Fig.9 where the "spaghetti" in the middle part corresponds to non-bonding states and the top band (mainly coming from oxygen) is only partly-filled. How to get around with this basic puzzle? There are two possible approaches. One is the weak coupling theory briefly described in the next subsection, and the other is the strong-coupling method based on Mott-Hubbard picture. The latter will be briefly mentioned in Subsection 2.4 and more extensively discussed in the next section. The entire set of Prof. Anderson's lectures is devoted to this approach.

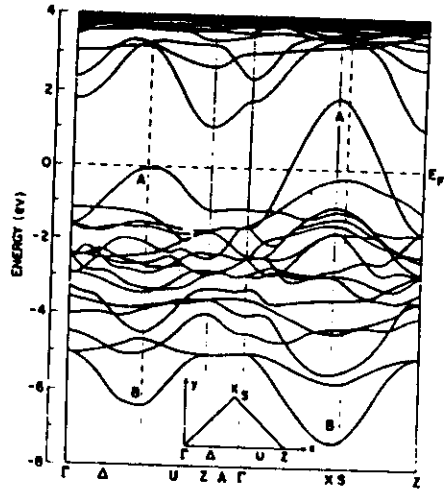

Fig. 9: LAPW energy bands for La_2CuO_4 along symmetry lines in the bct Brillouin zone. From L.F. Mattheiss, Phys. Rev. Lett. 58, 1028 (1987).

2.3 Weak Coupling Approach

The main features of the band structure calculations can be reproduced by a simple tight-binding approximation yielding the following spectrum

$$\varepsilon(k) = -2t\,(\cos k_x a + \cos k_y a) \qquad (3)$$

where a is the Cu-Cu lattice constant. The two-dimensional Brillouin zone is shown in Fig.10. At half-filling the Fermi surface (Fermi line is this case) is shown by bold lines. One notices immediately the nesting (parallel pieces) of Fermi lines in this case analogous to one-dimensional ($1D$) systems.

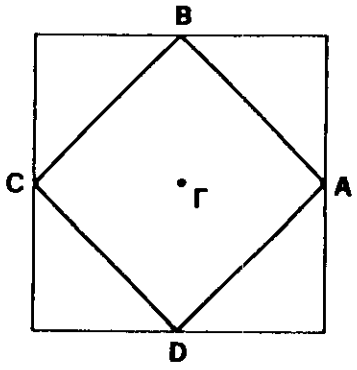

Fig. 10: The 2D Brillouin zone for a square lattice.

It was Peierls [25] who has first shown that a $1D$ metal is unstable with respect to transformation into an insulating state. Assume an $1D$ metal with lattice constant a is half-filled. Because of electron-lattice coupling, energetically it is more favorable to open a gap at the Fermi surface (two points here) with accompanying lattice distortion. The system loses potential energy due to lattice distortion, but gains kinetic energy as a result of gap opening. The lattice constant becomes $2a$, while the Brillouin zone is reduced by a factor of 2. This is schematically shown in Fig.11 and is explained with more details in Ref.26.

The $2D$ case under discussion is rather similar. The nesting vectors are given by $\boldsymbol{Q} = \pi/a(\pm 1, \pm 1)$ (all of them are equivalent to each other up to the reciprocal lattice vector). The new ingredient here is the presence of saddle points A,B,C,D, with coordinates $(0, \pm\pi/a)$ and $(\pm\pi/a, 0)$, which leads to a weak logarithmic "Van Hove singularity" in the density of states (Fig.12). As in the $1D$ case, the metallic state is unstable with respect to a transition into various condensation states.

