Spin-spectral-weight distribution and energy range of the parent compound $\text{La}_2\text{CuO}_4$

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Abstract – The spectral-weight distribution in recent neutron scattering experiments on the parent compound $\text{La}_2\text{CuO}_4$ (LCO), which are limited in energy range to about 450 meV, is studied in the framework of the Hubbard model on the square lattice. We find that the higher-energy weight extends to about 566 meV and is located at and near the momentum $[\pi, \pi]$. Our results confirm that the $U/t$ value suitable to LCO is in the range $U/t \in (6,8)$. The continuum weight energy-integrated intensity vanishes or is extremely small at momentum $[\pi, 0]$. This behavior of the intensity is consistent with that of spin waves, which are damped at $[\pi, 0]$.

It is natural to expect that a greater understanding of the physics of the high-$T_c$ superconductor undoped parent compounds, such as $\text{La}_2\text{CuO}_4$ (LCO), will lead to a greater understanding of the corresponding superconductors. In particular, the less complicated undoped systems can provide valuable information on which model Hamiltonians quantitatively describe the cuprates. Improved determination of the model Hamiltonians is essential because of the many nearby competing phases in the doped systems, easily affected by small parameters, which can now be seen because of continued improvements in numerical simulations [1]. A decade ago the neutron scattering experiments on LCO of Coldea et al. [2] first showed sufficient details of the spin-wave spectrum to demonstrate that a simple nearest-neighbor Heisenberg model must be supplemented by a number of additional terms, including ring exchanges. These terms arise naturally out of a single-band Hubbard model with finite $U/t$, and several detailed studies showed that the spin-wave data in the available energy window could be successfully described by the Hubbard model using a somewhat smaller value of $U/t \sim 6–8$ than originally thought appropriate [2–5]. However, part of the spectral weight was deduced to be outside the energy window.

Recently, improved neutron scattering experiments [6] with a much wider energy window of about 450 meV, have raised a number of questions. Surprisingly, these studies revealed that the high-energy spin waves are strongly damped near momentum $[\pi, 0]$ and merge into a momentum-dependent continuum. These results led the authors of ref. [6] to conclude that “the ground state of $\text{La}_2\text{CuO}_4$ contains additional correlations not captured by the Néel-SWT [spin-wave theory] picture”. This raises the important question of whether the more detailed results can still be described in terms of a simple Hubbard model. Here we address this question using a combination of a number of theoretical and numerical approaches, including, in addition to standard treatments, a new spinon approach for the spin excitations [5,7] and density matrix renormalization group (DMRG) calculations for Hubbard cylinders [8–10]. We show that the Hubbard model does describe the new neutron scattering results. In particular, at momentum $[\pi, 0]$ the continuum weight energy-integrated intensity is found to vanish or be extremely small. Furthermore, we find that beyond 450 meV, the spectral weight is mostly located around momentum $[\pi, \pi]$.

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and extends to about 566 meV, suggesting directions for future experiments.

The Hubbard model on a square lattice with $N \gg 1$ sites and periodic boundary conditions reads $\hat{H} = \hat{T} + U \hat{D}$. Here $\hat{T} = -t \sum_{\langle j,j' \rangle} \sum_{\sigma=\uparrow,\downarrow} c_{j,\sigma}^\dagger c_{j',\sigma} + \text{h.c.}$ is the kinetic-energy operator, $\hat{D} = \sum_{N_{j}=1}^{N} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}$ counts the number of electron doubly occupied sites, $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$ are electron creation and annihilation operators with site index $j = 1, \ldots, N$ and spin $\sigma = \uparrow, \downarrow$, and $\hat{n}_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$. The expectation values are
\begin{equation}
\begin{aligned}
d &= \langle \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \rangle, \\
m_{AF} &= \frac{1}{2} \langle (\hat{n}_{j,\uparrow} - \hat{n}_{j,\downarrow})^2 \rangle,
\end{aligned}
\end{equation}

play an important role in our study, following the strong evidence that for $U > 0$ and $N \rightarrow \infty$ the model ground state has antiferromagnetic long-range order [11]. In the last expression of eq. (1), $m_{AF}^0$ stands for a mean-field sublattice magnetization that does not account for the effect of transverse fluctuations and $\delta S$ accounts for such an effect, its value being estimated below. Moreover, the on-site spin operators read
\begin{equation}
\begin{aligned}
\hat{S}_{\uparrow j}^z &= \frac{1}{2} (\hat{n}_{j,\uparrow} - \hat{n}_{j,\downarrow}), \\
\hat{S}_{\uparrow j}^x &= \frac{1}{2} (\hat{S}_{\uparrow j}^z - \hat{S}_{\uparrow j}^y), \\
\hat{S}_{\downarrow j}^y &= \frac{1}{2} (\hat{S}_{\downarrow j}^z + \hat{S}_{\downarrow j}^x), \\
\hat{S}_{\downarrow j}^z &= c_{\downarrow j,\uparrow}^\dagger c_{\downarrow j,\downarrow}^\dagger c_{\downarrow j,\downarrow} c_{\downarrow j,\uparrow}.
\end{aligned}
\end{equation}

