

FERMI LIQUID DESCRIPTION OF $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

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We treat a model with orbitals on the copper and oxygen sites and hopping between them. In the limit of infinite U on the Cu site, the problem is treated using the slave boson method. In the presence of doping, we find a Fermi liquid solution with mass enhancement proportional to x^{-1} . Low frequency optical absorption shows deviation from a simple Drude behavior, with oscillator strength proportional to x . Interactions between quasi-particles via the exchange of slave bosons is calculated. The Heisenberg exchange interaction J arises as a second order boson exchange and may give rise to singlet pairing between quasi-particles. Our treatment is essentially a perturbation theory valid when J is less than the renormalized bandwidth. Consequently the Fermi liquid description may break down for small doping.

1. Introduction

The physics of the high T_c superconductor

$\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ is often discussed in terms of the Hubbard model. A number of authors have pointed out that it is important to include the copper and oxygen orbitals [1,2]. We consider a model in which $d_{i,\sigma}^\dagger$ creates a hole in the

Cu ($3d_{x^2-y^2}$) orbital at energy ϵ_d° , $c_{i,\sigma}^\dagger$ creates a hole in the

$O(2p_x \text{ or } 2p_y)$ orbital at energy ϵ_p and a hopping matrix element t_{pd} connects the nearest Cu and O neighbors. We introduce a Hubbard U_d and U_c on the copper and oxygen sites, but we shall treat the limits $U_d=\infty$ and $U_c=0$. U_d is generally agreed to be much larger than any other energy scale in the problem, so that $U_d=\infty$ (absence of Cu^{3+}) is a reasonable starting point. We also assume that $\epsilon_p - \epsilon_d^\circ > 0$ so that the undoped La_2CuO_4 nominally consists of Cu^{2+} and O^{2-} and the holes introduced by doping with Sr occupy the oxygen orbitals. As we shall see, $\epsilon_p - \epsilon_d^\circ \equiv D$ plays the role of U in the Hubbard model, and this is consistent with the analysis of the trends in transition metal oxides [3]. For x small U_c does not interfere with band formation because the probability of double occupation is small, so that setting

$U_c = 0$ would not change the physics qualitatively. We should keep in mind that U_c enters into the estimate of the super-exchange J between neighboring copper spins, because that involves double occupation of the oxygen site in between, so that

$$J = 4 t_{pd}^4 (\epsilon_p - \epsilon_d^\circ)^{-2} (\epsilon_p - \epsilon_d^\circ + U_c)^{-1}.$$

The $U_d = \infty$, $U_c = 0$ limit can be treated by introducing a slave boson on each Cu site. The problem is further simplified by noting that only a single combination of the two oxygen orbitals in the unit cell couples to the Cu, so

that we have a two-band model. For $U_d = 0$, we have the familiar band structure

$$E_{1,[2]}^\circ(k) = (\epsilon_p + \epsilon_d^\circ - [+] R_k^\circ) / 2 \quad (1)$$

where $R_k^\circ = ((\epsilon_p - \epsilon_d^\circ)^2 + 16 t_{pd}^2 \gamma_k^2)^{1/2}$ and $\gamma_k^2 = \sin^2(k_x/2) + \sin^2(k_y/2)$. For one hole per unit cell, the lower band E_1 is half filled.

2. Mean Field Theory

The present model is formally identical to the Anderson lattice and we can take over earlier work which treats the problem in a large orbital degeneracy (N) expansion [4,5,6]. We adopt a convention where the hopping matrix element is denoted by $t/N^{1/2}$, (so that when $N = 2$, $t = \sqrt{2} t_{pd}$). We assume that the N -fold degenerate d states can accommodate $Q = Nq_0$ holes and we set $q_0 = 1/2$. The deviation from half-filling δ is defined by writing the total number of holes per unit cell as $H = Q(1+\delta)$. We enforce the constraint

$$b_i^\dagger b_i + d_i^\dagger d_i = Q. \quad (2)$$

We consider the large N limit only as a formal device to produce a consistent loop expansion, and we set $N = 2$ for spin degeneracy in our final results. It is only when $N = 2$ and $Q = 1$ that the constraint Eq.(2) corresponds to the infinite U_d model.

