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LETTER TO THE EDITOR

The effective t - J Hamiltonian for the copper oxides

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Abstract. Starting from the Emery model, which is assumed to describe the copper–oxygen planes, and including direct oxygen hopping matrix elements, t_{pp} , we have been able to derive the effective t - J Hamiltonian for the copper orbitals using the linked cluster expansion method up to fourth order in t_{pd} , the hybridization matrix element. The spin-dependent part of the effective Hamiltonian is composed of two contributions: the superexchange interaction, and another one of RKKY type. The effective parameters (t and J) depend on doping, δ . This Hamiltonian can be used to study the magnetic properties of the high- T_c materials versus δ .

The study of high- T_c materials continues to attract attention from both the theoretical and the experimental point of view [1]. There is general agreement that the basic structure of these materials is composed of CuO_2 planes. There is evidence from both band-structure calculations and spectroscopy investigations that the generic properties of the CuO_2 planes can be described only in terms of the Cu $3d_{x^2-y^2}$ and the O $p_{x(y)}$ orbitals. These considerations lead us to the three-band Hubbard or Emery model. This is given by [2]:

$$H \equiv (\epsilon_d - \mu) \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + (\epsilon_p - \mu) \sum_{l\sigma} p_{l\sigma}^\dagger p_{l\sigma} + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} + t_{pp} \sum_{\langle l,l'\rangle\sigma} (-1)^{N_{ll'}} p_{l\sigma}^\dagger p_{l'\sigma} + t_{pd} \sum_{\langle l,i\rangle\sigma} (-1)^{M_{li}} (p_{l\sigma}^\dagger d_{i\sigma} + \text{HC}) \quad (1)$$

where t_{pd} is the hopping matrix element between the Cu and O orbitals, U_d is the Coulomb repulsion of two holes in a Cu $d_{x^2-y^2}$ orbital, $\Delta \equiv \epsilon_p - \epsilon_d$, or the charge transfer gap (CT), between the p and d orbitals, in the hole picture and t_{pp} is the direct oxygen hopping matrix element. These are the most important parameters of the model. These parameters are usually taken from LDA calculations [3] to be : $\Delta \simeq 3.5$ eV, $t_{pd} \simeq 1.35$ eV, $t_{pp} \simeq 0.65$ eV, and $U_d \simeq 9$ eV. In equation (1), the indices l and i refer to the oxygen and copper sites, respectively. μ is the chemical potential. The phase factors $N_{ll'}$ and M_{li} are either 0 or 1 [4].

The purpose of this letter is to give a derivation of the t - J model [5] starting from the Emery model of equation (1). The t - J model has excitations that correspond to the low-energy excitations of the Emery model [1].

To start our derivation, we Fourier analyse the oxygen orbitals. This gives

$$H \equiv (\epsilon_d - \mu) \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \sum_{k\nu\sigma} \epsilon_{k\nu} c_{k\nu\sigma}^\dagger c_{k\nu\sigma} + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} + H' \quad (2)$$

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where H' is given by

$$H' \equiv \frac{t_{pd}}{\sqrt{N}} \sum_{ik\nu\sigma} \gamma_{k\nu} \left(\exp(-ik \cdot R_i) d_{i\sigma}^\dagger c_{k\nu\sigma} + \text{HC} \right) \quad (3)$$

and

$$\epsilon_{k\nu} \equiv (\epsilon_p - \mu) + 4t_{pp}(-1)^\nu \sin \frac{k_x}{2} \sin \frac{k_y}{2} \quad \gamma_{k\nu} \equiv \sqrt{2} \left(\sin \frac{k_x}{2} + (-1)^\nu \sin \frac{k_y}{2} \right)^{1/2}. \quad (4)$$

In (3), N is the number of copper sites. This model is the three-band Anderson lattice model with the explicit oxygen band, $\epsilon_{k\nu}$ [4]. In contrast to the heavy-fermion systems, the oxygen bandwidth, $4t_{pp}$, has a magnitude of about of t_{pd} and the oxygen bands are lightly filled for $\delta \rightarrow 0$.