Our study involves the dynamical structure factors,
\begin{equation}
\begin{aligned}
S^{\alpha\alpha'}(\vec{k},\omega) &= \frac{(g^2\mu B)^2}{N} \sum_{j,j'=1}^{N} e^{-i\vec{k} \cdot (\vec{r}_j - \vec{r}_{j'})} \\
&\times \int_{-\infty}^{\infty} dt e^{i\omega t} \langle GS| \hat{S}_{\alpha j}^x(t) \hat{S}_{\alpha' j'}^x(0) |GS \rangle,
\end{aligned}
\end{equation}

where $\alpha = \alpha' = x, y, z$ or $\alpha = -$ and $\alpha' = +$ and below we consider $\sigma = 2$. It is straightforward to show that the sum rules $[1/N] \sum_{\vec{k}} S^{\alpha\alpha'}(\vec{k})$, where $S^{\alpha\alpha'}(\vec{k}) = [1/2\pi] \int_{-\infty}^{\infty} d\omega S^{\alpha\alpha'}(\vec{k},\omega)$, involve the average single occupancy $(1 - 2d)$ and read $[(g^2\mu B)^2/4] [\delta_{\alpha,-\alpha'} + 2 \delta_{0,0} \delta_{\alpha,-\alpha'}] \langle 1 - 2d \rangle$. In an ideal experiment one sees a transfer of weight from the longitudinal to the transverse part such that independently of the scattering geometry, the corresponding effective spin form factor satisfies the sum rule
\begin{equation}
\begin{aligned}
\frac{1}{N} \sum_{\vec{k}} \frac{1}{2 \pi} \int_{-\infty}^{\infty} d\omega \omega S^{exp}(\vec{k},\omega) = \mu_{B}^2 B (1 - 2d).
\end{aligned}
\end{equation}

That the coefficient involved is $2(1 - 2d)$ rather than $3(1 - 2d)$ follows from the experiment one mode being perpendicular to the plane and thus silent [4]. For $U/t \in (0, 8)$ the antiferromagnetic long-range order may be accounted for by a variational ground state with a SDW initial trial state, such as $|G\rangle = e^{-gD}|SDW\rangle$ or $|GB\rangle = e^{-hT/1 + e^{-gD}}|SDW\rangle$, where $|SDW\rangle$ is the ground state of a simple effective mean-field Hamiltonian, as that of eq. (18) of ref. [12]. For $U/t > 1$ such an order is as well accounted for by a Baeriswyl variational state $|B\rangle = e^{-hT/1 + e^{-gD}}|\infty\rangle$, where $|\infty\rangle$ is the exact $U/t \rightarrow \infty$ ground state [12]. The coefficients $h$ and $g$ multiplying the kinetic-energy and double-occupancy operators, respectively, are variational parameters. Similarly for the trial state $|SDW\rangle$, the relation $4|m_{AF}^0|^2 = (1 - 4d)^2$, holds for $|G\rangle$, $|GB\rangle$, and $|B\rangle$, while the function $d = d(U/t)$ is state dependent. This gives $d = \frac{1}{4} [1 - 4|m_{AF}^0|^2]$, consistent with $d$ not being affected by transverse fluctuations.

The evaluation of the ground-state energy for $|GB\rangle$ and $|B\rangle$ is for $N \gg 1$ an involved problem. Here we resort to an approximation, which corresponds to the simplest expression of the general form $E/N = T_0 q_U + U d$, where $T_0 = -\frac{U}{2} t$, compatible with three requirements: the relation $d = \frac{1}{2} [1 - 4|m_{AF}^0|^2]$; the occurrence of antiferromagnetic long-range order for the whole $U/t > 0$ range; and the lack of a linear kinetic-energy term in $U/t \ll 1$. Brinkman and Rice found $q_U = 8d(1 - 2d)$ for the original paramagnetic-state Gutwiller approximation [13], which is lattice insensitive and thus does not account for the square-lattice antiferromagnetic long-range order. The simplest modified form of the quantity $q_U$ suitable to a broken-symmetry ground state such that the three conditions are met is
\begin{equation}
q_U = \frac{U}{8t} a_{(+)} d \left[ \frac{(1 - 2d)}{4|m_{AF}^0|^2} - a_2 \right] - a_3,
\end{equation}