To lowest order in N^{-1} , we have mean field theory, where $\langle b \rangle = b_0 = \sqrt{N} r_0$, and the effective hopping matrix element becomes $\sigma_0 = (t/\sqrt{N})b_0 = tr_0$. At the same time the position of the d level is renormalized from ϵ_d° to ϵ_d so that the renormalized band structure $E_{1[2]}$ and R_k are given by Eq.(1) with $t_{pd} \rightarrow \sigma_0$ and $\epsilon_d^\circ \rightarrow \epsilon_d$. These bands describe the quasi-particles and the chemical potential is determined by filling the lower band by H/N holes. The Fermi surface then contains H holes and Luttinger's theorem is obeyed. The mean-field parameters r_0 and ϵ_d are given by the equations

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$$r_0^2 + \sum_k u_k^2 f(E_1(k)) = q_0 \quad (3)$$

$$(\epsilon_d - \epsilon_d^0) = (t/r_0) \sum_k u_k v_k \gamma_k f(E_1(k)) \quad (4)$$

where f is the Fermi factor and $u_k^2 [v_k^2] = (1 + [-]) (\epsilon_p - \epsilon_d)/R_k/2$ is the $d[c]$ weight in the E_1 band. Eq.(3) is just the constraint Eq.(2) in mean field. We have solved Eqs.(3) and (4) numerically, but we can learn much by examining the limit $4t \ll D$ where an analytic solution is possible. Our model contains two dimensionless parameters D/t and δ . For $\delta < 0$, the shift in ϵ_d can be calculated perturbatively from Eq.(4) and is small, of order t^2/D . Using $q_0 = H/N - q_0\delta$, Eq.(3) can be written as

$$r_0^2 = -\frac{\delta}{2} + \sum_k (1 - u_k^2) f(E_1(k)) \quad (5)$$

For $t \ll D$, $u_k^2 \approx 1$ and we obtain $r_0^2 = -\delta/2$. The bandwidth of the two bands are given by $8r_0^2 t^2 / (\epsilon_p - \epsilon_d^0)$ and we see that they are narrowed by the factor $|\delta|$ compared with the bare bandwidth $8t_{pd}^2/D$. This band narrowing is familiar in the Hubbard model in the large U/t limit. It represents the physical picture that in a Fermi-liquid picture which satisfies Luttinger theorem, we represent δ holes in the lower Hubbard band by $H = N/2 (1 + \delta)$ holes which must acquire a larger effective mass $m^*/m \approx \delta^{-1}$.

We can see from Eq.(4) that $r_0 = 0$ at $\delta = 0$ and the perturbative solution we found disappears for $\delta > 0$. It turns out that another solution can be found where ϵ_d is renormalized by a large amount until it is close to ϵ_p , i.e., $\epsilon_p - \epsilon_d = (4t^2/D) \sum_k \gamma_k^2 f(E_1)$. Provided $\sigma_0 \ll \epsilon_d - \epsilon_p$ (and this will be shown to be consistent), the term $\sum_k (1 - u_k^2) f$ in Eq.(4) can be expanded to give $\gamma_0^2 4t^2 / (\epsilon_d - \epsilon_p)^2 \sum_k \gamma_k^2 f(E_1)$ which is much greater than γ_0^2 . Combined with Eq.(3), Eq.(4) now has the solution $r_0^2 \approx (\delta/2) (2t/D)^2 \sum_k \gamma_k^2 f(E_1)$. Putting these solutions into the band structure, we find that the bandwidths are still given by $8\delta t_{pd}^2/D$ as in the $\delta < 0$ case. The picture, as shown in Fig.1, is that as δ changes signs, the lower band shifts discontinuously from near ϵ_d^0 to $(4t^2/D) \sum_k \gamma_k^2 f(E_1)$ below ϵ_p . The jump in ϵ_d is dictated by the physical requirement that the chemical potential must be near ϵ_p for $\delta > 0$, because the additional holes are expected to occupy oxygen sites. Indeed, the oxygen hole can delocalize by virtual hopping onto the copper sites and the energy gained is just $\approx 4t_{pd}^2/D$ from perturbation theory, thus explaining the

location of the narrow band below ϵ_p .

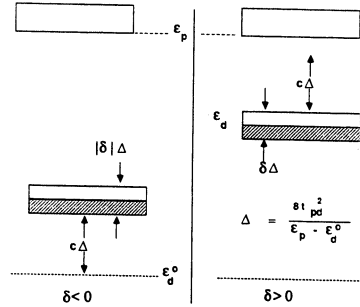


Fig. 1. Schematic illustration of the renormalized hole bands. Shaded area indicates filled states. The constant $C = \sum_k \gamma_k^2 f(E_1(k))$ is of order unity.