It can be shown that it is a good approximation to reduce the two oxygen bands to a single oxygen band [6]. This is done by means of a rotation given by $c_{k\sigma} \equiv \gamma_k^{-1} M_k \phi_{k\sigma}$, where M_k has the following form

$$M_k = \begin{bmatrix} \gamma_{k1} & \gamma_{k2} \\ \gamma_{k2} & -\gamma_{k1} \end{bmatrix}$$

where

$$\gamma_k^2 \equiv \gamma_{k1}^2 + \gamma_{k2}^2 = 4 \left(\sin^2 \frac{k_x}{2} + \sin^2 \frac{k_y}{2} \right). \quad (5)$$

Then, we end up with the following two-band Hubbard Hamiltonian

$$H \equiv (\epsilon_d - \mu) \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \sum_{k\sigma} \epsilon_k \phi_{k\sigma}^\dagger \phi_{k\sigma} + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} + H' \quad (6)$$

where H' is given by

$$H' \equiv \frac{t_{pd}}{\sqrt{N}} \sum_{ik\sigma} \gamma_k \left(\exp(-ik \cdot R_i) d_{i\sigma}^\dagger \phi_{k\sigma} + \text{HC} \right) \quad (7)$$

and

$$\epsilon_k \equiv (\epsilon_p - \mu) + 4t_{pp} \left| \sin \frac{k_x}{2} \sin \frac{k_y}{2} \right| \quad \gamma_k \equiv 2 \left(\sin^2 \frac{k_x}{2} + \sin^2 \frac{k_y}{2} \right)^{1/2} \quad (8)$$

where $|F|$ means the absolute value of F . We are going to work with one oxygen band for simplicity. The case of two oxygen bands can be treated similarly, but the final expressions become more involved. We are trying to keep the algebra as simple as possible.

Next, we want to obtain an effective Hamiltonian for the coupling between the copper atoms. For this purpose we use the linked cluster expansion method [7]. This theorem tells us that the thermodynamic potential, Ω , can be calculated from the following expression:

$$\Omega \equiv \Omega_0 - \frac{1}{\beta} \sum_{n=1}^{\infty} U_n \quad (9)$$

where Ω_0 is the unperturbed thermodynamic potential, β is the inverse of the temperature and U_n is given by

$$U_n \equiv \frac{(-1)^n}{n} \int_0^\infty d\tau_1 \cdots \int_0^\infty d\tau_n \langle T_\tau H'(\tau_1) \cdots H'(\tau_n) \rangle_c \quad (10)$$

and T_τ means time ordering [7]. The averages are performed with the oxygen orbitals and c means different connected diagrams.

Since

$$\langle \phi_{k\sigma}^{(2n+1)}(\tau) \rangle_c \equiv \langle \phi_{k\sigma}^{\dagger(2n+1)}(\bar{\tau}) \rangle_c \equiv 0 \tag{11}$$

only even terms of (10) contribute. Thus, in second order in t_{pd} , we have, with $H_2 \equiv U_2$,

$$H_2 \equiv -\frac{t_{pd}^2}{2\beta N} \sum_{\substack{ik\sigma \\ i'k'\sigma'}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \gamma_k \gamma_{k'} \times \left[\exp[-i(\mathbf{k} \cdot \mathbf{R}_i + \mathbf{k}' \cdot \mathbf{R}'_{i'})] \langle T_\tau \phi_{k\sigma}^\dagger(\tau_1) \phi_{k\sigma}^\dagger(\tau_2) \rangle d_{i\sigma}(\tau_1) d_{i'\sigma'}(\tau_2) \right. \\ + \exp[-i(\mathbf{k} \cdot \mathbf{R}_i - \mathbf{k}' \cdot \mathbf{R}'_{i'})] \langle T_\tau \phi_{k\sigma}^\dagger(\tau_1) \phi_{k\sigma}(\tau_2) \rangle d_{i\sigma}(\tau_1) d_{i'\sigma'}^\dagger(\tau_2) \\ + \exp[i(\mathbf{k} \cdot \mathbf{R}_i - \mathbf{k}' \cdot \mathbf{R}'_{i'})] \langle T_\tau \phi_{k\sigma}(\tau_1) \phi_{k\sigma}^\dagger(\tau_2) \rangle d_{i\sigma}^\dagger(\tau_1) d_{i'\sigma'}(\tau_2) \\ \left. + \exp[i(\mathbf{k} \cdot \mathbf{R}_i + \mathbf{k}' \cdot \mathbf{R}'_{i'})] \langle T_\tau \phi_{k\sigma}(\tau_1) \phi_{k\sigma}(\tau_2) \rangle d_{i\sigma}^\dagger(\tau_1) d_{i'\sigma'}^\dagger(\tau_2) \right] \tag{12}$$

