Calculation of the four-spin cyclic exchange in cuprates

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Starting from the three-band Hubbard model for the cuprates, we calculate analytically the four-spin cyclic exchange in the limit of infinite on-site Coulomb repulsion and zero O-O hopping t_{pp} using two methods: (i) perturbation theory in t_{pd}/Δ, where t_{pd} is the Cu-O hopping and Δ the Cu-O charge transfer energy and (ii) exact solution of a Cu_4O_4 plaquette. The latter method coincides with the first to order eight in t_{pd} and permits us to extend the results to t_{pd}/Δ of order one. The results are relevant to recent experimental and theoretical research that relate the splitting of certain spin excitations with Δ and the superconducting critical temperature.

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I. INTRODUCTION

Several works have studied the influence of the energy and existence of apical oxygen (O) atoms on the superconducting critical temperature T_c of the cuprates [1–3]. The absence of apical O atoms and larger separation between their on-site energy and that of the O atoms of the superconducting CuO_2 planes increases T_c. The absence of negatively charged apical O ions also renders it less favorable to add holes to the neighboring copper (Cu) ions reducing Δ, the energy necessary to transfer a hole from the Cu atom to a nearest-neighbor O atom in the CuO_2 planes. In turn, decreasing Δ is expected to increase considerably the four-spin cyclic exchange J_{4c} around the Cu_4O_4 square plaquettes, which has an important effect in the magnon dispersion [4,5] and magnetic Raman [6,7] and infrared [8] spectrum for insulating cuprates. In particular, the magnon splitting at the Brillouin zone boundary ΔE_{MBZB} in simple spin models is proportional to J_{4c} [4]. Therefore, it is natural to expect that the magnitude of J_{4c}, measurable through ΔE_{MBZB}, gives information on the charge-transfer energy Δ and the expected T_c in the cuprates, as shown by the recent work of Peng *et al.* [5]. The four-spin cyclic exchange also plays an important role in spin ladder cuprates [9–11]. It is also interesting to note that multiple spin exchange plays an essential role in the thermodynamic properties of solid ^{3}He in bulk [12] and in films [13].

Experimental evidence of the symmetry of holes in high-T_c superconductors [14,15], and first-principles constrained-density-functional calculations [16,17], indicate that the appropriate model to describe the electronic structure of superconducting CuO_2 planes is the three-band Hubbard model [18,19], which contains the 3d orbitals of the Cu atoms with $x^2 - y^2$ symmetry and the 2p orbitals of the O atoms which point towards the Cu atoms. In terms of perturbation theory in the Cu-O hopping t_{pd}, the four-spin cyclic exchange J_{4c} (although of order eight) is the nontrivial physical term of lowest order which does not involve double occupancy of holes at Cu or O sites. Therefore one expects that it pays an important role for small Cu-O charge-transfer energy Δ. However, to our knowledge, there is no calculation of J_{4c} in the three-band Hubbard model [18,19]. Instead, a calculation is available in the one-band Hubbard model, where J_{4c} is of fourth order in the hopping integral t [20]. However, this result cannot be extended to the cuprates. While efficient low-energy reductions of the three-band to the one-band Hubbard model exist which provide the values of $t \sim t_{pd}^2$ and the one-band on-site repulsion U [2,17,21,22], they include terms which are at most of order t_{pd}^4, and therefore some higher-order processes are lost if the one-band result for J_{4c} is used.

Recently, a numerical calculation of the magnon splitting ΔE_{MBZB} in a cluster of eight unit cells described by the three-band Hubbard model has been reported [23]. It shows that ΔE_{MBZB} increases as Δ decreases as expected, and the order of magnitude of the splitting agrees with that measured in several compounds [5]. In any case, this is an expensive calculation and if a simpler calculation of J_{4c} were available, this term could be introduced in spin models or successful generalized $t - J$ models [24–27], which have a much smaller Hilbert space for the same cluster size and can be attacked with other techniques [27–30].

