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SCHRIFFIER-WOLFF TRANSFORMATION OF THE p-d MODEL FOR OXIDE SUPERCONDUCTORS: CHARGE FLUCTUATION REGIME

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Преобразование Шриффера — Вольфа для p-d модели
оксидных сверхпроводников: режим зарядовых флуктуаций

На основе преобразования Шриффера — Вольфа дан систематический вывод эффективных взаимодействий до четвертого порядка по амплитуде V p-d гибридизации, описывающих низкоэнергетические свойства плоскости CuO_2 в оксидных сверхпроводниках. По сравнению с другими аналогичными выводами мы предполагаем, что амплитуда V сравнима с величиной щели $\Delta = \epsilon_p - \epsilon_d$, что соответствует режиму зарядовых (но не спиновых $V \ll \Delta$) флуктуаций в системе. Особое внимание уделено изучению проблемы магнитных фрустраций в системе Cu-спинов.

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Schriffier-Wolff Transformation of the p-d Model
for Oxide Superconductors: Charge Fluctuation Regime

To describe low-energy properties of the CuO_2 plane in oxide superconductors the effective interactions up to the fourth order in the p-d hybridization amplitude V are derived systematically by the Schrieffer-Wolff transformation. Contrary to other analogous derivations we assume the value of V to be comparable to the charge transfer gap $V \sim \Delta = \epsilon_p - \epsilon_d$ that corresponds to the charge fluctuation (not spin fluctuation $V \ll \Delta$) regime in the system. Among the variety of relevant phenomena we examine only a particular problem of magnetic frustrations in the system of Cu-spins.

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1. Introduction

It is now widely recognized that high-T_c superconductivity is deeply related to the problem of strong correlations. Some simplification in treating this problem is usually gained by transforming the starting one-band (or extended) Hubbard model into an approximate effective Hamiltonian which describes relevant low-energy properties of oxide superconductors. The simplest effective Hamiltonian is the well-known t-J model /1/ which is transformed in the canonical perturbation theory /2,3/ from the one-band Hubbard Hamiltonian in the strong correlation limit. More complicated examples appear /4-6/ when one considers highly hybridized orbitals in the CuO_2 plane on the basis of the p-d model suggested by Emery /7/. In this model the largest energy is the on-site Hubbard repulsion U_d at copper sites and an extra hole, introduced to the system by doping,goes to the oxygen p-level. One may highlight two different regimes for holes dynamics /8/. The first one,the so-called spin fluctuation regime, corresponds to a weak copper-oxygen hybridization parameter, $V \ll \Delta$, $U_d - \Delta$, where Δ is the charge transfer gap and $U_d - \Delta$ is energy of the higher Hubbard sublevel at copper sites with respect to the p-level. In this limit,one obtains a Kondo-type effective Hamiltonian /4/ that involves propagating oxygen holes which interact with the strongly localized copper spins. According to /5,9,10/ more representative values of the parameters in the Emery model give not so weak hybridization. In fact, $V < \Delta$, while $V \ll U_d - \Delta$ is fulfilled. Such a choice of the parameters i.e. the charge fluctuation regime, requires special attention because the charge degrees of freedom at copper sites should be taken into account.

The first systematic derivation of effective interactions up to the fourth order in V/Δ and $V/(U-\Delta)$ in the spin fluctuation regime was presented by Zaanen and Oles /11/.They applied the formalism of projection operators in the canonical perturbation theory, as it was done in obtaining the t-J model /3/. Recently, the same results /12/ have been rederived on the basis of the canonical Schrieffer-Wolff transformation. Besides, a great variety of other papers is devoted to the derivation and analysis of approximate effective Hamiltonians in the spin fluctuation limit of the Emery model.We mention only a few of them /4-6,9/. Particularly, a good deal of efforts are undertaken in the study of relation of the t-J model to the p-d, or even more general Hamiltonian containing Cu- and O-bands /8,11,13-16/.

To the author's knowledge, the systematic perturbation expansion consideration of the charge fluctuation regime for the Emery model like this is not so far presented in the literature. In this paper we fill partly this blank and obtain on the basis of the canonical Schrieffer-Wolff transformation the effective interactions to the fourth order in V. The effects of the direct oxygen-oxygen hopping (O-band) on the effective interactions are taken into account as well.

