Calculated magnetic exchange interactions in high-temperature superconductors

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Using a first-principles linear-response approach, we study the magnetic exchange interactions J for a series of superconducting cuprates. We reproduce the observed spin-wave dispersions together with other experimental trends, and show that different cuprates have similar J's regardless of their T_c. The nearest-neighbor J is not sensitive to the hole doping, which agrees with recent experiments. For the undoped cuprates, the second-nearest-neighbor J is ferromagnetic, but changes its sign with hole doping. We also find that, in contrast to the hopping integral, the exchange interaction is not sensitive to the position of apical oxygen. To see the effect of the long-range nature of the exchange on the superconducting T_c, we study the dynamical spin susceptibility $\chi(q,\omega)$ within the t-J model using a dynamical cluster approximation.

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I. INTRODUCTION

After more than two decades of intensive studies of high-temperature superconductors (HTSCs), it is now well accepted that magnetic exchange interactions in the cuprates play a fundamental role. Despite a general lack of consensus on the pairing mechanism in the cuprates, it is believed to be of magnetic origin.[1–5] In support of this scenario, a direct relationship $T_c \propto J$ between T_c and the in-plane exchange interaction J was extracted from magnetic measurements for one family of the cuprates in Ref. 6. Despite vast efforts devoted to understanding the magnetic properties of the cuprates,[7–21] there are still several important issues which need to be clarified. Among them is the long-range nature of the exchange interactions J between the Cu ions, and its effect on the dynamical spin susceptibility $\chi(q,\omega)$ and the critical temperature T_c. Studies of model Hamiltonians, such as the t-J model show a strong dependence of the calculated properties on the value of J.[22,23] In particular, numerical calculations suggest a direct relationship between the magnitude of the magnetic exchange coupling and the pair binding energy.[23] Therefore, obtaining accurate estimates for the exchange constants and studying their trends across different HTSCs including their doping dependence and influence on $\chi(q,\omega)$ and T_c is an interesting problem which we address in the present work.

Experiments provide estimates for the magnitude of the exchange interaction, but despite many studies there is a spread in obtained values even for the nearest-neighbor magnetic coupling J_1 in the most studied compound La_2CuO_4 where it varies from 110 to 150 meV.[8–11] The latter result does not only depend on the experimental technique being used but also on how the results are fitted, i.e., depending on whether higher order exchange terms are included. Nevertheless, based on recent high-resolution inelastic neutron-scattering (INS) experiments, there is an overall agreement that at least for the undoped La_2CuO_4,[11] a simple nearest-neighbor Heisenberg model is not sufficient and the high-order magnetic exchange interaction is quite important. However, all high-order terms have similar effects on the spin-wave dispersion and its intensity dependence, therefore, even INS, the most powerful technique for exploring magnetic excitations, cannot determine the magnetic exchange coupling very accurately. Worse than La_2CuO_4, for most other HTSC compounds, the difficulty in synthesizing large single crystals limits the capability of performing accurate measurements. Thus, the experimental information on the exchange interactions is very limited.

In addition to the experiment, the magnetic interactions of the undoped cuprates have been studied in a number of theoretical works.[19,24–26] However, most of them use a cluster approximation and map the total energy differences obtained by a first-principles calculation to a model Hamiltonian which prevents detailed studies of the long-range nature of the J's. It is, for example, well known that the long-range hopping integrals are very important for the electronic properties in the cuprates[27] and even the effective third nearest-neighbor hopping t'' has a considerable effect on the interatomic exchange.[28] Therefore it is desirable to reinvestigate the exchange interaction in cuprates by a first-principles calculation.

