Spin-wave dispersion in La_2CuO_4

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We calculate the antiferromagnetic spin-wave dispersion in a half-filled Hubbard model for a two-dimensional square lattice, and find it to be in excellent agreement with recent high-resolution inelastic neutron scattering performed on La_2CuO_4 [Phys. Rev. Lett. **86**, 5377 (2001)].

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After over a decade of intense research on the microscopic origin of high-temperature superconductivity in cuprates, there is no general consensus on the microscopic Hamiltonian suitable for describing these materials. Nevertheless, it appears that magnetic fluctuations must play an important role. Therefore, the study of magnetic fluctuations in the high-temperature superconductor parent compounds, such as La_2CuO_4, is an important field of research, both theoretical and experimental.

In two recent papers,[1,2] high-resolution inelastic neutron-scattering measurements were performed on two different two-dimensional spin-1/2 quantum antiferromagnets. These are copper deuteroformate tetradeuterate (CFTD) and La_2CuO_4. Surprisingly, the dispersion at the zone boundary 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_2CuO_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 this is so.[4] On the other hand, an explanation for the observed dispersion in La_2CuO_4 was proposed,[1] using an extended Heisenberg model[5,6] involving first-, second-, and third-nearest-neighbor interactions as well as interactions among four spins. This extended model was obtained from the Hubbard model, using perturbation theory, and is diagonalized afterward using classical (large-S) linear spin-wave theory.[1]

The La_2CuO_4 results clearly show that the usual Heisenberg model is insufficient to explain the experimental data, and that the Hubbard model is the correct Hamiltonian for describing the magnetic interactions in the cuprates.[7] In this work we do not use perturbation theory for deriving an effective magnetic Hamiltonian. Instead we work directly with the Hubbard model. We consider a half-filled Hubbard model in a spin-density-wave (SDW)-broken symmetry ground state and, by summing up all ladder diagrams, we compute the transverse spin susceptibility and from this obtain the spin-wave dispersion.

The Hubbard model for a square lattice of N sites is defined as

$$\begin{aligned} H=&-t\sum_{\langle i,j\rangle,\sigma}(c^\dagger_{i,\sigma}c_{j,\sigma}+c^\dagger_{j,\sigma}c_{i,\sigma})\\ &+\mu\sum_{i,\sigma}c^\dagger_{i,\sigma}c_{i,\sigma}+U\sum_i c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow},\\ =&\sum_{\vec k,\sigma}[\epsilon(\vec k)-\mu]c^\dagger_{\vec k,\sigma}c_{\vec k,\sigma}+H_U, \end{aligned} \tag{1}$$

where the sum over $\langle i,j\rangle$ counts each pair of nearest neighbors only once, the momentum $\vec k$ runs over the Brillouin zone, the electronic energy dispersion $\epsilon(\vec k)=-2t\cos k_x-2t\cos k_y$ has the nesting vector $\vec Q=(\pi,\pi)$, and

$$H_U=\frac{U}{N}\sum_{\vec k,\vec k',\vec q}c^\dagger_{\vec k,\uparrow}c_{\vec k-\vec q,\uparrow}c^\dagger_{\vec k',\uparrow}c_{\vec k'+\vec q,\downarrow}. \tag{2}$$

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

$$F_\sigma(\vec p;\tau-\tau')=-\langle T_\tau c_{\vec p\pm\vec Q,\sigma}(\tau)c^\dagger_{\vec p,\sigma}(\tau')\rangle. \tag{3}$$

in addition to the usual Green's function:

$$G_\sigma(\vec p;\tau-\tau')=-\langle T_\tau c_{\vec p,\sigma}(\tau)c^\dagger_{\vec p,\sigma}(\tau')\rangle. \tag{4}$$

In mean-field theory for a SDW, the two propagators are related as shown in the Feynman diagrams depicted in Figs. 1 and 2. Single (doubled) arrowed lines represent diagonal (off-diagonal) propagators. The single line represents the free propagator, whereas double lines represent mean-field propagators. The Hubbard interaction is represented by a dashed line. The solution to the mean-field equations yields the SDW staggered magnetic moment m, which is defined as

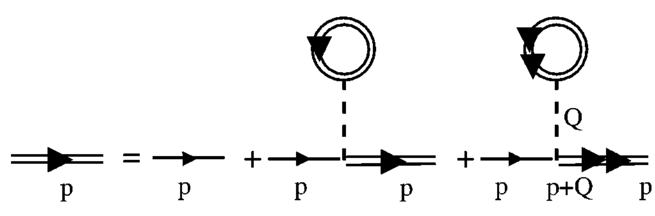

FIG. 1. Feynman diagrams corresponding to the SDW mean-field equation for $G_\sigma(\vec p;\tau-\tau')$.