where $4|m_{AF}^0|^2$ behaves as $4|m_{AF}^0|^2 = U/8t$ for $U/t \ll 1$, $a_{(+)} = \pi^2 / 4$, $a_2 = (1 - [\pi^2 / 2a_{(+)}])$, and $a_3 = a_3(U/8t)$ a function whose approximate limiting behaviors are
\begin{equation}
a_3 = \frac{a_{(+)}^{(-)}}{8} \left[ 1 - \text{tanh} \left( \frac{U}{8t} \right) \right],
\end{equation}

for $U$ smaller than the bandwidth $8t$ and $a_2 = -c_0/[\pi/2]^2 [8t/U]$ for $U/t \gg 1$. Here $c_0 = (\pi/4 + 1/8)/2 = 0.1462$ and the corresponding estimate $\alpha = 0.6696$ is that of the Heisenberg-model studies of ref. [11]. Minimization of the obtained ground-state energy with respect to $d$ leads indeed to $d = \frac{1}{2} [1 - 4|m_{AF}^0|^2]$. For $U/t < 1$ such a $q_U$ expression yields to second order in $U/t$, $E/N = T_0 U + \frac{U}{2} d (1 - 8\pi^2)^2 /[U^2/t^2]$, where $[1/8\pi^2] \approx 0.0127$. The coefficient $\approx 0.0127$ is that also obtained by second-order perturbation theory [14]. For $U/t \gg 1$ one recovers the known result $E/N = -4c_0[8^2/U]$, for $1/8\pi^2 \approx 0.0127$. That our approximation agrees with the known limiting behaviors.

For $U/t \in (0, 8)$, we find that $4|m_{AF}^0|^2$ gives quantitative agreement for the $(1 - 2d)$ dependence on $U/t$ with both our numerical DMRG calculations (see fig. 1) and the numerical results for the states $|G\rangle$ and $|GB\rangle$ (see fig. 4 of ref. [4]). For $U/t \gg 1$ we find the behavior $4|m_{AF}^0|^2 \approx e^{-2c_0[(8t/U)]^2}$ for the state $|B\rangle$, so that
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Fig. 1: (Colour on-line) Average single occupancy: approximate expression $[1 + \tanh(U/8t)]/2$ valid for $U/t \lesssim 8$ (full line), the limiting $U/t \gg 1$ expression $[1 - c_0(8t/U)^2]$ (dashed line), and from DMRG numerical results on two different width cylinders.

**Table 1:** Several spectral weights in units of $\mu_B^2$ as defined in the text and the sublattice magnetizations as calculated here for several $U/t$ values and some results from refs. [4,12].

| $U/t$ | 6.1 | 6.5 | 8.0 | 10.0 |
|-------|-----|-----|-----|------|
| $W_T$ | 1.643 | 1.671 | 1.762 ($1.778$ [4]) | 1.848 ($1.846$ [4]) |
| $W_{SW}$ | 0.808 | 0.799 | 0.761 | 0.714 |
| $W_{<450}$ | 1.571 | 1.593 | 1.663 | 1.730 |
| $W_{\geq450}$ | 0.072 | 0.078 | 0.099 | 0.118 |
| $m_{AF}^0$ | 0.401 | 0.410 | 0.436 ($0.43$ [4,12]) | 0.461 ($0.456$ [4]) |
| $m_{AF}^B$ | 0.329 | 0.342 | 0.384 ($0.39$ [12]) | 0.426 |
| $m_{\text{lower}}^B_{AF}$ | 0.200 | 0.207 | 0.233 | 0.258 |

$(1 - 2d) = [1 + \tanh(U/8t)]/2$ for approximately $U/t \lesssim 8$ and $(1 - 2d) = [1 - c_0(8t/U)^2]$ for $U/t \gg 1$. Furthermore, the states $|SDW\rangle$ and $|B\rangle$ give $m_{AF} = m_{AF}^0 = \frac{1}{2}\sqrt{1 - 4d}$, with an improved $d = d(U/t)$ dependence for the latter, whose $m_{AF}^0$ magnitudes are provided below in table 1 for several $U/t$ values. The states $|GB\rangle$ and $|B\rangle$ have $m_{AF}^B$ and $m_{AF}^B$ sublattice magnetization numerical values very close to those given by eq. (1) with $\delta S \approx d$ and $\delta S \approx d + \frac{1}{8}[1 - m_{HAF}/m_{HAF}^0] \approx d + 0.197$, respectively. Here $m_{HAF}^0 = 1/2$ and $m_{HAF} \approx 0.303$ is the Heisenberg-model sublattice magnetization magnitude [11]. Some $m_{AF}^B$ magnitudes are given below in table 1, along with those of $m_{\text{lower}} = (1 - 2d)[m_{HAF}/m_{HAF}^0] m_{AF}^0$, which we define for $U/t > 0$ and for $U/t \gg 1$ becomes $m_{AF}^B$. Probably $m_{AF}^B$ is closest to the exact $m_{AF}$, while $m_{AF}^B$ is consistent with our use of the RPA. In the DMRG calculations of $(1 - 2d)$ (see fig. 1), two different circumference cylinders were simulated as a function $U/t$, with open boundary conditions in $x$ and periodic in $y$, and the double occupancy measured in one of the middle columns. A maximum of $m = 4000$ states was kept, with an accuracy of $\sim 10^{-4}$ in $(1 - 2d)$ for the $10 \times 4$ system for the least accurate smaller $U/t$ values, and about $10^{-3}$ for the $10 \times 6$ system. We find that the value of $(1 - 2d)$ is relatively insensitive to cluster size, and these cluster sizes are representative of 2D behavior [15].