Effective Hamiltonian derived here involves a variety of different kinds of interactions and provides a basis for better understanding the low-energy properties of the CuO_2 plane. Among them we restrict ourselves to a particular problem of magnetic frustrations in the system of Cu-spins and calculate superexchange integrals as functions of the direct O-transfer and the O-hole concentration.

2. p-d Model and Canonical Transformation

Hamiltonian for the CuO_2 plane can be written as

$$H = \varepsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \sum_{im\sigma} V_{im}(d^+_{i\sigma}c_{m\sigma} + c^+_{m\sigma}d_{i\sigma}) + U_d \sum_i n_{i\uparrow}n_{i\downarrow}$$
$$+ \sum_{mn\sigma} t_{mn} c^+_{m\sigma} c_{n\sigma} \qquad (1)$$

where $d^+_{i\sigma}$ ($d_{i\sigma}$) and $c^+_{m\sigma}$ ($c_{m\sigma}$)are hole operators for copper (**i**) and oxygen (**m**) sites. The energy of the oxygen p-level is chosen to be zero, $\varepsilon_p=0$, hence for the copper d-level $\varepsilon_d<0$. The hybridization parameter V_{im} is non-zero only for the near-neighboring (n.n.) Cu-O sites. In comparison with the original Emery model /7/ we omit the on-site repulsion at O-ions ($U_p = 0$) and n.n. Cu-O repulsion ($U_{pd}=0$), while the direct hopping term ($\sim t_{mn}$) between n.n. O-sites is involved. The representative values (in eV) for the parameters are /5,9,10/: $|\varepsilon_d| \cong 2$, $|V| \cong 1.5$,$U_d \cong 8$ and $t \cong 0.5$, which provides the charge fluctuation regime $V << U_d + \varepsilon_d$ while $V/|\varepsilon_d| < 1$

To treat strong correlations at Cu-sites,it is natural to introduce the Hubbard operators $X^{pq}_i = |ip\rangle\langle qi|$ instead of $d^+_{i\sigma}$ ($d_{i\sigma}$) operators

$$d^+_{i\sigma} = X^{\sigma 0}_i + \varepsilon_{\sigma'\sigma} X^{2\sigma'}_i \qquad d_{i\sigma} = X^{0\sigma}_i + \varepsilon_{\sigma'\sigma} X^{\sigma' 2}_i \qquad (2)$$

where $\varepsilon_{\uparrow\downarrow} = - \varepsilon_{\downarrow\uparrow} = 1$ and $\varepsilon_{\uparrow\uparrow} = \varepsilon_{\downarrow\downarrow} = 0$. The operator $X^{\sigma 0}_i$ ($X^{0\sigma}_i$) creates (destroys) a hole with the spin σ on the lower d-sublewel with the energy ε_d and $X^{2\sigma}_i$ ($X^{\sigma 2}_i$)creates (destroys) a hole with the spin $\bar{\sigma}=-\sigma$ on the upper d-sublevel with the energy $U_d+\varepsilon_d$.

In terms of these operators Hamiltonian (1) can be rewritten in the following form :

$$H = H_0 + H_1 + H_2$$

$$H_0 = \varepsilon_d \sum_{i\sigma} X^{\sigma\sigma}_i + (U_d+2\varepsilon_d) \sum_i X^{22}_i + \sum_{mn\sigma} t_{mn} c^+_{m\sigma} c_{n\sigma} \qquad (3)$$

$$H_1 = H^+_1 + \text{h.c.} \qquad H^+_1 = \sum_{im\sigma} V_{im} X^{\sigma 0}_i c_{m\sigma} \qquad (4)$$

$$H_2 = H^+_2 + \text{h.c.} \qquad H^+_2 = \sum_{im} \sum_{\sigma\sigma'} V_{im} \varepsilon_{\sigma'\sigma} X^{2\sigma'}_i c_{m\sigma} \qquad (5)$$

Our aim is to obtain an effective Hamiltonian (to the fourth order in V) which works in the (low in energy) subspace of states with no doubly occupied copper sites. Just the term H_2 corresponds to the admixure of the high-energy states, and hence, we consider this term in (5) as the perturbation. As the first step we remove from the transformed Hamiltonian $H' = \exp(S_1)H\exp(-S_1)$ the term linear in H_2. This gives for the generator $S_1 = S_1^+ -$ h.c. of the Schrieffer-Wolff transformation the following equation:

$$\mathrm{ad}_{S_1} H_0 = -H_2 \tag{6}$$

with the notation

$$\mathrm{ad}_A B \equiv [A,B]. \tag{7}$$

Then, Hamiltonian H' can be represented in the form

$$H' = H_0 + H_1 + \sum_{n=1}^{\infty}\left[\frac{n}{(n+1)!}\,\mathrm{ad}^n_{S_1} H_2 + \frac{1}{n!}\,\mathrm{ad}^n_{S_1} H_2\right] \tag{8}$$