In contrast to the undoped cuprates, investigations of J's in doped HTSCs are scarce, regardless the superconductivity actually happens only after introducing doping. Based on a model calculation, Si *et al.*[29] suggested that J_1 will decrease rapidly with doping. On the other hand, the commonly used t-J model uses the same J for different doping levels,[22] therefore study the effect of doping on the exchange interaction based on a first-principles calculation is quite interesting. Unfortunately, *ab initio* techniques for extracting J's (like the cluster approximations mentioned above) are not efficient for the doped case, and there are no extensive calculations of this type reported in the literature. In this work, we use a recently developed linear-response approach,[30] and perform detailed studies of exchange interactions for both parent and doped HTSCs. Beyond this, we also investigate the effect of the long-range J' s on the spin susceptibility $\chi(q,\omega)$ and the superconducting transition temperature T_c within the frame-

work of the dynamical cluster approximation (DCA) for the t-J model.

II. EXCHANGE INTERACTION AND SPIN WAVES

A. Method

We perform our electronic structure calculations based on density-functional theory (DFT) LMT

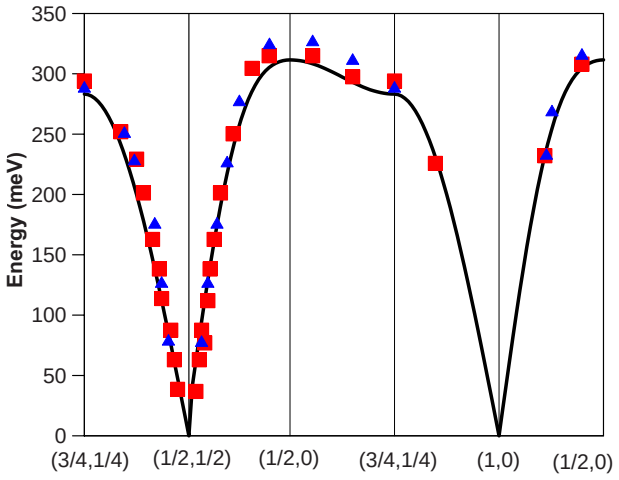

FIG. 2. (Color online) Comparison between calculated (solid lines) and experimental (symbols) spin-wave dispersions for La_2CuO_4. The triangles and squares are the experimental results at $T=10$ and 295 K, respectively (Ref. 11).

$$A_q = J_1 - J_2[1 - \cos(2\pi q_x)\cos(2\pi q_y)] - J_3\left(1 - \tfrac{1}{2}[\cos(4\pi q_x) + \cos(4\pi q_y)]\right),$$

$B_q = \frac{1}{2}J_1[\cos(2\pi q_x) + \cos(2\pi q_y)]$, and Z_c is the renormalization factor, respectively. Here based on the above formula with the quantum renormalization factor $Z_c = 1.18$,[35] and using the obtained numerical J_1, J_2, and J_3, we calculate the spin-wave dispersion for La_2CuO_4, and display the result in Fig. 2 by the solid line. For comparison, in Fig. 2 we also show the INS data by symbols.[11] Our results agree well with the experiments near the zone center. A small discrepancy exists around the zone boundary which may be due to the four-particle cyclic exchange interaction J_r, which recently attracted much attention.[17,19]

We now turn to our predictions of exchange interactions for other HTSC materials where the experimental values of J are limited. The experiment[14,15] shows the J_1 of $Sr_2CuO_2Cl_2$ is about 10 meV smaller than that of La_2CuO_4. This is reproduced by our numerical calculation as shown in Table I. The J_1 of $YBa_2Cu_3O_{6.15}$ has been measured by neutron scattering, and the obtained value is about 120 meV.[12,13] After considering the quantum renormalization effect,[35] the experimental J_1 will be reduced to 100 meV, which is very close to our numerical result 93 meV. It is interesting to note that our theoretical study reproduces the experimental trend across the materials studied (La_2CuO_4 has largest J_1, $Sr_2CuO_2Cl_2$ is intermediate, and J_1 in $YBa_2Cu_3O_6$ is smallest[15]). As it is seen from Table I, all parent HTSCs have almost the same J_1 (around 110 meV) regardless of their number of CuO_2 layers and their different T_c's. J_2 is also similar and shows FM behavior while J_3 is AFM-like. Using the quantum renormalization factor[35] and linear spin-wave theory, we also calculate the spin-wave dispersion for all other compounds and show the results for $HgBa_2CaCu_2O_6$, $Sr_2CuO_2Cl_2$, and $YBa_2Cu_3O_6$ in Fig. 3. Since different compounds have similar exchange interactions the shape of the spin-wave curve is quite similar while $YBa_2Cu_3O_6$ has smaller spin-wave excitation.