But

$$\langle \phi^\dagger \phi^\dagger \rangle_c \equiv \langle \phi \phi \rangle_c \equiv 0 \tag{13}$$

$$\langle T_\tau \phi_{k\sigma}^\dagger(\tau_1) \phi_{k'\sigma}(\tau_2) \rangle \equiv \delta_{kk'} \delta_{\sigma\sigma'} \langle T_\tau \phi_{k\sigma}^\dagger(\tau_1) \phi_{k\sigma'}(\tau_2) \rangle \text{ etc.} \tag{14}$$

Thus, equation (11) reduces to

$$H_2 \equiv -\frac{t_{pd}^2}{2\beta N} \sum_{\substack{ik\sigma \\ i'k'\sigma'}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \gamma_k^2 \left[\exp(-i\mathbf{k} \cdot \mathbf{R}_{ii'}) \langle T_\tau \phi_{k\sigma}^\dagger(\tau_1) \phi_{k\sigma}(\tau_2) \rangle_c d_{i\sigma}(\tau_1) d_{i'\sigma}^\dagger(\tau_2) \right. \\ \left. + \exp(i\mathbf{k} \cdot \mathbf{R}_{ii'}) \langle T_\tau \phi_{k\sigma}(\tau_1) \phi_{k\sigma}^\dagger(\tau_2) \rangle_c d_{i\sigma}^\dagger(\tau_1) d_{i'\sigma}(\tau_2) \right]. \tag{15}$$

Since

$$G_c^0(\mathbf{k}, \tau) \equiv -\langle T_\tau \phi_{k\sigma}(\tau_1) \phi_{k\sigma}^\dagger(\tau_2) \rangle_c \tag{16}$$

equation (11) is transformed to

$$H_2 \equiv \sum_{i(\mathbf{R})\sigma} t_{\text{eff}}(\mathbf{R}) \left(d_{i\sigma}^\dagger d_{i+\mathbf{R}\sigma} + \text{HC} \right) \tag{17}$$

where the effective hopping matrix element, $t_{\text{eff}}(\mathbf{R})$, is given by

$$t_{\text{eff}}(\mathbf{R}) \equiv \frac{t_{pd}^2}{2N} \sum_{\mathbf{k}} \gamma_k^2 \cos(\mathbf{k} \cdot \mathbf{R}) \left[\frac{1}{(\epsilon_k - \epsilon_d)} (n_F(\epsilon_d) - n_F(\epsilon_k)) \right. \\ \left. - \frac{1}{(\epsilon_k - \epsilon_d - U_d)} (n_F(\epsilon_d + U_d) - n_F(\epsilon_k)) \right] \tag{18}$$

with $n_F(\epsilon)$ being the Fermi-Dirac distribution function and $\langle \mathbf{R} \rangle$ meaning nearest-neighbour atoms (NN).

Next, let us evaluate the fourth-order term, $H_4 \equiv U_4$. It is given by

$$H_4 \equiv -\frac{1}{4\beta} \int_0^{\beta_1} \dots \int_0^{\beta_4} \langle T_\tau H'(\tau_1) \dots H'(\tau_4) \rangle_c. \tag{19}$$

After a straightforward calculation, we arrive at the following result:

$$H_4 \equiv \frac{t_{pd}^4}{4N^2} \sum_{\substack{ikp\sigma \\ i'k'p'\sigma'}} (\gamma_k \gamma_{k'})^2 \hat{A}(\mathbf{k}, \mathbf{k}'; \beta)$$

$$\begin{aligned}
& \times \left[\exp[-i(\mathbf{k} \cdot \mathbf{R}_{ip} + \mathbf{k}' \cdot \mathbf{R}_{i'p})] d_{i\sigma}^\dagger d_{p\sigma'}^\dagger d_{i'\sigma}^\dagger d_{p'\sigma}^\dagger \right. \\
& + \exp[-i(\mathbf{k} \cdot \mathbf{R}_{ip} + \mathbf{k}' \cdot \mathbf{R}_{i'p'})] d_{i'\sigma}^\dagger d_{p\sigma}^\dagger d_{i\sigma}^\dagger d_{p'\sigma'}^\dagger \\
& + \exp[-i(\mathbf{k} \cdot \mathbf{R}_{i'i} + \mathbf{k}' \cdot \mathbf{R}_{p'p})] d_{i\sigma}^\dagger d_{p'\sigma'}^\dagger d_{p\sigma}^\dagger d_{i'\sigma}^\dagger \\
& + \exp[-i(\mathbf{k} \cdot \mathbf{R}_{i'p'} + \mathbf{k}' \cdot \mathbf{R}_{pi'})] d_{i\sigma}^\dagger d_{i'\sigma}^\dagger d_{p\sigma}^\dagger d_{p'\sigma'}^\dagger \\
& + \exp[-i(\mathbf{k} \cdot \mathbf{R}_{ip} + \mathbf{k}' \cdot \mathbf{R}_{p'i})] d_{i\sigma}^\dagger d_{i'\sigma}^\dagger d_{p'\sigma'}^\dagger d_{p\sigma}^\dagger \\
& \left. + \exp[-i(\mathbf{k} \cdot \mathbf{R}_{i'i} + \mathbf{k}' \cdot \mathbf{R}_{p'p})] d_{i\sigma}^\dagger d_{p\sigma}^\dagger d_{p'\sigma'}^\dagger d_{i'\sigma}^\dagger + \text{HC} \right] \quad (20)
\end{aligned}$$