The linear in V Hamiltonian H_1 gives the residual hybridization which mixes hole's states at the lower d-sublevel with the p-level states. This linear term cannot be removed by a canonical perturbation transformation because the change-transfer gap $|\varepsilon_d|$ is not as large as $U_d+\varepsilon_d$. However, being the part of the main interactions in H_0+H_1 the term H_1 gives higher order in V contributions.

To satisfy equation (6) the generator S_1^+ should be chosen in the form

$$S_1^+ = \sum_{i\sigma} X_i^{2\sigma}\lambda_{i\sigma}$$

and for the operator $\lambda_{i\sigma}$ we obtain from (6) the equation

$$[H_0,S_1^+] = \sum_{i\sigma} X_i^{2\sigma}(U_d+\varepsilon_d+\mathrm{ad}_{H_0})\lambda_{i\sigma} = \sum_{im\sigma\sigma'} V_{im}\varepsilon_{\sigma'\sigma} X_i^{2\sigma'} c_{m\sigma}$$

This equation is satisfied if

$$\lambda_{i\sigma'} = \sum_{m\sigma} V_{im}\varepsilon_{\sigma'\sigma}(U_d+\varepsilon_d+\mathrm{ad}_{H_0})^{-1}c_{m\sigma}$$

Taking into account that

$$\mathrm{ad}_{H_0} c_{m\sigma} = -\sum_n t_{mn}\, c_{n\sigma}$$

and introducing the $\hat{t}$ -matrix with elements t_{mn} we finally obtain the result

$$S_1^+ = \sum_{inm}\sum_{\sigma\sigma'} V_{in}\, X_i^{2\sigma'}\varepsilon_{\sigma'\sigma}[(U_d+\varepsilon_d-\hat{t})^{-1}]_{nm}\, c_{m\sigma} \tag{9}$$

Note that the Schriffer -Wolff transformation with the generator (9) takes into account effects of the narrow O-band to any given order in $t/(U_d+\varepsilon_d) \ll 1$, because

$$[(U_d+\varepsilon_d-\hat{t})^{-1}]_{nm} = \sum_{k=0}^{\infty}\frac{1}{(U_d+\varepsilon_d)^{k+1}}\,(\hat{t}^k)_{nm} \tag{10}$$

For clarity below we put following notation :$U_d+\varepsilon_d-\hat{t} = \hat{U}_1$.

Let us examine the second order effective interactions corresponding to n=1 terms in (8). The straightforward calculations gives first the result

$$\begin{aligned}\mathrm{ad}_{S1}H_2 = {} & \sum_{ij}\sum_{\sigma}\left(V\frac{1}{U_1}V\right)_{ij} X_i^{2\sigma}X_j^{\sigma 2} \\ & -\sum_{iml}\sum_{\sigma}\left(V\frac{1}{U_1}\right)_{im}V_{il}\, X_i^{22}\, c^+_{m\sigma}c_{l\sigma} \\ & -\sum_{iml}\sum_{\sigma\sigma'\alpha\nu}\left[\left(V\frac{1}{U_1}\right)_{im}V_{il}\, X_i^{\sigma\sigma'}c^+_{m\alpha}\, c_{l\nu}\,\varepsilon_{\sigma\alpha}\,\varepsilon_{\sigma'\nu} + \text{h.c.}\right]\end{aligned} \tag{11}$$

Here

$$\left(V\frac{1}{U_1}V\right)_{ij} = \sum_{mn} V_{im}\left(\frac{1}{U_1}\right)_{mn} V_{jn}$$

$$\left(V\frac{1}{U_1}\right)_{in} = \sum_{m} V_{im}\left(\frac{1}{U_1}\right)_{mn} \tag{12}$$