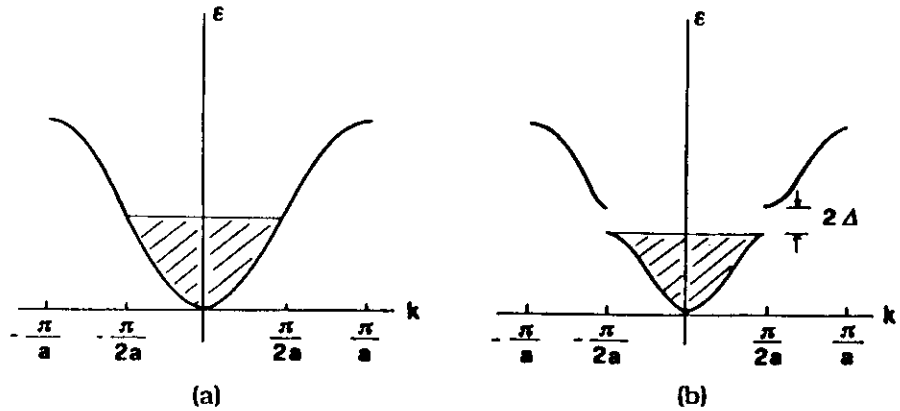

Fig. 11: The illustration of Peierls instability
(a) Unstable metallic state with periodicity a;
(b) Stable insulating state with periodicity 2a and an energy gap 2Δ

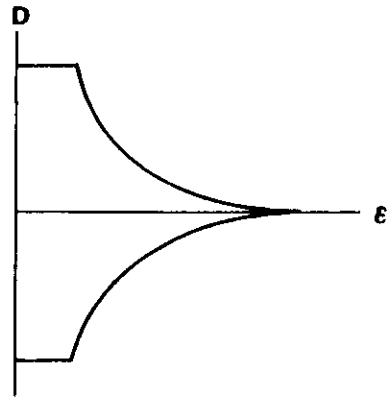

Fig. 12: Van Hove singularity of the density of states.

A general analysis can be carried out in the weak coupling limit when the band width is much greater than the Coulomb interaction, either using the renormalization group [27] or the parquette diagram [28] techniques. There are singlet and triplet SC fluctuations in the particle-particle channel and spin-density wave (SDW) and charge density wave (CDW) fluctuations in the particle-hole channel. Unlike the $1D$ case where the critical temperature is proportional to exp (g^{-1}) with g as dimensionless coupling constant, here $T_C \sim \exp(-g^{-1/2})$. It turns out that the d-wave pairing (i.e. order parameters satisfy the relation $\Delta_x = -\Delta_y$) is preferred in this case [27]. On the other hand, the spin bag model proposed by Schrieffer et al. [29] and based on longitudinal spin fluctuations, implies an extended s-wave pairing. Yet in another analysis [30], emphasizing the diverging transverse spin fluctuations, a p-wave pairing was proposed. Further studies in more realistic situations are needed to clarify this matter.

To sum up, the weak coupling approach is based on the assumption that the FL description is a good starting point, and the metallic state of the reference compound is destroyed by instabilities. Usually a gap opens in the spectrum, but the main characteristics of quasi-particles still remain. Recently, this approach has been extended to higher doping concentration [31] where antiferromagnetic fluctuations only lead to opening a pseudogap in the spectrum. Within this framework, the BCS-like superconducting behavior and photoemission experiments can be easily understood, but the normal state properties, especially the anomalous behavior of Hall constant, are much more difficult to describe.

2.4 Strong Coupling Approach

Very soon after the discovery of high T_C superconductors, P.W. Anderson suggested [32] that our starting point should be a Mott insulator because SC occurs near the metal-insulator transition.

Hence the physics involved should be very different from the FL picture. Moreover, he proposed that the one-band Hubbard model given by

$$H = -t\sum_{<i,j>,\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+h.c.) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{4}$$

where

$$n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma} \tag{5}$$

t is the nearest neighbor hopping and U is the on-site Coulomb repulsion, can bring about the essential physics. Also, this would allow us to describe SC and magnetism in a unified fashion. Furthermore, he speculated that the SC occuring in such doped insulators could be entirely different from the BCS behavior.

The anomalous behavior of oxide superconductors in the normal state can be, at least qualitatively, understood within this picture. Take, for example, the Hall measurements in La-compounds. The concentration of free charge carriers in the reference compound is zero, because at half-filling there is only one hole per site in localized state. Upon doping additional holes are introduced to give a positive R_H, which is inversely proportional to the doping concentration x. At higher doping there might be deviation from this simple law and at some critical concentration a transition from a doped Mott insulator to a normal metal may occur which would explain the change of R_H sign discussed in the first section. However, it is not easy for this approach to explain the fairly well defined Fermi surface observed in the angle-resolved photoemission, and especially, why the SC behavior is so much BCS like. Enormous efforts have been applied to develop the strong-coupling approach and the current status will be discussed in Prof. Anderson's lectures.

2.5 Heavy Fermion Approach

Before concluding this section I would like to mention very briefly another alternative approach.

