Spin waves in La$_2$CuO$_4$: band structure and correlation effects

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Abstract

We calculate the antiferromagnetic spin wave dispersion in the half-filled (electronic density $n = 1$) Hubbard model for a two-dimensional square lattice, using the random phase approximation (RPA) in a broken symmetry (spin density wave) ground state. Our results for the spin wave dispersion, $\omega(\mathbf{q})$, are compared with high-resolution inelastic neutron scattering performed on La$_2$CuO$_4$. The effects of different band structures and different values of the on-site Coulomb interaction on the spin wave spectrum is studied. Particular attention is put on the high energy dispersion values $\omega(\pi/2, \pi/2)$ and $\omega(0, \pi$).

Introduction: In two recent papers, [1, 2] high-resolution inelastic neutron scattering measurements have been performed on two different two-dimensional spin 1/2 quantum antiferromagnets. These are copper deuterofomate tetradeuterate (CFTD) and La$_2$CuO$_4$. Surprisingly, the dispersion at the zone boundary that has been observed in the two materials, does not agree with spin-wave theory predictions [3]. Moreover the amount of dispersion is not the same for both materials. In CFTD the dispersion is about 6% from $\omega(\pi/2, \pi/2)$ to $\omega(\pi, 0)$, whereas in La$_2$CuO$_4$ it is about -13% along the same direction. In the case of CFTD the dispersion at the zone boundary can be explained using the nearest-neighbor Heisenberg model alone, [2] and high precision quantum Monte Carlo simulations have confirmed that it is so.[4] On the other hand, an explanation for the observed dispersion in La$_2$CuO$_4$ has been proposed [1] using an extended Heisenberg model [5, 6] involving first-, second-, and third-nearest-neighbor interactions as well as interactions among four spins.

In a previous paper [7], we have shown that it possible to obtain the observed dispersion difference of -13% for La$_2$CuO$_4$ using the single band Hubbard model at half filling, with nearest neighbor hopping. In our formulation the extended Heisenberg model used in ref. [1] is incorporated by means of the virtual excursions of the electrons on the lattice. Fitting our results to the experimental data the obtained values of $U$ and $t$ agree well with those of ref. [1] and where confirmed by Quantum Monte Carlo calculations in the Hubbard model [8].

In this paper we generalize our previous study incorporating in the calculations the effect of a second nearest neighbor hopping $t'$ in the electronic spectrum (in high-$T_c$ materials the ratio $|t'/t|$ ranges roughly from 0.1 to 0.5). The effect of $U$ on the spin wave dispersion at the special points $\omega(\pi/2, \pi/2)$ and $\omega(0, \pi)$ is also studied.

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Model Hamiltonian: The Hubbard model for a square lattice of \( N \) sites is defined as

\[
H = \sum_{\vec{k},\sigma} \left[ \epsilon(\vec{k}) - \mu \right] c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} + U \sum_{i} c_{i,\uparrow}^\dagger c_{i,\uparrow}^\dagger c_{i,\downarrow} c_{i,\downarrow},
\]

where \( \epsilon(\vec{k}) \) defines the energy dispersion for independent electrons. In this work we consider two different electronic energy dispersions given by

\[
\epsilon(\vec{k}) = -2t \cos k_x - 2t \cos k_y \tag{2}
\]

and by

\[
\epsilon(\vec{k}) = -2t \cos k_x - 2t \cos k_y - 4t' \cos(k_x)\cos(k_y). \tag{3}
\]

The first energy dispersion has the nesting vector \( \vec{Q} = (\pi, \pi) \); the second one is not nested.

The broken symmetry state is introduced by considering the existence of an off-diagonal Green's function given by

\[
F_{\sigma}(\vec{p}; \tau - \tau') = -< T_{\tau} c_{\vec{p} + \vec{Q}, \sigma}(\tau) c_{\vec{p}, \sigma}^\dagger(\tau') >.
\]

in addition to the usual Green's function:

\[
G_{\sigma}(\vec{p}; \tau - \tau') = -< T_{\tau} c_{\vec{p}, \sigma}(\tau) c_{\vec{p}, \sigma}^\dagger(\tau') >.
\]

At the mean field level the Fourier transform of these two Green's functions are given by

\[
G(\vec{p}, i\omega_n) = \frac{u_{\vec{p}}}{i\omega_n - E_+(\vec{p})} + \frac{v_{\vec{p}}}{i\omega_n - E_-(\vec{p})},
\]

\[
F_{\sigma}(\vec{p}, i\omega_n) = \frac{\tilde{u}_{\vec{p},\sigma}}{i\omega_n - E_+(\vec{p})} + \frac{\tilde{v}_{\vec{p},\sigma}}{i\omega_n - E_-(\vec{p})},
\]

where the energies \( E_{\pm} \) are given by

\[
E_{\pm}(\vec{p}) = \frac{\xi(\vec{p}) + \xi(\vec{p} + \vec{Q})}{2} + U \frac{n}{2} \pm \frac{1}{2} \sqrt{[\xi(\vec{p}) - \xi(\vec{p} + \vec{Q})]^2 + U^2 m^2},
\]

\[
\xi(\vec{p}) = \epsilon(\vec{p}) - \mu, \quad \text{and the coherence factors read}
\]

\[
u_{\vec{p}} = \frac{E_+ - \xi(\vec{p}) - U n/2}{E_+ - E_-}, \quad \nu_{\vec{p}} = \frac{E_- - \xi(\vec{p}) - U n/2}{E_+ - E_-},
\]

\[
\tilde{u}_{\vec{p},\sigma} = -\frac{U m \sigma/2}{E_+ - E_-}, \quad \tilde{v}_{\vec{p},\sigma} = \frac{U m \sigma/2}{E_+ - E_-}.
\]