The physical meaning of the processes involved in (11) is clear. It should be only stressed that each of the terms in (11) works either in the subspase of highly excited states with double occupancy (the first and the second line in (11)) or in the subspace of low-lying states (the third line in (11)). The rest of the second order interactions are given by

$$\mathrm{ad}_{S_1} H_1 = \sum_{ij} \sum_{\sigma\sigma'} \Big[(V \frac{1}{U_1} V)_{ij} \, X_i^{2\sigma'} X_j^{0\sigma} \varepsilon_{\sigma\sigma'}$$

$$+ \sum_{ml} (V \frac{1}{U_1})_{im} V_{il} \, X_i^{20} \, c^+_{m\sigma} c_{l\sigma'} \varepsilon_{\sigma\sigma'} + \mathrm{h.c.} \Big] \qquad (13)$$

Both kinds of the processes involved in (13) lead to mixing of the highly excited and low-lying states in the sustem. These second order hybridization terms should be removed from the resulting effective Hamiltonian. We make this by applying the second Schrieffer-Wolff transformation $\tilde{H} = \exp(S_2) H' \exp(-S_2)$. Requiring that the transformed Hamiltonian $\tilde{H}$ does not include the term linear in $\mathrm{ad}_{S_1} H_1$ we obtain by the procedure developed before the generator S_2 in the following form:

$$S_2 = S_2^{(1)} + S_2^{(2)}$$

$$S_2^{(1)} = \sum_{ij} \sum_{\sigma\sigma'} \Big[(V \frac{1}{U_1} V)_{ij} \frac{1}{U_d} X_i^{2\sigma'} X_j^{0\sigma} \varepsilon_{\sigma\sigma'} - \mathrm{h.c.} \Big] \qquad (14)$$

$$S_2^{(2)} = \sum_{\substack{iml \\ m'l'}} \sum_{\sigma\sigma'} \Big[(V \frac{1}{U_1})_{im} V_{il} \Big[\frac{1}{U_2} \Big]_{mm'll'} X_i^{20} \, c^+_{m'\sigma} c_{l'\sigma'} \varepsilon_{\sigma\sigma'} - \mathrm{h.c.} \Big]$$

where

$$\Big[\frac{1}{U_2} \Big]_{mm'll'} = \sum_{n=0}^{\infty} \Big[\frac{1}{(U_d + 2\varepsilon_d - \hat{t}\,)^{n+1}} \Big]_{mm'} (\hat{t}^n)_{ll'} \qquad (15)$$

Introducing the operator P projecting out the highly excited states, we obtain the effective Hamiltonian expanded in V as

$$\tilde{H}_{eff} = P \exp(S_2) \exp(S_1) H \exp(-S_1) \exp(-S_2) P = \sum_{n=0}^{\infty} \tilde{H}^{(n)} \qquad (16)$$

Up to the fourth order one has

$$\tilde{H}^{(0)} = P H_0 P, \qquad \tilde{H}^{(1)} = P H_1 P,$$

$$\tilde{H}^{(2)} = \frac{1}{2} P \, \mathrm{ad}_{S_1} H_2 P, \qquad \tilde{H}^{(3)} = \frac{1}{2} P \, \mathrm{ad}^2_{S_1} H_1 P, \qquad (17)$$

$$\tilde{H}^{(4)} = \frac{1}{8} P \, \mathrm{ad}^3_{S_1} H_2 P + \frac{1}{2} P \, \mathrm{ad}_{S_2} \mathrm{ad}_{S_1} H_1 P$$

3. Effective Interactions

After performing some lengthy calculation and classifying different kinds of interactions we present the transformed Hamiltonian in the final form

$$\tilde{H}_{eff} = \tilde{H}_0 + \tilde{H}_{Cu-O} + \tilde{H}_{Cu-Cu} + \tilde{H}_{S-S} \qquad (18)$$

The zero order Hamiltonian is

$$\tilde{H}_0 = \varepsilon_d \sum_{i\sigma} N_i + \sum_{mn\sigma} t_{mn} c^+_{m\sigma} c_{n\sigma} \qquad (19)$$

where

$$N_i = \sum_{\sigma} X_i^{\sigma\sigma}$$

The effective Cu-O Hamiltonian $\tilde{H}_{Cu-O}$ includes four terms

$$\tilde{H}_{Cu-O} = \sum_{n=1}^{4} \tilde{H}^{(n)}_{Cu-O} \qquad (20)$$

The first term is the first-order residual hybridization interaction with $V^{(1)}(i|m) \equiv V_{im}$

$$\tilde{H}^{(1)}_{1} = \sum_{im\sigma} V^{(1)}(i|m)\, X_i^{\sigma 0} c_{m\sigma} + \text{h.c.} \qquad (21)$$