In this work we report on two analytical results for the four-spin cyclic exchange and the magnon splitting starting from the three-band Hubbard model for infinite Cu (U_d) and O (U_p) on-site Coulomb repulsions and zero O-O hopping t_{pp}: perturbation theory in the Cu-O hopping t_{pd} up to order eight and exact solution of a Cu_4O_4 plaquette. The latter is equivalent to include all higher order perturbation terms that are contained in this plaquette and leads to a considerable improvement of the results for small Δ. For realistic and small values of Δ (of the order of 3.6 eV or smaller [1,16,17]), the assumption of infinite on-site repulsions is not essential. In fact it has been shown that our results are insensitive to the Coulomb repulsion at the Cu sites U_d [23], while perturbative processes involving O on-site repulsion U_p do not contribute at order eight and involve large denominators at higher order. The exact solution of the cluster permits us to extend the validity of the results to smaller values of $\Delta > 2t_{pd}$. For $\Delta < 2t_{pd}$ other terms like the six-spin cyclic exchange affect the magnon splitting.

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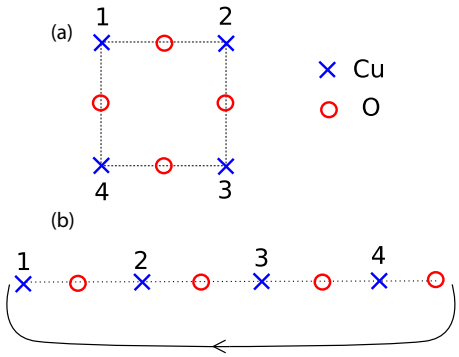

FIG. 1. (a) Basic plaquette to calculate the four-spin cyclic exchange. (b) Equivalent linear chain with periodic boundary conditions.

In Sec. II we describe the three-band Hubbard model. In Sec. III we explain the origin of the four-spin cyclic exchange. Section IV contains the result of perturbation theory in t_{pd}/Δ in lowest nontrivial order. In Sec. V we obtain the exact spectrum of a Cu_4O_4 cluster from which a calculation of the four-spin cyclic exchange beyond perturbation theory is obtained and discuss the range of validity and limitations of this calculation. Section VI contains a summary.

II. MODEL

Our starting Hamiltonian corresponds to the three-band Hubbard model for cuprate superconductors [18,19]

$$H = \Delta \sum_{j\sigma} n_{j\sigma} - \sum_{\langle ij\rangle} t_{pd}(p^{\dagger}_{j\sigma} d_{i\sigma} + \text{H.c.}) + U_d \sum_i n_{i\uparrow} n_{i\downarrow} + U_p \sum_j n_{j\uparrow} n_{j\downarrow}. \quad (1)$$

Here $d^{\dagger}_{i\sigma}$ creates a hole with spin sigma in the 3d orbital of Cu at site i with symmetry $x^2 - y^2$. Similarly $p^{\dagger}_{j\sigma}$ creates a hole in the O orbital at site j which is directed to the nearest-neighbor Cu atoms (they are usually called p_σ orbitals). The relevance of these orbitals over the rest is justified by experimental evidence [14,15] and first-principles calculations [16,17]. The hole number operators are $n_{i\sigma} = d^{\dagger}_{i\sigma} d_{i\sigma}$ and $n_{j\sigma} = p^{\dagger}_{j\sigma} p_{j\sigma}$. In this work we neglect the O-O hopping t_{pp} and take $U_d, U_p \to \infty$. The consequences of these approximations are discussed in Sec. V.