Physically we do not expect the band narrowing to continue for arbitrarily small $|\delta|$, and we expect a Neel ground state at and near half filling. Thus we should compare J with the delocalization energy $4\delta t_{pd}^2/D$ and we expect that the above Fermi liquid picture will be a good starting point for $\delta > t_{pd}^2/D(D + U_C)$.

3. Optical Properties

We now focus on $\delta > 0$, since $\delta = x$ for Sr doping. Our mean-field solution predicts an interesting new structure in the conductivity $\sigma(\omega)$ corresponding to transition between bands E_1 and E_2 . The conductivity can be computed using the Kubo formula in terms of the current operator

$$j = i \sum_{jk} t_{jk} (b_j d_j^\dagger c_k - c.c.) \quad (5)$$

where t_{jk} is the nearest neighbor hopping matrix element t_{pd} . For low frequency excitation we replace b_j with b_0 and $\sigma(\omega)$ can be computed using the renormalized band structure. We find a Drude term at $\omega = 0$ corresponding to particle-hole excitation in the lower band and an excitation with a gap $\approx \epsilon_p - \epsilon_d \approx (4t^2/D) \sum_k \gamma_k^2 f(E_1)$ for $4t \ll D$ corresponding to interband absorption. This latter feature is severely broadened because the final state includes a hole in the E_2 band which decays rapidly by making particle-hole excitations in the E_1 band. Our estimate shows that the decay rate is of the same order of magnitude as $\epsilon_p - \epsilon_d$, so that the gap is not well defined. In addition, we recall that there exists a dispersionless oxygen band at ϵ_p corresponding to the linear combination which does not hybridize with the copper. We find optical transition between the occupied band E_1 and this band as well.

Again we expect the gap to be severely broadened. These two features and the Drude term have approximately equal oscillation strength of $e^2 n \delta 4t^2 / D k_F^2$ where n is the density of holes per volume (approximately 1 per Cu). It is convenient to introduce a band mass m_b by $k_F^2 / m_b = 4t^2 / D$ which corresponds to the unrenormalized bandwidth. Then the oscillation strength can be written as $(e^2 n / m_b) \delta$.

On the other hand, for high frequency excitations we must use the boson propagation

$\int \langle b^+(t) b(0) \rangle e^{i\omega t}$ which has a pole at $\omega \approx \epsilon_d - \epsilon_d^0$ in computing $\sigma(\omega) \approx \int \langle j(t) j(0) \rangle e^{i\omega t} dt$. This gives rise to absorption at $\epsilon_p - \epsilon_d^0$ with oscillation strength $\approx (e^2 / n m_b) (1 - \delta)$. Since this term involves the boson propagator, it is formally of order $1/N$, but it is of order unity as far as its δ dependence is concerned.

To understand physically the weight δ associated with the low frequency optical transition, we note that the excitation in the E_1 bands consist mainly of Cu states with a small admixture proportional to δ of O-states. Since for $t \ll D$ the charge on the Cu is fixed, the Cu states contribute only spin, and the oxygen states spin and charge (both of order δ), to the excitation. Thus, the optical transition involves only charge transfer between O sites, with an effective matrix element via the Cu site.

Recent optical reflectivity [7] on single crystals revealed an onset of absorption at $\approx 2eV$ in the doped as well as undoped sample. We interpret this as $\epsilon_p - \epsilon_d^0$, with some reduction due to excitonic effects. Thus we estimate $\epsilon_p - \epsilon_d^0$ to be $\geq 2eV$. An additional broad feature with width $\approx 0.5eV$ and oscillator strength proportional to δ is observed. There is some disagreement at present on whether an additional narrower Drude term is needed at low frequencies. It is tempting for us to interpret the broad feature as a severely broadened interband transition, so that

$$\epsilon_p - \epsilon_d \approx 0.5eV.$$

4. Fluctuations

We have followed ref (5,6) and extended the theory to include boson fluctuations. Expanding about the mean field solution, the Lagrangian is given by

$$L = L_0 + L_b + L_1 + N (\sigma_0^2 / t^2 - q_0) (\epsilon_d - \epsilon_d^0) \quad (7)$$

where (with $m = 1$ to N)

$$L_0 = \sum_{k,m} c_{k,m}^\dagger \left(\frac{\partial}{\partial \tau} + \epsilon_p \right) c_{k,m} + d_{k,m}^\dagger \left(\frac{\partial}{\partial \tau} + \epsilon_d \right) d_{k,m} + \sum_{k,q,m} \sigma_0 \gamma(k) c_{k,m}^\dagger d_{q,m} \quad (8)$$