The second-order term is

$$\tilde{H}^{(2)}_{Cu-O} = \sum_{imn} J^{(2)}(i|m\ n) \left[\mathbf{S}_i \mathbf{s}_{mn} - \frac{1}{4} N_i n_{mn} \right] \qquad (22)$$

where

$$S_i^{\alpha} = \frac{1}{2} X_i^{\sigma\sigma'} \sigma^{\alpha}_{\sigma\sigma'} \ , \quad s^{\alpha}_{mn} = \frac{1}{2} c^{+}_{m\sigma} c_{n\sigma'} \sigma^{\alpha}_{\sigma\sigma'} \ , \quad n_{mn} = c^{+}_{m\sigma} c_{n\sigma}$$

and

$$J^{(2)}(i|m\ n) = \left(V\frac{1}{U_1}\right)_{im} V_{in} + \left(V\frac{1}{U_1}\right)_{in} V_{im} \qquad (23)$$

Hamiltonian $\tilde{H}^{(2)}_{Cu-O}$ involves at $m \neq n$ the oxygen hopping three-site O-Cu-O interaction and at m=n the antiferromagnetic exchange interaction with the constant $J^{(2)}(i|m\ m)$ between copper ($\mathbf{S}_i$) and oxygen ($\mathbf{s}_m$) spins. Due to expansion (10) of the matrix $\left(\frac{1}{U_1}\right)_{lm}$ in powers of the oxygen hopping integral t_{nm} these interactions connect not only nearest-neighboring, bat more distant sites. The next contribution is the third order Cu-O hybridization-type interactions

$$\tilde{H}^{(3)}_{Cu-O} = \sum_{ijm} \sum_{\sigma\sigma'} V^{(3)}(ij|m) \left[X_i^{\sigma 0} X_j^{\bar{\sigma}\bar{\sigma}'} c_{m\sigma'} \varepsilon_{\sigma\bar{\sigma}} \varepsilon_{\sigma'\bar{\sigma}'} + \text{h.c.} \right] \qquad (24)$$

$$+ \sum_{ilmn} \sum_{\sigma\sigma'} V^{(3)}(i|l\ n\ m) \left[X_i^{\sigma 0} c^{+}_{l\bar{\sigma}} c_{n\bar{\sigma}'} c_{m\sigma'} \varepsilon_{\sigma\bar{\sigma}} \varepsilon_{\sigma'\bar{\sigma}'} + \text{h.c.} \right]$$

where

$$V^{(3)}(ij|m) = -\frac{1}{2} \left(V\frac{1}{U_1} V\right)_{ij} \left(V\frac{1}{U_1}\right)_{jm}$$

$$V^{(3)}(i|l\ n\ m) = \frac{1}{2} \left(V\frac{1}{U_1}\right)_{il} \left(V\frac{1}{U_1}\right)_{in} V_{im} \qquad (25)$$

The fourth order term is

$$\tilde{H}^{(4)}_{Cu-O} = \sum_{imnll'} A^{(4)}(i|m\ n\ l\ l') \left[\mathbf{S}_i \mathbf{s}_{mn} - \frac{1}{4} N_i n_{mn} \right] n_{ll'} + \text{h.c.} \qquad (26)$$

$$+ \sum_{ijmn} \left\{ \frac{1}{2} \left[B^{(4)}(ij|mn) + B^{(4)}(ij|nm) \right] N_j - B^{(4)}(ii|mn) \right\} \times$$

$$\times \left[\mathbf{S}_i \mathbf{s}_{mn} - \frac{1}{4} N_i n_{mn} \right]$$

and involves different kinds of exchange-type Cu-O interactions and oxygen hopping-type O-Cu-O interactions. Here

$$A^{(4)}(i|mnll') = \frac{1}{4} \left(V\frac{1}{U_1}\right)_{im} \left[V_{in} \left(V\frac{1}{U_1}\right)_{il} \left(V\frac{1}{U_1}\right)_{il'} \right.$$

$$\left. - V_{il'} \left(V\frac{1}{U_1}\right)_{in} \left(V\frac{1}{U_1}\right)_{il} \right] \qquad (27)$$

$$B^{(4)}(ij|mn) = \frac{3}{2} \left(V\frac{1}{U_1} V\right)_{ij} \left(V\frac{1}{U_1}\right)_{im} \left(V\frac{1}{U_1}\right)_{jn}$$

$$+ \frac{1}{4} \left(V \frac{1}{U_1^2} V\right)_{ij} \left[\left(V\frac{1}{U_1}\right)_{im} V_{jn} + \left(V\frac{1}{U_1}\right)_{jn} V_{im} \right] \qquad (28)$$