III. FORM OF THE FOUR-SPIN CYCLIC EXCHANGE

The cyclic exchange acting on the four spins at the Cu sites in a square plaquette as represented in Fig. 1 is

$$H_{4c} = J_{4c}\left(C_4 + C_4^{-1}\right), \quad (2)$$

where C_4 is a cyclic permutation of the position of the four spins ($C_4|\sigma_1\sigma_2\sigma_3\sigma_4\rangle = |\sigma_4\sigma_1\sigma_2\sigma_3\rangle$). The extension to the whole lattice of Cu sites is straightforward [20]. Expressing C_4 as a product of transpositions one has

$$C_4 + C_4^{-1} = P_{12}P_{23}P_{34} + P_{34}P_{23}P_{12}. \quad (3)$$

Noting that $P_{il} = (1/2 + 2\mathbf{S}_i \cdot \mathbf{S}_l)$ transposes the spins i and l and performing the products of repeated Pauli matrices in Eq. (3) one obtains after some algebra

$$H_{4c} = J_{4c}[4\{(\mathbf{S}_1 \cdot \mathbf{S}_2)(\mathbf{S}_3 \cdot \mathbf{S}_4) + (\mathbf{S}_1 \cdot \mathbf{S}_4)(\mathbf{S}_2 \cdot \mathbf{S}_3) - (\mathbf{S}_1 \cdot \mathbf{S}_4)(\mathbf{S}_2 \cdot \mathbf{S}_3)\} + \sum_{i<l} \mathbf{S}_i \cdot \mathbf{S}_l + 1/4]. \quad (4)$$

In some papers only the four-spin term is included explicitly (with the prefactor $4J_{4c}$ denoted as J_{ring} in Ref. [11] or J_c in Refs. [4,5]), leaving the other terms as corrections to nearest-neighbor and next-nearest-neighbor exchange. In the one-band Hubbard model fourth-order perturbation theory leads to $J_{4c} = 20t^4/U$, t being the hopping integral and U the on-site Coulomb repulsion [20].

IV. PERTURBATION THEORY IN THE CU-O HOPPING

We split the Hamiltonian into the perturbation $H_t = -\sum_{\langle ij\rangle} t_{pd}(p^{\dagger}_{j\sigma} d_{i\sigma} + \text{H.c.})$ and $H_0 = H - H_t$. The degenerate ground state of H_0 consists of a hole occupying each Cu site and has energy $E_f^0 = 0$. The processes of lowest order in the Cu-O hopping t_{pd} that contribute to H_{4c} are of order t_{pd}^8 and involve each of the plaquettes of the form represented in Fig. 1. We can restrict the analysis to one of them and label the sites as in Fig. 1. The perturbation processes that mix a state $|i\rangle = d^{\dagger}_{1\sigma_1} d^{\dagger}_{2\sigma_2} d^{\dagger}_{3\sigma_3} d^{\dagger}_{4\sigma_4}|0\rangle$ (with spin configuration $|\sigma_1\sigma_2\sigma_3\sigma_4\rangle$) with the final state $-|f\rangle = -d^{\dagger}_{2\sigma_1} d^{\dagger}_{3\sigma_2} d^{\dagger}_{4\sigma_3} d^{\dagger}_{1\sigma_4}|0\rangle = d^{\dagger}_{1\sigma_4} d^{\dagger}_{2\sigma_1} d^{\dagger}_{3\sigma_2} d^{\dagger}_{4\sigma_3}|0\rangle$ (with spin configuration $C_4|i\rangle = |\sigma_4\sigma_1\sigma_2\sigma_3\rangle$) involves two hoppings of each electron in the clockwise direction (Fig. 1). Adding all contributions (or the analogous ones in the anticlockwise direction) one can obtain J_{4c}. From standard degenerate perturbation theory one has

$$J_{4c} = \frac{\langle i|H_t|e_1\rangle \prod_{j=1}^{6} \langle e_j|H_t|e_{j+1}\rangle \langle e_7|H_t|f\rangle}{\prod_{j=1}^{7}\left(-E_j^0\right)}, \quad (5)$$