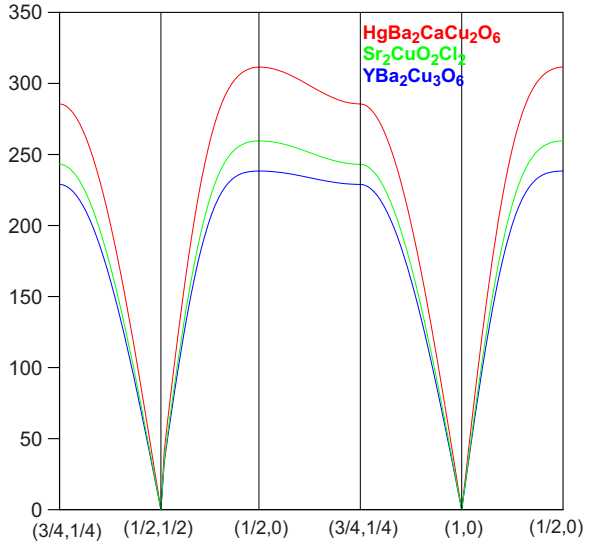

FIG. 3. (Color online) Calculated spin-wave dispersions for $HgBa_2CaCu_2O_6$, $Sr_2CuO_2Cl_2$, and $YBa_2Cu_3O_6$.

To further check the possible relationship between J and T_c, we also study a high-pressure phase of $HgBa_2Ca_2Cu_3O_8$, for which T_c increases considerably.[37] Applying pressure reduces the lattice parameter, and, as a result, increases the magnitude of J, but this enhancement is too weak to relate it with rising T_c. For example, we find the values of J_1 are 114.3 and 116.4 meV at 3 and 8 GPa, respectively, which is very close to the value at ambient pressure as shown in Table I.

C. Effect of apical oxygen

It is believed that the apical oxygen has a dramatic effect on T_c.[38–41] However, there is a debate on whether T_c is positively correlated with the magnitude of the effective next-nearest-neighbor hopping t',[40] or if an intersite super-repulsion term is important.[41] We therefore study the effect of the position of the apical oxygen on the exchange interaction. The apical oxygen in La_2CuO_4 is located at the $(0,0,z_o)$ site. By adjusting the internal atomic coordinate z_o we perform the calculation for different distances d_A between the apical oxygen and Cu.

Our results are shown in Table II. In contrast to the hopping integral, which is quite sensitive to the position of the

TABLE II. The calculated exchange interaction in La_2CuO_4, with different d_A, where d_A is the distance between apical oxygen and Cu atom. d_A is in Å and J is in meV.

d_A	J_1	J_2	J_3
2.5	111.1	−12.4	−0.4
2.6	112.9	−13.1	0.1
2.7	114.2	−13.8	1.2
2.8	116.0	−14.6	2.1

apical oxygen,[40,41] the magnitude of the exchange interaction in the CuO_2 plane only slightly increases with d_A as shown in Table II. In the Hg-based cuprates with $d_A \sim 2.7$ Å, J is found smaller than the one in La_2CuO_4 with the same d_A, so it is likely that the exchange interaction is more sensitive to the detail of the electronic structure, rather than just to the distance d_A.