The Cu-Cu effective Hamiltonian $\tilde{H}_{Cu-Cu}$ contains three kinds of fourth-order interactions

$$\tilde{H}_{Cu-Cu} = \sum_{k=1}^{3} \tilde{H}^{(4)}_{Cu-Cu}(k) \qquad (29)$$

Two of them are given by

$$\tilde{H}^{(4)}_{Cu-Cu}(1)=\sum_{ij} J^{(4)}(ij)\left[S_iS_j - \frac{1}{4} N_iN_j \right] \qquad (30)$$

$$\tilde{H}^{(4)}_{Cu-Cu}(2)=-\sum_{ijmn} \frac{1}{4} \left[B^{(4)}(ij|mn)+B^{(4)}(ij|nm)\right]\left[S_iS_j- \frac{1}{4} N_iN_j\right]n_{mn} \qquad (31)$$

Here

$$J^{(4)}(ij)= \frac{2}{U_d} (V\frac{1}{U_1} V)^2_{ij} \qquad (32)$$

and (30) gives the familiar Cu-Cu superexchange interaction while (31) incorporates explicitly the oxygen operator n_{mn} and, hence, causes a renormalization for the Cu-Cu superexcenge depending on an oxygen hole doping .

The third term in (29) presents an effective highly correlated d-hole hopping interaction

$$\tilde{H}^{(4)}_{Cu-Cu}(3)= \frac{1}{2}\sum_{ikj\sigma} J^{(4)}(ikj)\left[X_i^{\bar{\sigma}0} X_k^{\sigma\bar{\sigma}} X_j^{0\sigma}- X_i^{\bar{\sigma}0} X_k^{\sigma\sigma} X_j^{0\bar{\sigma}} \right] \qquad (33)$$

where

$$J^{(4)}(ikj)= \frac{2}{U_d} (V\frac{1}{U_1} V)_{ik}(V\frac{1}{U_1} V)_{kj}(1-\delta_{ij}) \qquad (34)$$

Hamiltonian (33) is anologous to the three-site extra term one obtains in deriving perturbatively the well-known t-J model /3/.

To make the physical meaning of the interactions presented by $\tilde{H}_{S-S}$ more clear, the last term in (18), let us first introduce the singlet combinations of oxygen and copper hole operators, respectively,

$$\phi_{nm} = \sum_{\sigma\sigma'} c_{n\sigma'} c_{m\sigma}\, \varepsilon_{\sigma\sigma'}\ , \qquad \psi_{ji} = \sum_{\sigma\sigma'} X_j^{0\sigma'} X_i^{0\sigma}\, \varepsilon_{\sigma\sigma'}$$

Then the effective Hamiltonian $\tilde{H}_{S-S}$ contains two fourth order parts

$$\tilde{H}_{S-S}= \tilde{H}_{S-S}(1)+ \tilde{H}_{S-S}(2)$$

and gives singlet-singlet interactions

$$\tilde{H}_{S-S}(1)=\sum G^{(4)}(i|mnll')\ X_i^{00}\ \phi^+_{mn}\ \phi_{ll'} \qquad (36)$$

$$\tilde{H}_{S-S}(2)= \sum \left[F^{(4)}(ij|mn)\ \ \phi^+_{mn}\ \psi_{ij}+ h.c.\right] \qquad (37)$$

Here

$$G^{(4)}(i|mnll')=\frac{1}{2} \sum_{m'n'} V_{im'}(V\frac{1}{U_1})_{in'}\Big[V_{im}(V\frac{1}{U_1})_{in} (\frac{1}{U_2})_{m'l\ n'l'}$$

$$+ V_{il}(V\frac{1}{U_1})_{il'}(\frac{1}{U_2})_{m'm\ n'n}\Big]. \qquad (38)$$

$$F^{(4)}(ij|mn)= - \frac{1}{2} (V\frac{1}{U_1}V)_{ij} \Big[V_{im}(V\frac{1}{U_1})_{in}\frac{1}{U_d} +$$

$$\sum_{ll'} V_{il}(V\frac{1}{U_1})_{il'}(\frac{1}{U_2})_{ln\ l'm} \Big] \qquad (39)$$

We see the Hamiltonian (18)-(39) derived here involves a variety of different kinds of effective interactions and serves as a good starting point to investigate low-energy properties of the CuO_2 plane in oxide superconductors. This work remains to be done elsewhere.