This term is diagonalized to give the quasi-particle bands E_1 and E_2 .

$$L_b = \frac{N}{t^2} \sum_k (\sigma_k, \lambda_k) \begin{bmatrix} \epsilon_d - \epsilon_d^0 & i\sigma_0 \\ i\sigma_0 & 0 \end{bmatrix} \begin{pmatrix} \sigma_k \\ \lambda_k \end{pmatrix} \quad (9)$$

There are two fluctuating boson fields, the σ field which represents magnitude fluctuation (ie, deviation from the mean field value σ_0) and the λ field, which takes care of phase fluctuations. The interaction is

$$L_1 = \sum_{k_1 k_2} \gamma(k_1) (c_{k_1 m}^\dagger d_{k_2 m} \sigma(k_2 - k_1) + d_{k_2 m}^\dagger c_{k_1 m} \sigma(k_1 - k_2)) + i \sum_{k_1 k_2} \lambda(k_1 - k_2) d_{k_1}^\dagger d_{k_2} \quad (10)$$

To first order in $1/N$, the boson propagator is given by (the boson Matsubara frequency)

$$D_{ij}^{-1}(q, \omega) = D_{0,ij}^{-1} - \sum_{ij} (q, \omega) \quad (11)$$

where $ij = \sigma$ or λ and from Eq.(9), $D_{0,\sigma\sigma}^{-1} = (N/t^2) (\epsilon_p - \epsilon_d^0)$,

$D_{0,\sigma\lambda}^{-1} = i (N/t^2) \sigma_0$ and $D_{0,\lambda\lambda}^{-1} = 0$. The self energy Σ_{ij} is

the polarization bubble, ie particle-hole excitation coupled to boson propagators via Eq.(10). Upon transforming to the E_1 and E_2 bands we obtain

$$D_{\sigma\sigma}^{-1} = N \left\{ \sum_k \frac{\gamma_k^2}{R_k} f(E_1(k)) - \frac{1}{2} \sum_k (\gamma(k+q) uv' + \gamma(k) u'v)^2 R_{11}(k, q, \omega) + \sum_k (\gamma(k+q) uu' - \gamma(k) vv')^2 R_{12}(k, q, \omega) \right\} \quad (12a)$$

$$D_{\lambda\lambda}^{-1} = \frac{1}{2} N \left\{ \sum_k u^2 u'^2 R_{11}(k, q, \omega) - \sum_k u^2 v^2 R_{12}(k, q, \omega) \right\} \quad (12b)$$

$$D_{\lambda\sigma}^{-1} = D_{\sigma\lambda}^{-1} = i N \sigma_0 \left\{ \frac{1}{t^2} + \sum_k \gamma^2(k+q) \frac{u^2}{R_{k+q}} R_{11}(k, q, \omega) - \sum_k \left(\frac{\gamma^2(k+q) u^2}{R_{k+q}} - \frac{\gamma^2(k) v^2}{R_k} \right) R_{12}(k, q, \omega) \right\} \quad (12c)$$

In these equations we have used the short-hand notation $u = u_k$, $v = v_k$, $u' = u_{k+q}$ and $v' = v_{k+q}$ and we have introduced the intraband particle-hole excitation

$R_{11}(k, q, \omega) = (f(E_1(k+q)) - f(E_1(k))) / (E_1(k+q) - E_1(k) - i\omega)$ and the interband function

$$R_{12}(k, q, \omega) = -\frac{1}{2} (f(E_1(k+q)) - f(E_2(k)))$$

$$\left[\frac{1}{E_1(k+q) - E_2(k) - i\omega} + \frac{1}{E_1(k+q) - E_2(k) + i\omega} \right]$$