Spin susceptibility and spin waves: In order to describe the spin dynamics of the system we consider the transverse spin susceptibility \( \chi_{-+}(\vec{q}, i\omega_n) \), which is defined as

\[
\chi_{-+}(\vec{q}, i\omega_n) = \mu_B^2 \int_0^\beta d\tau e^{i\omega_n \tau} < T_\tau S^- (\vec{q}, \tau) S^+ (\vec{q}, 0) >,
\]
where $\beta = 1/T$ is the inverse temperature, $T_\tau$ is the chronological order operator (in imaginary time), $S^-(\vec{q}) = \sum_{\vec{p}} c_{\vec{p} \downarrow}^{\dagger} c_{\vec{p} + \vec{q} \uparrow}$ and $S^+(\vec{q}) = [S^-(\vec{q})]^\dagger$. The above expression can be written as

$$
\chi_{\pm}(\vec{q}, \omega_n) = \mu_B \sum_{n=0}^{\infty} \int_0^\beta d\tau \sum_{\vec{p}, \vec{p}'} e^{i\omega_n \tau} \left< T_\tau \left[ - \int_0^\beta d\bar{\tau} H_U(\bar{\tau}) \right]^{n} c_{\vec{p} \downarrow}(\tau) c_{\vec{p} + \vec{q} \uparrow}(\tau) c_{\vec{p}' \downarrow}(0) c_{\vec{p}' + \vec{q} \uparrow}(0) \right> \overset{d.c.}{}.
$$

where d.c. stands for differently connected diagrams. The susceptibility is evaluated at the RPA level \cite{Ref} and the spin wave spectrum $\omega(\vec{q})$ is determined from the poles of $\chi_{\pm}(\vec{q}, \omega + i0^+)$.

In Figure 1 the spin wave spectrum is plotted along high symmetry directions of the Brillouin zone for both dispersions (2) and (3). For the case of the dispersion (2) the values of $t$ and $U$ giving the best fit to the experimental data are, for $T = 0$ K, $U = 1.8$ eV, $t = 0.295$ eV. The dashed line is the analytical result (at 0 K) for $U = 1.8$ eV, $t = 0.295$ eV. The solid line is the analytical result (at 0 K) for $U = 1.8$ eV, $t = 0.295$ eV. The momentum is in units of $2\pi$ and $M = (1/2, 1/2)$, $X = (1/2, 0)$, and $\Gamma = (0, 0)$.

In Figure 1 the spin wave spectrum is plotted along high symmetry directions of the Brillouin zone for both dispersions (2) and (3). For the case of the dispersion (2) the values of $t$ and $U$ giving the best fit to the experimental data are, for $T = 0$ K, $U = 1.8$ eV, $t = 0.295$ eV, with $U/t = 6.1$ (we note that there is no measurable change between the calculation at $T = 0$ K and $T = 10$ K). For the dispersion (3), which does not present nesting, the experimental data can be fitted using $U = 2.1$ eV, $t = 0.34$ eV, with $U/t = 6.2$, and $t'/t = -0.25$. These last set of values agree with those determined in ref. \cite{Ref}, from an perturbative calculation of the poles of $\chi_{\pm}(\vec{q}, \omega + i0^+)$.

It is clear from these results that the introduction of a more realistic band structure, given by (3), leads to larger values of $t$ and $U$. 

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{spin_wave_dispersion.png}
\caption{Spin wave dispersion, in meV, along high symmetry directions in the Brillouin zone. The circles are the data reported in Ref. \cite{Ref1} at 10 K. The dashed line is the analytical result (at 0 K) for $U = 1.8$ eV, $t = 0.295$ eV. The solid line is the analytical result (at 0 K) for $U = 1.8$ eV, $t = 0.295$ eV. The momentum is in units of $2\pi$ and $M = (1/2, 1/2)$, $X = (1/2, 0)$, and $\Gamma = (0, 0)$.}
\end{figure}
Let us now consider the effect of the Coulomb interaction $U$ on the energy difference $\omega(0, \pi) - \omega(\pi/2, \pi/2)$. Experimentally the dispersion, in CFTD, is about 6% from $\omega(\pi/2, \pi/2)$ to $\omega(\pi, 0)$, whereas in La$_2$CuO$_4$ it is about -13% along the same direction. The question is whether it is possible to obtain these very different behaviors from a single model Hamiltonian. In Figure 2 we study the evolution of $\omega(0, \pi)$ and $\omega(\pi/2, \pi/2)$ as function of $U/t$ for the dispersions (2) and (3). For the dispersion (2) it is clear that $\omega(0, \pi)$ is always larger then $\omega(\pi/2, \pi/2)$, except in the limit $U \to \infty$ where they become equal. This behavior was confirmed by Quantum Monte Carlo [8]. On the other hand, for the dispersion (3), $\omega(0, \pi)$ and $\omega(\pi/2, \pi/2)$ become equal for a finite value of $U/t$, which for the chosen parameters is $U/t \simeq 10.5$. For larger values of $U/t$ the dispersion at $\omega(\pi/2, \pi/2)$ becomes larger than $\omega(0, \pi)$.

In conclusion, our results shown that it is possible to fit the spin wave spectrum with the $t - t' - U$ Hubbard model and that the two different behaviors for $\omega(0, \pi)$ and $\omega(\pi/2, \pi/2)$ observed in La$_2$CuO$_4$ and in Cu(DCOO)$_2$·4D$_2$O follow from a single model Hamiltonian.

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