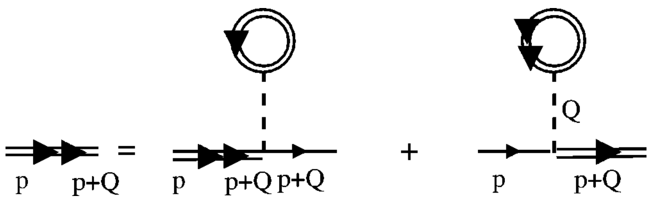

FIG. 2. Feynman diagrams corresponding to the SDW mean-field equation for $F_\sigma(\vec{p};\tau-\tau')$

$$\frac{1}{N}\sum_{\vec{p}}\langle c^\dagger_{\vec{p}+\vec{Q},\sigma}c_{\vec{p},\sigma}\rangle=\frac{m}{2}\sigma. \tag{5}$$

The staggered magnetic moment m is reduced from its Néel value for finite values of t/U, and its behavior as function of t/U at zero temperature is shown in Fig. 3. Both the above Green's functions have two-pole structures given by

$$G_\sigma(\vec{p},i\omega_n)=\frac{u_{\vec{p}}}{i\omega_n-E_+(\vec{p})}+\frac{v_{\vec{p}}}{i\omega_n-E_-(\vec{p})}, \tag{6}$$

$$F_\sigma(\vec{p},i\omega_n)=\frac{\tilde{u}_{\vec{p},\sigma}}{i\omega_n-E_+(\vec{p})}+\frac{\tilde{v}_{\vec{p},\sigma}}{i\omega_n-E_-(\vec{p})}, \tag{7}$$

where the energies $E_\pm$ are given by

$$E_\pm(\vec{p})=\frac{\xi(\vec{p})+\xi(\vec{p}+\vec{Q})}{2}+U\frac{n}{2}\pm E(\vec{p}), \tag{8}$$

where $E(\vec{p})=\frac{1}{2}\sqrt{[\xi(\vec{p})-\xi(\vec{p}+\vec{Q})]^2+U^2m^2}$ and $\xi(\vec{p})=\epsilon(\vec{k})-\mu$, and the coherence factors read

$$u_{\vec{p}}=\frac{E_+-\xi(\vec{p}+\vec{Q})-Un/2}{E_+-E_-},\quad v_{\vec{p}}=\frac{E_+-\xi(\vec{p})-Un/2}{E_+-E_-} \tag{9}$$

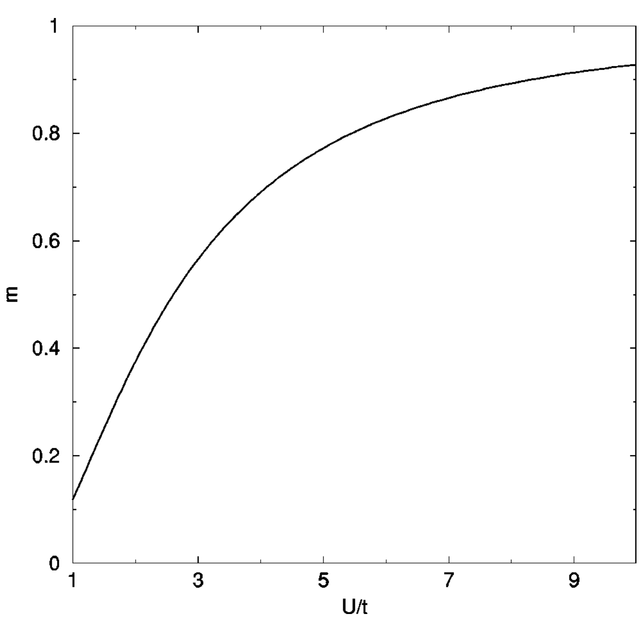

FIG. 3. Staggered magnetization as function of U/t at $T=0$ K.

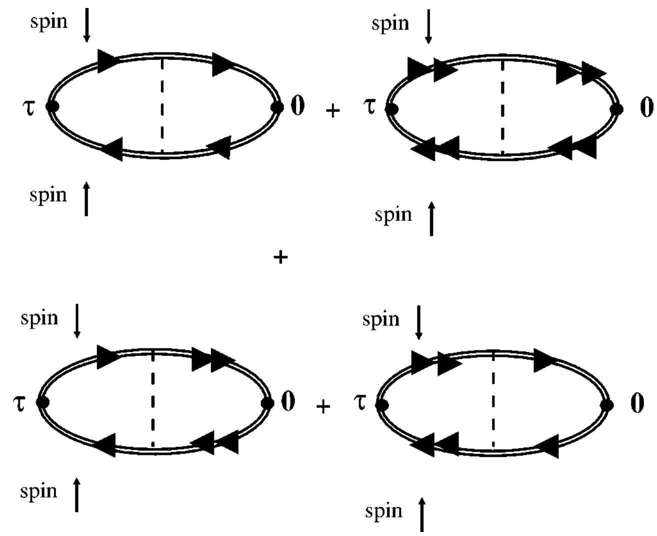

FIG. 4. The four first-order bubble diagrams for $\chi^1_{+-}(\vec{q},i\omega_n)$ in the SDW state. A summation over the internal momentum along the interaction line is implied.