The boson propagator D is obtained by inverting the 2×2 matrix elements given by Eq.(12). Two quasi-particles with incoming momenta k, \bar{k} are scattered by the exchange of a boson of momentum q and frequency ω into outgoing states of $k+q$ and $\bar{k}-q$. The effective interaction potential is given by

$$V_{\text{eff}} = -(\gamma(k+q) v' u + \gamma(k) u' v)$$

$$(\gamma(\bar{k}-q) \bar{v}' \bar{u} + \gamma(\bar{k}) \bar{u}' \bar{v}) D_{\sigma\sigma}(q, \omega)$$

$$+ u' u \bar{u}' \bar{u} D_{\lambda\lambda}(q, \omega)$$

$$+ i u' u (\gamma(\bar{k}-q) \bar{v}' \bar{u} + \gamma(\bar{k}) \bar{u}' \bar{v}) D_{\lambda\sigma}(q, \omega)$$

$$+ i (\gamma(k+q) v' u + \gamma(k) u' v) \bar{u}' \bar{v}) D_{\sigma\lambda}(q, \omega) \quad (13)$$

where $\bar{u} = \underline{u}_{\bar{k}}$ and $\bar{u}' = \underline{u}_{\bar{k}-q}$ etc. Note that all the k and \bar{k} dependent factors in Eq.(13) are all functions only of the energy $E_1(k)$, $E_1(\bar{k})$ etc, so that for scattering between quasi-particles on the Fermi surface, V_{eff} depends only on the momentum and frequency transfer of q and ω .

We can make some analytic progress by specializing to $q, \omega \rightarrow 0$ and the limit $t_{pd} \gg D$. As in Fermi Liquid theory, the interband term $R_{11}(k, q, \omega)$ is singular in this limit and $R_{11}(k, q, \omega) \approx \delta(E_1(k) - \mu) \nabla(\partial E_1/\partial k \cdot q, \partial E/\partial k \cdot q - i\omega)$. First consider the limit $\omega = 0, q \rightarrow 0$, in which case $\sum_k R_{11}$ simply gives the renormalized single particle density of states ρ , which as we saw earlier is enhanced from the bare density of states ρ_0 derived from the band structure by $|\delta|^{-1}$. After much delicate cancellations, we obtain (for $\delta > 0$)

$$\det(D^{-1}) \approx 2\rho\sigma_0^2(I_2 - \gamma^2(k_F)I_1)$$

$$- 2\rho\gamma^4(k_F)\sigma_0^4I_1/(\epsilon_p - \epsilon_d)^2$$

$$+ \sigma_0^2(\epsilon_p - \epsilon_d)^2I_1^2 + \dots \quad (14)$$

$$\rho V_{\text{eff}}(\omega = 0, q \rightarrow 0)$$

$$= \frac{1}{N} \left(1 - \frac{(\epsilon_d - \mu)^2 I_1 + \sigma_0^2 I_1^2 (\epsilon_p - \epsilon_d)^2 / \rho}{2\sigma_0^2 I_2 - 2(\epsilon_d - \mu)(\epsilon_p - \epsilon_d) I_1} \right) \quad (15)$$

where $I_n = \sum_k (\gamma_k^{2n} / R_k^3) f(E_1(k))$ are integrals encountered in the interband terms R_{12} and are of order $\rho / (\epsilon_p - \epsilon_d)^3$. The final result is that $\rho V_{\text{eff}}(\omega = 0, q \rightarrow 0) = \frac{1}{N} (1 - A\delta)$

where A is a number of order unity. We can identify the Fermi liquid parameter A_0^s as $A_0^s = N\rho V_{\text{eff}}(\omega = 0, q \rightarrow 0)$,

so that

$$A_0^s \approx 1 - A\delta. \quad \text{According to Fermi liquid theory,}$$

$$\frac{dn}{d\mu} = \rho (1 - A_0^s) \approx \rho A\delta = A\rho_0 \quad (16)$$

We thus obtain the result that $dn/d\mu$ is given by the unrenormalized band density of states. This situation is familiar in the heavy Fermion problem and reflects the physical picture that the mass enhancement moves with the Fermi level as carriers are added to the system. Using the identity $1 - A_0^s = (1 + F_0^s)^{-1}$, we conclude that $F_0^s \approx \delta^{-1}$ is

very large. This latter quantity is related to

$V_{\text{eff}}(q = 0, \omega \rightarrow 0)$. Its computation is actually easier because $R_{11}(q = 0, \omega \rightarrow 0) = 0$ and the remaining terms in Eq.(12) can be easily estimated to give the desired result. The same effective interaction when considered in a different spin channel gives rise to F_0^a which is of order $1/N$ and therefore small. Thus the magnetic susceptibility χ is given by ρ and is enhanced. Again this is correct only if

$4\delta t_{pd}^2 / D > J$ and we expect χ to saturate at J^{-1} in the opposite limit.