D. Effect of doping

It may not be surprising that the J's of the parent HTSCs do not directly correlate with their T_c's which characterize the corresponding doped materials. We therefore study the effect of hole doping for La_2CuO_4 using the virtual-crystal approximation (VCA), which has been used successfully for the phonon properties of $La_{2-x}Ba_xCuO_4$.[42] For the doped case, our scheme is rough, but nevertheless does include major ingredients of the system, such as, superexchange, double exchange, and Ruderman-Kittel-Kasuya-Yoshida (RKKY) exchange interactions.[29] Naively, one may think the hole induced by doping can hop through the Cu ion, and result in a ferromagneticlike double-exchange interaction, which would consequently suppress J_1. But if the doping level is not high, this effect is not large as seen in Table III. Since the spin-wave velocity is mainly controlled by J_1, our results agree with the recent INS experiments, which showed clearly that for $La_{2-x}Sr_xCuO_4$ the spin-wave velocity is doping insensitive.[16] Hole doping enhances J_3 slightly as seen in Table III. Different from J_1 and J_3, doping has a large affect on J_2, which changes from FM-like to AFM-like resulting in considerable spin fluctuation.

III. EFFECT ON T_c

Now, we aim to address the following questions: (1) can the variation in exchange parameters for different materials explain the difference in T_c? (2) What is the effect of varying exchange parameters on the dynamic spin-fluctuation spectrum? To answer these questions, we use a dynamic cluster approximation (DCA) (Refs. 43 and 44) to calculate the properties of a t-J model. A similar study was performed in Ref. 45. There, a combined DFT-LDA and DCA-QMC approach was used to study the parameter dependence of T_c in a three-band Hubbard model. These calculations showed that T_c is a very strong function of the hopping parameters, and very sensitive to even small variations in the long-range hopping integrals.

Here, we want to study the dependence of T_c on the exchange parameters J. We therefore consider a two-dimensional t-J model,

$$H = -t \sum_{\langle ij \rangle, s} (\tilde{c}^{\dagger}_{is}\tilde{c}_{js} + \tilde{c}^{\dagger}_{is}\tilde{c}_{js}) + \sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_\mathbf{j}, \qquad (2)$$

where $\mathbf{S_i}=\tilde{c}^{\dagger}_{is}\sigma_{ss'}\tilde{c}_{is'}$ and $\tilde{c}^{\dagger}_{is}$ is a projected fermion operator c

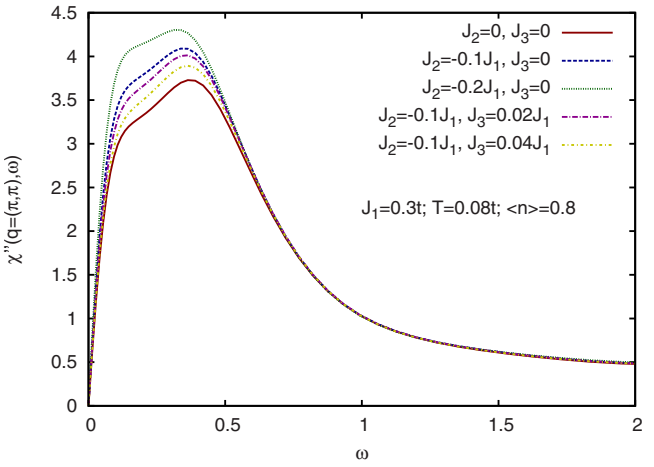

FIG. 4. (Color online) Spin susceptibility $\chi''(q,\omega)$ for $q=(\pi,\pi)$ versus ω for different exchange interactions J_2 and J_3. Here, $J_1=0.3t$ is fixed and a filling $\langle n\rangle=0.8$ and temperature $T=0.08t$ have been used.

$$V_d(k,\omega,k',\omega') = \frac{3}{2}\bar{U}^2\chi(k-k',\omega-\omega') - \bar{J}(\cos k_x - \cos k_y) \times(\cos k'_x - \cos k'_y). \quad (3)$$