where

$$\hat{A}(\mathbf{k}, \mathbf{k}'; \beta) \equiv \frac{1}{\beta} \sum_{ik_n} G_c^0(\mathbf{k}, ik_n) G_c^0(\mathbf{k}', ik_n) g_d^2(ik_n) \quad (21)$$

and

$$G_c^0(\mathbf{k}, ik_n) \equiv \frac{1}{(ik_n - \epsilon_k)} \quad (22)$$

$$g_d(ik_n) \equiv \frac{1}{2(ik_n - \epsilon_d)} + \frac{1}{2(ik_n - \epsilon_d - U_d)} \quad (23)$$

where we have taken the atomic limit for the copper sites [8].

By performing the Matsubara summation, we obtain

$$\hat{A}(\mathbf{k}, \mathbf{k}'; \beta) \equiv \hat{A}_1(\mathbf{k}, \mathbf{k}'; \beta) + \hat{A}_2(\mathbf{k}, \mathbf{k}'; \beta) \quad (24)$$

with

$$\begin{aligned}
\hat{A}_1(\mathbf{k}, \mathbf{k}'; \beta) & \equiv \frac{n_F(\epsilon_d)}{2(\epsilon_k - \epsilon_d)(\epsilon_{k'} - \epsilon_d)} \left[\frac{1}{(\epsilon_{k'} - \epsilon_d)} - \frac{1}{U_d} \right] \\
& \times \frac{n_F(\epsilon_d + U_d)}{2(\epsilon_d + U_d - \epsilon_k)(\epsilon_d + U_d - \epsilon_{k'})} \left[\frac{1}{(\epsilon_k - \epsilon_d - U_d)} + \frac{1}{U_d} \right] \quad (25)
\end{aligned}$$

$$\begin{aligned}
\hat{A}_2(\mathbf{k}, \mathbf{k}'; \beta) & \equiv \frac{n_F(\epsilon_k)}{2(\epsilon_k - \epsilon_{k'})} \left[\frac{1}{(\epsilon_k - \epsilon_d)^2} \right. \\
& \left. + \frac{1}{(\epsilon_k - \epsilon_d - U_d)^2} + \frac{2}{(\epsilon_k - \epsilon_d)(\epsilon_k - \epsilon_d - U_d)} \right]. \quad (26)
\end{aligned}$$

In order to obtain a $\cos((\mathbf{k} - \mathbf{k}') \cdot \mathbf{R})$ dependence from (20), we need to make the following identifications

$$\begin{aligned}
i' & \equiv p' & p & \equiv i & (\text{first term}) \\
i' & \equiv p & p' & \equiv i & (\text{second term}) \\
i' & \equiv p & p' & \equiv i & (\text{third term etc.})
\end{aligned}$$

Then, we arrive at the following result

$$H_4 \equiv \frac{1}{2} \sum_{\substack{i(R) \\ \sigma\sigma'}} J(\mathbf{R}) d_{i\sigma}^\dagger d_{i+\mathbf{R}\sigma'}^\dagger d_{i+\mathbf{R}\sigma}^\dagger d_{i\sigma}^\dagger \quad (27)$$

where

$$J(\mathbf{R}) \equiv \frac{3t_{pd}^4}{N^2} \sum_{kk'} \hat{A}(\mathbf{k}, \mathbf{k}'; \beta) (\gamma_k \gamma_{k'})^2 \cos((\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}). \quad (28)$$

On the other hand, the spin summation can be rewritten as

$$\sum_{\sigma\sigma'} d_{i\sigma} d_{i\sigma}^\dagger d_{j\sigma'} d_{j\sigma'}^\dagger \equiv \frac{1}{2} n_i n_j + 2 \mathbf{S}_i \cdot \mathbf{S}_j. \quad (29)$$