and

$$\tilde{u}_{\vec{p},\sigma}=\frac{Um\sigma/2}{E_+-E_-},\qquad \tilde{v}_{\vec{p},\sigma}=-\frac{Um\sigma/2}{E_+-E_-}. \tag{10}$$

It is known that the mean-field treatment of the spin dynamics of itinerant strongly correlated electronic systems yields satisfactory results, as in the study of the dynamic spin-response function of the cuprates' superconducting state.[8] 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

$$\chi_{-+}(\vec{q},i\omega_n)=\mu_B^2\int_0^\beta d\,\tau e^{i\omega_n\tau}\langle T_\tau S^-(\vec{q},\tau)S^+(\vec{q},0)\rangle, \tag{11}$$

where $\beta=1/T$ is the inverse temperature, T_τ is the chronological order operator (in imaginary time), $S^-(\vec{q})=\Sigma_{\vec{p}}c^\dagger_{\vec{p},\downarrow}c_{\vec{p}+\vec{q},\uparrow}$, and $S^+(\vec{q})=[S^-(\vec{q})]^\dagger$. The above expression can be written as

$$\chi_{+-}(\vec{q},i\omega_n)=\mu_B^2\sum_{n=0}^{\infty}\int_0^\beta d\,\tau\sum_{\vec{p},\vec{p}'}e^{i\omega_n\tau}\Big\langle T_\tau\Big[-\int_0^\beta d\,\overline{\tau}H_U(\overline{\tau})\Big]^n \times c^\dagger_{\vec{p},\downarrow}(\tau)c_{\vec{p}+\vec{q},\uparrow}(\tau)c^\dagger_{\vec{p}'+\vec{q},\uparrow}(0)c_{\vec{p}',\downarrow}(0)\Big\rangle_{d.c.}, \tag{12}$$

where $d.c.$ stands for differently connected diagrams.

We now compute $\chi_{-+}(\vec{q},i\omega_n)$ by summing up all ladder diagrams and taking into account the existence of two possible Green's-function lines. The first-order bubble diagrams are shown in Fig. 4. The complete ladder summation is given by

$$\chi^{ladder}_{+,-}(\vec{q},i\omega_n) = \frac{-(x+y)[1+\lambda(\overline{x}+y)]+\lambda(z_1+z_2)^2}{[1+\lambda(x+y)][1+\lambda(\overline{x}+y)]-\lambda^2(z_1+z_2)^2}, \tag{13}$$

with $\lambda = U/N$ and

$$x(\vec{q},i\omega_n)=\frac{1}{\beta}\sum_{n',\vec{p}} G_\downarrow(\vec{p},i\omega'_n)G_\uparrow(\vec{p}+\vec{q},i\omega'_n+i\omega_n),$$

$$y(\vec{q},i\omega_n)=\frac{1}{\beta}\sum_{n',\vec{p}} F_\downarrow(\vec{p},i\omega'_n)F_\uparrow(\vec{p}+\vec{q},i\omega'_n+i\omega_n),$$

$$z_1(\vec{q},i\omega_n)=\frac{1}{\beta}\sum_{n',\vec{p}} G_\downarrow(\vec{p},i\omega'_n)F_\uparrow(\vec{p}+\vec{q},i\omega'_n+i\omega_n),$$

$$z_2(\vec{q},i\omega_n)=\frac{1}{\beta}\sum_{n',\vec{p}} F_\downarrow(\vec{p},i\omega'_n)G_\uparrow(\vec{p}+\vec{q},i\omega'_n+i\omega_n),$$

$$\overline{x(\vec{q},i\omega_n)}=\frac{1}{\beta}\sum_{n',\vec{p}} G_\downarrow(\vec{p},i\omega'_n)G_\uparrow(\vec{p}+\vec{q}+\vec{Q},i\omega'_n+i\omega_n).$$

The retarded susceptibility is obtained from Eq. (13), performing the analytical continuation $i\omega_n \rightarrow \omega + i0^+$. The poles of the retarded susceptibility give the energy $\omega(\vec{q})$ of the spin excitations of the system as well as their lifetimes. The equation for the poles is

$$\{1+\lambda[x(\vec{q},\omega)+y(\vec{q},\omega)]\}\{1+\lambda[\overline{x(\vec{q},\omega)}+y(\vec{q},\omega))]\} - \lambda^2[z_1(\vec{q},\omega)+z_2(\vec{q},\omega)]^2=0. \tag{14}$$