In the Anderson lattice problem, interaction via a single boson exchange leads to a q dependent interaction which leads to a very weak d -wave pairing.[8] The computation of $V_{\text{eff}}(q, \omega = 0)$ would require extensive numerical work. However, we note that the R_{11} terms in Eq.(12) is larger than the remaining terms by at least δ^{-1} . For $q \rightarrow 0$, it is essential to keep the remaining terms because the leading contribution to $\det D^{-1}$ and to V_{eff} cancelled leading to $\rho V_{\text{eff}}(q \rightarrow 0, \omega = 0) \approx 1$. However, for general q this cancellation does not occur and it will be a reasonable approximation to keep only the R_{11} terms. This in fact corresponds closely to the infinite U one band Hubbard model treated by Kotliar and Liu[9], where one can make a similar argument that the R_{11} terms dominate for general q . Thus we expect that for $t_{pd} \ll D$ and $\delta \ll 1$, the Kotliar-Liu result will describe the two-band model also, namely, a weak attraction in the d -wave like channel with a gap parameter $\Delta(k) \approx \sin k_x \sin k_y$. In the case $\delta < 0$, examination of Eq.(12) indeed shows directly that in the limit $D \rightarrow \infty$ and $t_{pd}^2 / D \approx t_{\text{eff}}$ constant, Eq.(12) reduces to

the Kotliar-Liu result for the infinite U model with t_{eff} .

Recently, Houghton, Read and Won[10] showed that in the Anderson lattice problem, the RKKY interaction between local f moments via the polarization of the

conduction electrons is recovered in second order of $1/N$ by including the exchange of two boson propagators. Similar considerations yield the analogous process in the present problem, leading to the super-exchange J between copper moments via the oxygen orbitals. Alternatively, the exchange term can be added to the originally Hamiltonian via a canonical transformation. As noted earlier, the quasi-particles are mostly spin excitations on the copper, and so they retain the exchange interaction in the local moment picture. It has previously been noted that antiferromagnetic exchange when treated in a Hartec-Fock factorization in the particle-particle channel leads to d-wave superconductivity[11]. Our theory shows that this interaction survives in the quasi-particle picture, and that the residual hard core repulsion between the quasi-particles (as represented by single boson exchange) is small and even weakly attractive in the $sink_x sink_y$ channel. At the same time, it is clear that our theory is essentially an expansion in the parameter ρJ and the transition temperature

$$\approx (\delta t_{pd}^2 / D) \exp - (\rho J)^{-1} \text{ is low where the theory is valid.}$$

In the opposite limit when $J \gg \delta t_{pd}^2 / D$,

Anderson[12] has emphasized that the antiferromagnetism must be taken into account first, and the introduction of holes into system can lead to new possibilities, including superconducting ground state and strong deviation from Fermi liquid behavior in the normal state. A number of normal state properties, such as the linear dependencies of the Hall coefficient on doping, the fact that $\chi \approx J^{-1}$ and the linear T dependence of the resistivity have been cited as evidence for strong deviation Fermi from Fermi liquid behavior. Experimentally, the maximum T_c appears to occur in the intermediate range, when $\delta t_{pd}^2 / D \approx J$. Much

work remains to be done to develop a quantitative theory in the large

$J \gg \delta t_{pd}^2 / D$ limit and to decide whether the cross-over to

Fermi liquid behavior is a continuous one.

We conclude by remarking that many features of our solution of the two band model obtained in the limit $t_{pd} \ll D$ where we can make analytic progress, resembles what one expects for a single band model with $t_{\text{eff}} \approx 4 t_{pd}^2 / D$ and $U \approx D$. This is in agreement with the analysis of Zhang and Rice[13], carried out in the $t_{pd} \ll D$ limit. It is worth

remarking, however, that with some numerical work, our formalism is applicable also to the intermediate regime

$t_{pd} \approx D$ which we believe to be the experimental situation.

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