where $|e_j\rangle$, E_j^0 denote the seven intermediate eigenstates of H_0 and their energies. None of the intermediate states involve double occupancy at an O site. Since we take $U_d \to +\infty$, we neglect intermediate states with double occupancy at any Cu site. With the help of a computer program we have obtained the remaining 1088 processes and added the corresponding contributions to J_c. The result is

$$J_{4c} = 20\frac{t_{pd}^8}{\Delta^7}. \quad (6)$$

V. EXACT RESULTS FOR Cu_4O_4

The exact solution of the plaquette represented in Fig. 1 permits us to extend the perturbation result to the covalent region in which t_{pd} is not much smaller than Δ. The procedure, similar to that followed in other works [11,31], is to fit the lowest energy levels of H with all those of H_{4c} in the Cu_4O_4 cluster. It is equivalent to include all perturbation terms that are contained in the cluster. Fortunately, as we shall show, the form Eq. (2) [or the equivalent one Eq. (4)] still describes the corresponding contribution to the effective Hamiltonian in a wide range of values of Δ.

The spectrum of H_{4c} is easy to obtain. Starting from any of the 16 states $|e\rangle = |\sigma_1\sigma_2\sigma_3\sigma_4\rangle$, one constructs eigenstates of C_4

$$|k, e\rangle = N \sum_{j=0}^{3} (e^{-ik} C_4)^j |e\rangle, \tag{7}$$

such that $C_4|k, e\rangle = e^{ik}|k, e\rangle$, where N is a normalization factor and $k = m\pi/2$, where m is an integer with nonequivalent values 0, ± 1, 2. Using Eq. (2) the energies become

$$E_k = 2J_{4c} \cos k. \tag{8}$$

They only depend on k. An analysis of the other quantum numbers shows that the ground state, which has wave vector $k = \pi$ and energy $E_\pi = -2J_{4c}$, contains a singlet and a triplet. The first excited states with $k = \pm\pi/2$ and $E_k = 0$ are two triplets and the remaining six states with $k = 0$ and $E_0 = 2J_{4c}$ are the quadruplet and the other singlet.

To solve the fermion multiband model H in the cluster we follow a simple extension of the elegant procedure of Caspers and Ilske for the exact solution of the Hubbard chain with infinite U [32]. Here we describe the main idea. The details can be found in Ref. [32]. The Cu_4O_4 cluster is equivalent to a linear chain with periodic boundary conditions (see Fig. 1). Imagine for the moment that the Cu-O hopping between the last atom in the chain and the first one is set to zero, leaving a chain with open boundary conditions. Then the holes hop between different atoms in the chain but the order of the four spins $(\sigma_1\sigma_2\sigma_3\sigma_4)$ is kept, since the infinite Coulomb repulsion at each site does not allow us to exchange spins. Furthermore, there is a one to one correspondence between any state of the system and that obtained replacing the spin configuration $(\sigma_1\sigma_2\sigma_3\sigma_4)$ by $(\uparrow\uparrow\uparrow\uparrow)$. The Hamiltonian matrix in both spaces have the same form and since the problem in the latter subspace is a spinless fermion problem, it can be solved trivially, and the mapping provides a solution to the original problem.

When the hopping between the first and the last atom is restored, one is faced with the difficulty that when the hole of the last atom hops to the first one, the spin configuration $(\sigma_1\sigma_2\sigma_3\sigma_4)$ is changed to $(\sigma_4\sigma_1\sigma_2\sigma_3) = C_4(\sigma_1\sigma_2\sigma_3\sigma_4)$, where C_4 is a cyclic permutation of the spin configuration (without affecting the charge distribution) and in general, the above one to one correspondence is lost. However, for any charge configuration, one can construct eigenstates of C_4 [similar to Eq. (7)]. It is easy to realize that for these eigenstates, the mapping to the spinless Hamiltonian is still possible but the hopping from the last atom to the first one becomes multiplied by e^{ik}, the eigenvalue of C_4. Clearly the reverse process has a factor e^{-ik}. Then, the problem becomes equivalent to spinless fermions under a magnetic flux. While the original argument was developed for the Hubbard model, clearly it is still valid if the on-site energies of the different sites differ.