It is not possible to solve Eq. (14) analytically for arbitrary U and t. In the limit $t/U \rightarrow 0$ at half-filling, from Eq. (14) we recover the same result as in linear spin-wave theory for the nearest-neighbor Heisenberg model,

$$\omega(q_x,q_y) \rightarrow \frac{4t^2}{Um}\sqrt{4-(\cos q_x+\cos q_y)^2}, \tag{15}$$

which predicts that $\omega(0,\pi)=\omega(\pi/2,\pi/2)$, in disagreement with the experimental data,[1] and $m \rightarrow 1$, showing no magnetic moment reduction from the Néel state value. Of course Eq. (15) holds asymptotically for $t/U \ll 1$. We remark that the factor $1/m$ plays the role of the quantum renormalization factor Z_c.[1]

On the other hand, for finite t/U, Eq. (14) has to be solved numerically. Considering the half-filled case ($\mu=0$), appropriate for La_2CuO_4, we computed the spin-wave dispersion $\omega(\vec{q})$ for $U=1.8$ eV and $t=0.295$ eV along the high-symmetry directions, in the two-dimensional Brillouin zone, considered in Ref. 1. These values agree with those used in Ref. 1: $U=2.2\pm0.4$ eV and $t=0.30\pm0.02$ eV. The results (solid line) are given in Fig. 5 together with the experimental results (in circles) at $T=10$ K. It is clear that $\omega(0,\pi) > \omega(\pi/2,\pi/2)$, that is, a dispersion at the zone boundary is obtained. For these values of t and U the staggered magnetic moment is $m=0.832$, and therefore $1/m=1.20$, which agrees well with $Z_c=1.18$ used to fit the data in Ref. 1.

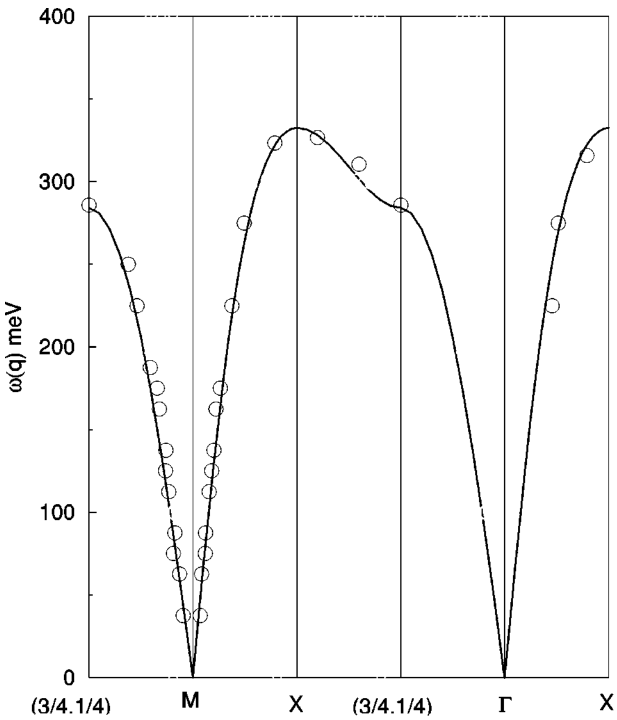

FIG. 5. Spin-wave dispersion, in meV, along high-symmetry directions in the Brillouin zone. The circles are the data reported in Ref. 1 at 10 K. The solid line is the analytical result (at 0 K) for $U=1.8$ eV and $t=0.295$ eV. The momentum is in units of 2π, and $M=(1/2,1/2)$, $X=(1/2,0)$, and $\Gamma=(0,0)$.

In their interpretation of the experimental data, the authors of Ref. 1 considered an effective Hamiltonian incorporating ring exchange. In such a model the electron not only makes a virtual trip to its nearest neighbor, but also makes virtual excursions around a loop visiting its second neighbors. If we had written the transverse susceptibility in coordinate space, it would be clear that in a ladder summation the electron goes around larger and larger rings before it comes back to the original site with its spin flipped. Therefore, such a good agreement between the perturbation theory calculation in Ref. 1 and our ladder summation is not surprising. Althought we have not presented the results here, Eq. (14) also predicts a continuum of excitations which are gapped relatively to the ground state.

In summary, we have shown that a ladder summation based on the SDW state can account satisfactorily for the measured spin-wave dispersion of La_2CuO_4 at all energies. The quality of the fitting points out that it is not needed to derive an effective spin Hamiltonian from the Hubbard model in order to obtain agreement with the data.

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