Here, $\bar{U}$ and $\bar{J}$ are effective coupling constants of the retarded spin-fluctuation part and the nonretarded exchange contribution, respectively. It was shown that the dominant contribution to the pairing interaction V_d comes from the spin fluctuations.[51]

From this one would expect that variations in the spectral weight in $\chi''(q,\omega)$ will directly affect the strength of V_d and thus T_c. Figure 5 shows the DCA/NCA results for T_c for different values of the next-nearest-neighbor and third-nearest-neighbor exchange integrals J_2 and J_3. Here, we have fixed the nearest-neighbor exchange $J_1=0.3t$ and the filling $\langle n\rangle=0.8$. Consistent with Eq. (3), one finds that the magnitude of T_c tracks the magnitude of the spectral weight in $\chi''(q,\omega)$ for $q=(\pi,\pi)$. E.g., the highest T_c is obtained for $J_2=-0.2J_1$, $J_3=0$, i.e., when the spectral weight in $\chi''(q,\omega)$ is maximal for $q=(\pi,\pi)$.

We emphasize, however, that T_c is rather insensitive to changes in the long-range exchange parameters J_2 and J_3. E.g., a change in J_2 from $J_2=0$ to $J_2=-0.2J_1$ only induces a $\approx 5\%$ increase in T_c and the effects of J_3 on T_c are almost negligible. Note, however, that the third-nearest-neighbor exchange J_3 is not directly represented on a 4-site 2×2 cluster. In this approximation, the spins on the cluster only know about J_3 through their effective coupling to the spin-fluctuation host. Therefore, it is possible that larger variations in T_c would be found in larger cluster simulations. From the present results, however, we conclude that the differences in the long-ranged exchange terms cannot explain the differences in T_c between different cuprates.

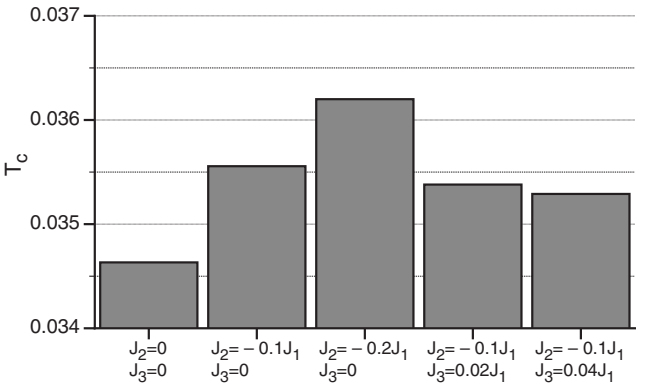

FIG. 5. Superconducting transition temperature for different exchange interactions J_2 and J_3. Here, we have used the same values for J_1, J_2, and J_3 and the filling as in Fig. 4

IV. CONCLUSION

In summary, we have calculated the magnetic exchange interactions for a series of HTSC cuprates using the LDA+U based linear-response approach. Our calculated spin-wave dispersions were found in good agreement with high-resolution inelastic neutron-scattering experiments. Our simulations show that for different parent HTSCs, the nearest-neighbor and next-nearest-neighbor exchange constants are similar, while the third-nearest-neighbor J appears to be material dependent. Furthermore, we find that J_1 is insensitive to the hole doping, which agrees with recent experiments and supports the implicit assumption of the t-J model with a fixed magnitude of J. In contrast to the hopping integral, which strongly depends on the position of the apical oxygen, our results show that the magnetic exchange interaction is rather insensitive to the position of the apical oxygen. In addition to the LDA+U calculations, we studied the dependence of the dynamic spin susceptibility $\chi(q,\omega)$ and superconducting transition temperature T_c on the exchange parameters in a t-J model using a dynamic cluster approximation. We find that both $\chi(q,\omega)$ and T_c are only weakly affected by variations in the exchange parameters beyond nearest neighbor. Based on these results, we conclude that differences in long-range exchange terms between different materials cannot explain their different superconducting transition temperatures.

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