It was a long standing puzzle to explain the anomalous properties of some dilute magnetic alloys (say Fe in Cu or Mn in Au). This is the so-called Kondo problem [33]. Later on, a class of mixed-valence compounds (e.g.$CeCu_2Si_2$, UBe_{13} etc.) were discovered which showed Curie-Weiss magnetic susceptibility at high temperatures, but anomalously large Pauli susceptibility and electronic specific heat at low temperatures [34]. It turned out that the Anderson model with strong Hubbard U on the localized orbits and mixing of localized and itinerant orbits [35], or its large U-equivalent for spin S=1/2, the Kondo model [36], is a good description. At high temperatures (greater than the characteristic Kondo temperature) the behavior of such systems is very different from what one would expect for a FL. On the other hand, at low temperatures, as a result of renormalization, the system is well described by a U=0 fixed point with FL characteristics (although the density of states is greatly enhanced). This transition from non-FL to FL behavior is also discussed in Prof. Anderson's lecture.

There have been several attempts to apply this approach (generalized to lattice version) to high T_C superconductors. At the early stage of high T_C endeavor, the slave boson technique was used to study the possible Mott transition at half-filling and the renormalization of band width upon doping [37]. Later on, the model was refined by including various factors [38]. However, there are some fundamental differences between heavy-fermion and high T_C superconductors. The charge carriers in the latter are not so "heavy" (about twice the free electron mass) and the density of states is not inversely proportional to concentration as one would expect from heavy fermion analogy. Anyway, whether oxide superconductors are another example of renormalization from non-FL to FL picture, is an entirely open question.

3. Working Models in Strong-Coupling Approach

In this section we consider the relationship between the Hubbard model and t - J model as well as reduction of a multi-band Hubbard model to an effective one-band model. These models are widely used in the current literature, but mostly without detailed explanation.

3.1 Hubbard and t - J Models

The simple looking Hubbard Hamiltonian (4) is very difficult to solve. The exact solution is available only in 1D case [39]. It is thus natural to seek equivalent models in the strong coupling limit $U >> t$. In this case, it can be reduced to the so-called t - J model. The essential constraint in the large U limit is to remove the double occupancy. This can be achieved by using a canonical transformation

$$H' = e^{iS} H e^{-iS} = H + [iS, H] + [iS, [iS, H]]/2! + \ldots \tag{6}$$

which was discussed by many authors [40,41]. Here we follow the procedure given in Ref.41.

The Hubbard Hamiltonian (4) can be presented as

$$H = T + V, \tag{7}$$

$$T = -t \sum_{i,j,\sigma} l_{ij}\, c_{i\sigma}^{\dagger} c_{j\sigma}, \tag{8}$$

$$V = U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{9}$$

where $I_{ij} = 1$ for nearest neighbors and 0 otherwise. Multiplying (8) by $n_{i,-\sigma} + h_{i,-\sigma} = 1$ from the left and $n_{j,-\sigma} + h_{j,-\sigma} = 1$ from the right, the hopping term can be rewritten as

$$T = T_0 + T_1 + T_{-1}, \tag{10}$$

where

$$T_0 = -t\sum_{i,j,\sigma} I_{ij} \left(n_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}n_{j,-\sigma} + h_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}h_{j,-\sigma}\right), \tag{11}$$

$$T_1 = -t\sum_{i,j,\sigma} I_{ij} n_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}h_{j,-\sigma}, \tag{12}$$

$$T_{-1} = -t\sum_{i,j,\sigma} I_{ij} h_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}n_{j,-\sigma}, \tag{13}$$

$$h_{i\sigma} = 1 - n_{i\sigma} = 1 - c^{\dagger}_{i\sigma}c_{i\sigma}. \tag{14}$$

Obviously, T_0 describes hopping between two doubly occupied (first term) or two singly occupied (second term) sites i and j, while T_1 term increases the number of doubly occupied sites by 1 and T_{-1} term decreases it by 1.