4. Magnetic Frustration in CuO_2 Plane

Here, we restrict ourselves to one of the phenomena, namely, to the problem of magnetic frustration effects in the system of Cu-spins. These effects are described by two fourth-order interactions (30) and (31). To estimate the dependence of the effective Cu-Cu superexchange integral $J^{(4)}(ij)$ on the oxygen doping we ignor the subtle effects of O-hole hoping by putting for site indices n=m in (31). After replacing in a mean-field approximation the O-hole operator n_{mm} by the average hole occupation number for O-sites $\langle n_{mm}\rangle = \sum_{\sigma} \langle c^{+}_{m\sigma} c_{m\sigma}\rangle \equiv n_p$ one gets the Heisenberg Hamiltonian

$$\tilde{H}^{(4)}_{Cu-Cu}(1) + \tilde{H}^{(4)}_{Cu-Cu}(2) \cong \sum_{ij} \tilde{J}^{(4)}(ij) \left[S_i S_j - \frac{1}{4} N_i N_j \right] \qquad (40)$$

where

$$\tilde{J}^{(4)}(ij) = J^{(4)}(ij) - n_p \frac{1}{2} \sum_{m} B^{(4)}(ij|mm) \qquad (41)$$

It is worth noting that the residual hybridization term, H_1 in (4), being considered perturbatively at $V \ll |\varepsilon_d|$, provides additional contributions (proportional to $V^4/|\varepsilon_d|^3$) to the superexchange constant $\tilde{J}^{(4)}(ij)$ in (40). At this limit Ihle and Kasner /17/ have investigated frustrations effects in Cu-spin system. However, treating the problem at $U_d \to \infty$ they missed the contribution (40)-(41). Here we examine separately the frustration effects giving by (40),(41) at finite value of U_d in the same manner as it was done in /17/.

From (28) and (32) we obtain for the nearest neighbours, (i,j)=n.n., the following form for the superexchange integral

$$\tilde{J}^{(4)}(ij=n.n.) = \tilde{J}^{(4)}_1 = \frac{2V^4}{(U_d+\varepsilon_d)^2} \frac{1}{U_d} \left\{ \left[1 - 8 \frac{|t|}{(U_d+\varepsilon_d)} \right] - \frac{U_d}{2(U_d+\varepsilon_d)} \left[1 - 12 \frac{|t|}{(U_d+\varepsilon_d)} \right] n_p \right\} \qquad (42)$$

Due to $|t|/(U_d+\varepsilon_d) \ll 1$ only the linear in t contributions are taken into account in (42). For the second neighbours (diagonal bond) the superexchange constant is given by

$$\tilde{J}^{(4)}(ij=n.n.n.) = \tilde{J}^{(4)}_2 = \frac{8V^2t^2}{(U_d+\varepsilon_d)^2 U_d} \left[1 - \frac{U_d}{(U_d+\varepsilon_d)} n_p \right] \qquad (43)$$

At t=0 only the n.n. antiferromagnetic coupling $\tilde{J}^{(4)}_1$ (>0) occurs and there is no frustration $\tilde{J}^{(4)}_2 = 0$ for all n_p. Moreover, the coupling $\tilde{J}^{(4)}_1$ drops with increasing O-hole concentration n_p, but does not change the sign in the range of reasonable values of n_p (<1). This result is in accord with that by Ihle and Kasner /17/.

At $t \neq 0$ the n.n. coupling $\tilde{J}^{(4)}_1$ decreases with direct O-band dispersion and the antiferomagnetic coupling $\tilde{J}^{(4)}_2$ appears that results in frustration measured by $\tilde{J}^{(4)}_2/\tilde{J}^{(4)}_1 \sim$ 0.03 - 0.05. However, taking into account the relevant values of the parameters, quoted before, one can see that with increasing n_p the exchange integral $\tilde{J}^{(4)}_2$ decreases faster then $\tilde{J}^{(4)}_1$, so that $\tilde{J}^{(4)}_2/\tilde{J}^{(4)}_1$ decreases too. From this result we conclude, like in /17/, that frustration in the superexchange cannot explain the drop in Neel temperature T_N with doping, and additional frustration mechanisms must be invoked.

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