For the solution of the equivalent spinless problem, it is convenient to distribute the phase $e^{\pm ik}$ of the hopping term equally in all the eight Cu-O links by a gauge transformation, so that translation symmetry with periodic boundary conditions is restored in the equivalent spinless model and the hopping term takes the form $H_t = -\sum_{i\delta} t_{pd}(e^{ik\delta/4} p^\dagger_{i+\delta} d_i +$ H.c.), where $\delta = \pm 1/2$ and $p^\dagger_{i+1/2}$ ($p^\dagger_{i-1/2}$) creates a spinless O hole half a lattice parameter at the right (left) of Cu site i.

The spinless problem is solved as usual in a basis of Cu and O one-particle states with charge wave vector $q = n\pi/2$ with $n = 0$, ± 1, 2. There are eight different one-particle eigenvalues, two for each q. Since the system has four holes, one has to fill the four one-particle states of lowest energy to obtain the low-energy spectrum that maps onto H_{4c}. It turns out that for all q only the lowest one-particle state is occupied. The resulting many-body energies that map onto those of H_{4c} for each spin wave vector k become

$$E^H_k = 2\Delta - \sum_{n=-1}^{2} \sqrt{\left(\frac{\Delta}{2}\right)^2 + 4t^2_{pd} \cos^2\left(\frac{n\pi}{4} + \frac{k}{8}\right)}. \tag{9}$$

For small t_{pd} this result can be expanded in powers of t_{pd}/Δ. Only even powers of t_{pd} enter. Although it is not apparent from Eq. (9), the terms of second, fourth, and sixth order give a result independent of k, so that the first nontrivial term is of order eight. Except for an irrelevant constant, this expansion to order eight gives $E^H_k = E_k$, where E_k is the result obtained previously by perturbation theory [Eqs. (6) and (8)]. Thus, as expected, for small t_{pd}/Δ, Eq. (9) reproduces the perturbative result up to order eight in t_{pd}, but with much less effort. Furthermore defining

$$J_{4c} = \frac{E^H_0 - E^H_\pi}{4} \tag{10}$$

permits us to extend the validity of the low-energy Hamiltonian H_{4c} to larger values of t_{pd}/Δ.

Note that for a general Hamiltonian with spin SU(2) symmetry the 16 low-energy eigenstates for 4 Cu spins in a square lattice are expected to be split in five different eigenvalues (corresponding to either different wave vectors k or different total spin), while the eigenstates of H_{4c} split only in three different energies according to the value of k. This property is retained by the low-energy eigenstates of the full Hamiltonian H in the Cu_4O_4 cluster, indicating that H_{4c} continues to be a good representation of this low-energy subspace. However, a shortcoming of H_{4c} in reproducing the eigenvalues of H for large t_{pd}/Δ is that in the latter the difference

$$D = \left(E^H_0 + E^H_\pi\right)/2 - E^H_{\pi/2} \tag{11}$$

is larger than zero while the corresponding difference vanishes in H_{4c}. However, D is very small for $\Delta > t_{pd}$ (see dashed line in Fig. 2). The first correction to D in powers of t_{pd} [obtained evaluating numerically Eq. (9)] is $6864 t^{16}_{pd}/\Delta^{15}$.