Noting that

$$[V,T_1] = UT_1, \quad [V,T_{-1}] = -UT_{-1}, \tag{15}$$

we can choose

$$iS = U^{-1}(T_1 - T_{-1}) \tag{16}$$

to remove terms changing the number of doubly occupied sites in the leading order of t/U. The resulting Hamiltonian becomes

$$H' = V + T_0 + U^{-1}([T_1,T_{-1}] + [T_0,T_{-1}] + [T_1,T_0]) + O(U^{-2}). \tag{17}$$

If no double occupancy is allowed, the only remaining term would be $-T_{-1}T_1$, and the effective Hamiltonian becomes

$$H_{eff} = -t\sum_{i,j,\sigma} h_{i,-\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}h_{j,-\sigma} + J\sum_{i,j} (S_i S_j - 1/4), \tag{18}$$

where

$$S_i = c^{\dagger}_i \frac{\sigma}{2} c_i \tag{19}$$

$$J = 2t^2/U \tag{20}$$

with σ as Pauli matrices. This is the widely used t - J model.

A technical detail: the coefficient given in (20) is different from the standard one ($J = 4t^2/U$), the reason being that the summation here is over nearest neighbors (twice on each bond), while in the Heisenberg model, it is over bonds only. One can also add a next-to-nearest neighbor hopping term, in which case it is called t - t' - J model.

A few remarks are in order. Firstly, at exact half-filling, each site is occupied by one hole, so the first term of (18) vanishes, and we recover the antiferromagnetic Heisenberg Hamiltonian. Secondly, this equivalency has been established in the limit $U >> t$. As an independent model, the t - J Hamiltonian can be considered in both limits $J >> t$ and $t >> J$, but only the latter corresponds to the Hubbard model.

Enormous amount of work has been done to study the Hubbard and t - J models, especially in $2D$. The related references can be found in recent conference proceedings [2 - 4]. Here we limit ourselves to mentioning a few points.

The ground state of the $2D$ Heisenberg model does show antiferromagnetic long-range order [42]. It is not a classical Neél

antiferromagnet, but can be well-described by including quantum fluctuations, say, in the spin wave approximation or using nonlinear σ - models [43]. An alternative approach is to consider the resonance-valence-bond (RVB) states first suggested by Anderson [35]. Extensive studies have been carried out using the mean field [44] and variational Monte-Carlo [45] techniques, and different singlet states (with s, d, $s + id$ symmetries) have been considered, but the energy is still higher than the exact result on small clusters [42]. It has been realized only later that the fermion representation of the RVB order parameters does not comply with the Marshall sign rule and replacing them by spin variables yielded the correct answer [47]. A simple way out is to introduce staggered magnetization in addition to the RVB parameters. Such "coexistence" studies have been done in the mean-field [48] and variational Monte-Carlo [49] approximations. Yet another useful technique to study the magnetic properties is the Schwinger boson (or slave fermion) formalism [50] which is consistent with the Marshall sign rule.

The motion of a few additional holes on an antiferromagnetic background is an old problem [51] with strong revival of interest recently [52-56]. The main factors to be considered include: (1) The static distortion of the spin background caused by holes; (2) the quantum fluctuations of spins; (3) the renormalization of hole motion due to virtual process of emitting and reabsorbing spin waves. It turns out that these holes can propagate but the effective mass is renormalized by a factor of t/J. It is natural to consider the possibility of hole pairing by calculating the energies of single and paired holes. However, in view of the renormalization and retardation effects one has to be rather cautious about the conclusions.

States with finite hole concentration are much more difficult to describe, and will be discussed in Prof. Anderson's lectures.

3.2 Multi-Band versus One-Band Models

What is the appropriate microscopic Hamiltonian for describing oxide superconductors has been one of issues under debate. Most people would agree with Anderson's suggestion of involving Hubbard model for this purpose. However, the CuO_2 plane contains both Cu and O, and moreover, there has been quite strong evidence that additional holes are mainly located on O, while no Cu^{3+} state showing up [57]. Thus several authors have proposed a more general model including both Cu and O bands [58] which can be written as

$$
\begin{aligned}
H = & -\sum_{i,l,\sigma} t_{il}\,(d^{\dagger}_{i\sigma}p_{l\sigma} + h.c.) - \sum_{l,l',\sigma} t'_{ll'}\,(p^{\dagger}_{l\sigma}p_{l'\sigma} + h.c.) \\
& + \varepsilon_d \sum_{i,\sigma} d^{\dagger}_{i\sigma}d_{i\sigma} + \varepsilon_p \sum_{l,\sigma} p^{\dagger}_{l\sigma}p_{l\sigma} \\
& + U_d \sum_{i} n_{di\uparrow}n_{di\downarrow} + U_p \sum_{l} n_{pl\uparrow}n_{pl\downarrow} \\
& + V \sum_{i,l,\sigma,\sigma'} n_{di\sigma}n_{pl\sigma'}
\end{aligned}
\tag{21}
$$