So, H_4 can be expressed in a compact form as:

$$H_4 \equiv \sum_{i(\mathbf{R})} J(\mathbf{R}) \left(\mathbf{S}_i \cdot \mathbf{S}_{i+\mathbf{R}} + \frac{1}{4} n_i n_{i+\mathbf{R}} \right). \quad (30)$$

From (30), we can conclude that the fourth-order contribution to the effective Hamiltonian has the form of a spin-dependent part $J(\mathbf{R})$, as in the t - J model. This $J(\mathbf{R})$ term has two contributions (see equations (24), (25) and (26)). If we make the following approximation

$$\epsilon_k - \epsilon_d \simeq \Delta \quad (31)$$

we see that $\hat{A}_m(\mathbf{k}, \mathbf{k}'; \beta)$, $m = 1, 2$, is given by

$$\hat{A}_1(\mathbf{k}, \mathbf{k}'; \beta) \simeq D_1 \quad (32)$$

$$\hat{A}_2(\mathbf{k}, \mathbf{k}'; \beta) \simeq D_2 \frac{1}{(\epsilon_k - \epsilon_{k'})} \quad (33)$$

where D_1 and D_2 are constants, with $D_1 > 0$.

$J(\mathbf{R})$ has two contributions: (i) a superexchange type of interaction due to $\hat{A}_1(\mathbf{k}, \mathbf{k}'; \beta)$ [9]; and (ii) a RKKY type of interaction [6] ($\hat{A}_2(\mathbf{k}, \mathbf{k}'; \beta)$) which is strongly dependent upon doping rate, δ , and has an oscillatory behaviour at very long distances between the copper atoms. It is this doping dependency of $J(\mathbf{R})$ that makes it interesting. It is possible to study the magnetic properties as functions of doping, as was done in [6]. In particular, the J_{RKKY} interaction might lead to a frustration of the long-range antiferromagnetic ordering with doping (small δ). In addition to the $J(\mathbf{R})$ term, we find a local repulsion given by the U_d term.

At this point, we have the effective Hamiltonian, H_{eff} , on the copper sites, given by

$$H_{\text{eff}} \equiv (\epsilon_d - \mu) \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + H_2 + H_4 + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow}. \quad (34)$$

In the large- U_d limit, we can enforce no double occupancy at half filling, by using perturbation theory on virtual states [10]. The result is

$$\begin{aligned} \hat{H}_{\text{eff}} \equiv & (\epsilon_d - \mu) \sum_{i\sigma} \hat{d}_{i\sigma}^\dagger \hat{d}_{i\sigma} + t \sum_{i(\mathbf{R})\sigma} \hat{d}_{i+\mathbf{R}\sigma}^\dagger \hat{d}_{i\sigma} \\ & + (J_1 + J_2) \sum_{i(\mathbf{R})} \mathbf{S}_i \cdot \mathbf{S}_{i+\mathbf{R}} + (J_1 - J_2) \sum_{i(\mathbf{R})} n_{i+\mathbf{R}} n_i + \text{three-site terms} \end{aligned} \quad (35)$$

where

$$t \equiv t_{\text{eff}}(\mathbf{R}) \quad J_1 \equiv J(\mathbf{R}) \quad J_2 \equiv \frac{4t^2}{U_d} \quad \hat{d}_{i\sigma} \equiv d_{i\sigma} (1 - n_{i-\sigma}). \quad (36)$$

In conclusion, we have been able to derive and extend the t - J Hamiltonian starting from the three-band Hubbard or Emery model. Our effective parameter J_1 contains the superexchange interaction of the t - J model derived by Zhang and Rice [5] in the limit of $t_{\text{pp}} \rightarrow 0$. However, t_{pp} is a key element in the description of the physics of high- T_c superconductors and it should not be taken equal to zero. The effective parameters depend on doping by means of the Fermi level. The spin-dependent part of the effective Hamiltonian is composed of two contributions, one mainly antiferromagnetic given by \hat{A}_1 , and a second one given by \hat{A}_2 , which is of the RKKY type. To our knowledge, it is the first

time that the latest contribution has been derived simultaneously with the superexchange contribution. There is a calculation by Eskes and Jefferson [11] where they have included t_{pp} and then used fifth-order perturbation theory. However, they did not obtain the RKKY-type interaction. The existence of the two contributions is of interest for studies of the evolution of magnetic properties upon doping.

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