A magnitude of interest in recent works [5,23] is the magnon splitting at the Brillouin zone boundary which for the spin model is given by [4,5]

$$\Delta E_{\mathrm{MBZB}} = \frac{12}{5} Z_c J_{4c}, \tag{12}$$

where $Z_c = 1.18$ is a renormalization factor accounting for quantum fluctuations [33]. This quantity using J_{4c} given by Eq. (10) is represented by the full line in Fig. 2 as a function of Δ. The corresponding perturbative result using J_{4c} given by Eq. (6) (dotted line in Fig. 2) largely overestimates the splitting for realistic values of Δ (smaller than $4t_{pd}$). Taking into account that estimated values of Δ (t_{pd}) are in the range

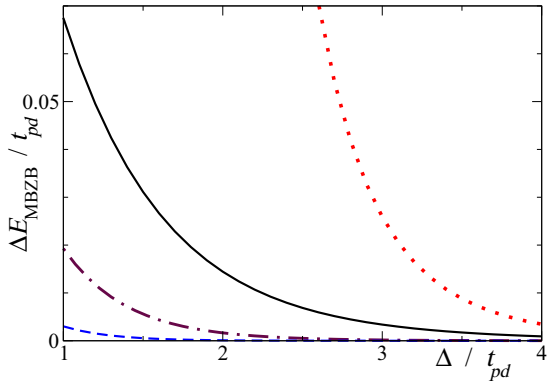

FIG. 2. Magnon splitting (full black line) and perturbative result (dotted red line) as a function of Δ. Also shown for comparison (see text) are $0.706D$ (dashed blue line) and $0.706S_6$ (dashed-dotted brown line).

1.3–3.6 (1.1–1.6) eV [16], our results for $\Delta E_{\rm MBZB}$ due to J_{4c} are approximately in the range 2–110 meV, which can be compared with the values between 30 and 150 meV measured in four parent compounds of high-T_c superconductors [5]. Our result is qualitatively similar to the splitting calculated in small clusters described by the three-band Hubbard model [Fig. 2(b) in Ref. [23]]. The result in that work is larger due to the inclusion of the O-O hopping t_{pp} which we have neglected here. We believe that to a first approximation, the main effect of t_{pp} is similar to decrease Δ by $1.46|t_{pp}|$, as suggested by a change of basis to O orbitals centered on Cu sites [24].

For small Δ, other perturbative processes of high order in t_{pd}/Δ, which are not contained in the Cu_4O_4 plaquette, might become important. The dominant one is probably the six-spin cyclic exchange, which can be calculated as above in a Cu_6O_6 cluster. In Fig. 2 we also show the energy difference given by Eq. (11) and the magnitude of the six-spin cyclic exchange $S_6 = E_0 - E_\pi$ calculated as above in a Cu_6O_6 ring rescaled by the factor $f = Z_c \times 3/5$ to evaluate their relative magnitude compared to $\Delta E_{\rm MBZB}$ (neglecting S_6, $\Delta E_{\rm MBZB} = f(E_0^H - E_\pi^H)$). The conclusion of this comparison is that while the effective Hamiltonian H_{4c} represents accurately the effects of the four-spin cyclic exchange for $\Delta > t_{pd}$, other terms, like the six-spin cyclic exchange become important for $\Delta < 2t_{tpd}$ and affect $\Delta E_{\rm MBZB}$.

VI. SUMMARY

In summary, for the three-band Hubbard model with infinite Coulomb repulsions U_d and U_p, O-O hopping $t_{pp} = 0$, and $\Delta \geqslant 2t_{pd}$, the magnon splitting at the Brillouin zone boundary is accurately described by the analytical expressions Eqs. (12), (10), and (9). Finite Coulomb repulsions are expected to have a very minor effect. Inclusion of t_{pp} increases the splitting. We expect that the main effect of increasing t_{pp} is equivalent to a decrease in Δ. For $\Delta < 2t_{pd}$, the six-spin cyclic exchange (which can be calculated following the lines of this work) also becomes important and affects the magnon splitting, The analytical expressions permit a rapid estimation of the magnon splitting (a lower bound for sizable t_{pp}). Conversely, given a magnon splitting measured experimentally one can infer the magnitude of Δ, and from it, one might have a qualitative idea of the expected superconducting critical temperature.

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