where t_{il} is Cu-O nearest neighbor hopping, $t'_{ll'}$ is O-O direct hopping. U_d, U_p, V are Cu, O on-site and Cu-O Coulomb repulsion, respectively, while indices i and l are Cu and O coordinates. These energy values are not exactly known and can only be estimated roughly by model studies. The possible range would be: t = 1+1.5 eV, t' = 0.5 eV, U_d = 5 +10 eV, U_p = 3 + 6 eV, V = 1.5 eV, $\Delta = \varepsilon_p - \varepsilon_d$ = 3 eV. Here we use hole representation, i.e., the starting configuration is $3d^{10}$ for Cu and $2p^6$ for O. This model is very complicated and one would like to simplify it as much as possible without sacrificing the essential physics. One possible choice is to keep only t, U_d (in the following we drop the subscript) and Δ, while ignoring other effects for the time being. Zhang and Rice [59] have shown that although the additional holes are primarily on oxygen,

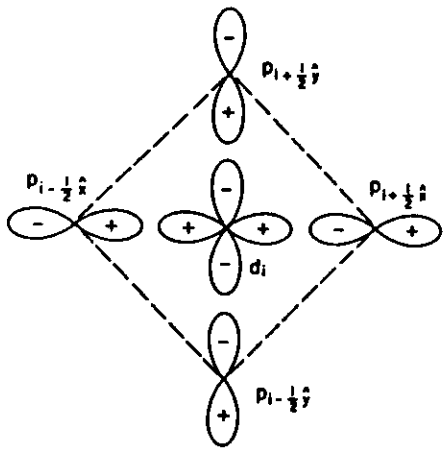

Fig. 13: Schematic diagram of the hybridization of the O hole ($2p^5$) and Cu hole ($3d^9$). The signs + and - represent the phase of the wave functions.

the strong Cu-O hybridization with proper symmetry consideration would still lead to an effective one-band model. In the following we reproduce briefly their arguments.

If we consider the CuO_2 square with Cu ion at the centre, one should take into account that the hopping integral depends on the relative sign of wave functions (See Fig.13), i.e.

$$t_{il} = t_o (-1)^{M_{il}} \tag{22}$$

where $M_{il} = 1$ for $l = i + \hat{x}/2$ and $i + \hat{y}/2$, while $M_{il} = 2$ for $l = i - \hat{x}/2$ and $i - \hat{y}/2$. Here the Cu-Cu distance is used as the length unit. The interesting limit is U, Δ, $U - \Delta >> t$.

If $t = 0$, the reference compound will have one hole on each Cu site and no holes on O. At further doping additional holes will be on

O sites, if $U > \Delta$. For non-vanishing t, the system will gain energy by Cu-O hybridization. Consider symmetric and anti-symmetric combinations of four oxygen wave functions surrounding a given copper

$$p_{i\sigma}^{(S,A)} = \frac{1}{2}\sum_l (\pm 1)^{M_{il}} p_{l\sigma}, \tag{23}$$

where -(+) correspond to $S(A)$ states. The symmetric state can form bonding (singlet) and antibonding (triplet) states with central Cu. i.e.

$$\varphi_i^{s,t} = \frac{1}{\sqrt{2}}(p_{i\uparrow}d_{i\downarrow} \pm p_{i\downarrow}d_{i\uparrow}). \tag{24}$$

Using second order perturbation theory one can calculate the energy of the singlet state to be

$$\varepsilon^{(S)} = -8\,(t_1 + t_2) \tag{25}$$

with

$$t_1 = t_0^2/\Delta, \quad t_2 = t_0^2/(U - \Delta), \tag{26}$$

while $\varepsilon^{(t)} = 0$. On the other hand, the antisymmetric state does not hybridize with Cu and has a non-bonding state energy equal to $-4t_1$. For comparison, the binding energy of a singlet combination with O at the centre and two Cu at the two ends would be $2(t_1 + t_2)$, i.e. 1/4 of the present value. The difference is due to the coherence effect. If we assume that the effective band width due to residual wave function overlap is smaller than the binding energy, only singlet states should be considered.

This is true for an isolated square. In the real system there is a complication due to sharing O by two neighboring Cu squares.

This difficulty can be overcome by introducing the Wannier function

$$\phi_{i\sigma} = N^{-1/2} \sum_k p_{k\sigma} \exp(ik \cdot R_i), \tag{27}$$

$$p_{k\sigma} = N^{-1/2} \beta_k \sum_i p_{i\sigma}^{(S)} \exp(-ik \cdot R_i), \tag{28}$$

where

$$\beta_k = [1 - 1/2 (\cos k_x + \cos k_y)]^{-1/2} \tag{29}$$

is the renormalization factor.

The functions $\phi_{i\sigma}$ are orthonormalized and one can combine them with d_i to form singlet (-) and triplet (+) states

$$\Psi_i^{\pm} = \frac{1}{\sqrt{2}} (\phi_{i\uparrow} d_{i\downarrow} \pm \phi_{i\downarrow} d_{i\uparrow}), \tag{30}$$

and the corresponding energies are

$$E\pm = -8 (1 + \lambda^2) t, \tag{31}$$

where for simplicity an assumption $t_1 = t_2 = t$ was made and $\lambda \approx 0.96$. We see that the orthonormalization does not change much the result.

Therefore, the additional hole on O is forming a strongly bound singlet state with Cu which is a spin zero entity. As far as the motion of this singlet state is concerned, it is very similar to an empty state in the Heisenberg antiferromagnet formed by Cu holes.

The effective Hamiltonian is

$$H_t = \sum_{i \neq j, \sigma} t_{ij} (\Psi_j^{\dagger} d_{i\sigma})^{\dagger} \Psi_i^{\dagger} d_{j\sigma}, \tag{32}$$

which is almost the same as the hopping term in the t - J model discussed in the previous subsection.

This reduction of the two-band (or three-band if one counts two O) Hubbard model to an effective one-band model is very instructive, but not everybody agreed with their conclusions. The main objection was that the charge carriers in CuO_2 plane also have spin, so the low-energy physics is different from the one-band model [60]. In particular, Emery and Reiter found an exact solution of a single hole with spin moving on a ferromagnetic background [60]. Very recently, we have shown that this solution can be almost exactly reproduced by hybridization of the singlet and triplet states [61]. Therefore, the basic argument of Zhang and Rice is still justified.

4. Concluding Remarks

In spite of the immense efforts made in High-T_C research, we do not have a theory for it yet. However, the range of acceptable models is narrowing down very quickly.

As mentioned earlier, if the weak coupling approach works, the main issue would be the explanation of various anomalies in normal state. On the contrast, if the strong coupling theory is justified, one has to explain the BCS-type SC behavior and the existence of Fermi surface.

Very recently, Varma and his collaborators [62] suggested a phenomenological "marginal FL" theory as an attempt to resolve this dilemma. Their basic assumption is that there are spin and charge fluctuations described by the polarization function

$$\begin{aligned} \mathrm{Im}\, P\,(q,\omega) &\sim -N(0)\,\frac{\omega}{T} \qquad \text{for } |\omega| < T \\ &\sim -N(0)\,\mathrm{sgn}\,\omega \quad \text{for } |\omega| > T \end{aligned} \tag{33}$$

which is q independent over a wide range. Here $N(0)$ is the unrenormalized one-particle density of states. The (retarded) self-energy due to scattering on these fluctuations would be

$$\Sigma(k,\omega) \sim g^2 N^2(0)\,(\omega \ln \frac{x}{\omega_c} - i\frac{\pi}{2}x), \tag{34}$$

where $x = \max(|\omega|, T)$, ω_c is the ultraviolet cut-off, and g is a coupling constant. These authors claim that all anomalies in the normal state can be explained by this hypothesis. According to this ansatz, the residue of the quasiparticle pole at the Fermi surface is proportional to $1/\ln|\omega_c/E_k|$, i.e. vanishes logarithmically. This is the origin of the name "marginal FL". This proposal is certainly very interesting, and a careful study of its consequences and possible microscopic justification is worthwhile to pursue. One should mention that Anderson has observed in his lectures that such behavior of self-energy is dictated by experiments.

A related issue is the study of the 1D Hubbard model. As discussed in Anderson's lectures, many peculiar properties of oxide superconductors are very similar to what one should expect from this model. Whether these features will remain in more realistic 2D case is an open and challenging question.

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