To study the coherent spin-wave weight distribution and spectrum, we have calculated by RPA the transverse dynamical susceptibility,

$$
\chi^{-}\left(\vec{k},\tau\right) = \frac{(g\mu_B)^2}{N} \sum_{j,j'=1}^{N} e^{-i\vec{k} \cdot (\vec{r}_j - \vec{r}_{j'})} \langle \hat{S}^-(\vec{r}_j,\tau) \hat{S}^+(\vec{r}_{j'},0) \rangle,
$$

(7)
where $\tau$ denotes the imaginary time in Matsubara formalism (we shall take the zero-temperature limit). In the case of the present model, the coherent spin-wave spectral weight in units of $\mu_B^2$ is $Z_d 2(1 - 2d)$. Here,

$$Z_d = 1 - \frac{2}{N(1 - 2d)} \sum_{\vec{k}} \sum_{\nu \neq \nu'} |\langle \nu | \hat{S}_{\vec{k}}^+ (\hat{G} \hat{S}) | \nu' \rangle|^2,$$

where the sum over energy eigenstates excludes those that generate the coherent spin-wave weight, $|\nu \rangle = |\nu, \omega(\vec{k})\rangle$. In the $U/t \to \infty$ limit, $Z_d$ may be identified with the corresponding $Z_d = Z_c Z_{\chi}$ factor of the Heisenberg model on the square lattice. According to the results of ref. [16], $Z_c \approx 1.18$ and $Z_{\chi} \approx 0.48$, respectively, so that $Z_d \approx 0.57$. The limiting values $Z_d = 1$ for $U/t \to 0$ and $Z_d \approx 0.57$ for $U/t \to \infty$ and the approximate intermediate value $Z_d \approx 0.65$ at $U/t = 8$ [4] are recovered as solutions of the equation $Z_d = e^{-Z_d \tanh(\sqrt{\pi \tau})}$, which is used here for finite $U/t$. In the thermodynamic limit the upper-Hubbard-band processes generate nearly no spin weight. Hence the longitudinal (elastic contribution to) spectral weight within $\mu_B^2 2(1 - 2d)$, eq. (4), is in units of $\mu_B^2$ approximately given by $\approx 4(m_{AF})^2$ and the spin-wave intensity reads $W_{SW} = Z_d [2(1 - 2d) - 4(m_{AF})^2]$. The GA+RPA method used in ref. [4] accounts for the quantum fluctuations that control the longitudinal and transverse relative weights, so that the spin-wave intensity factor is $Z_d$. The RPA used here leads to a similar spin-wave intensity momentum distribution but its experimentally determined factor $Z_{SW}^{exp} < Z_d$ is such that $W_{SW} = Z_d [2(1 - 2d) - 4(m_{AF})^2] = Z_{SW}^{exp} 2(1 - 2d)$.

Within the two-sublattice description the susceptibility becomes a $2 \times 2$ tensor and the above original susceptibility $\chi^{-}(\vec{k}, \tau)$ is the average of its four elements. After Fourier-transforming to $(\vec{k}, i\omega)$ space, within the RPA the susceptibility tensor obeys $\tilde{\chi}_{\nu \nu'}^{RPA} = [1 - U \tilde{\chi}^{(0)}]^{-1} \tilde{\chi}^{(0)}$. Here $\tilde{\chi}^{(0)}$ denotes the susceptibility tensor in the noninteracting system. $\tilde{\chi}_{\nu \nu'}^{RPA}$ has a pole $i\omega = \omega(\vec{k})$ obtained from the equation $\det [1 - U \tilde{\chi}^{(0)}] = 0$, which provides the dispersion relation $\omega(\vec{k})$ for the spin waves. It has been shown in ref. [3] that an excellent agreement with the spin-wave spectrum from ref. [2] is achieved. In fig. 2 upper panel we show a fit to the more recent experimental data of ref. [6] (full line) along with the results from the s1 fermion method reported below (dashed line) for $U/t = 6.1$ and $t = 295$ meV. Provided that the $t$ magnitude is slightly increased for increasing values of $U/t$, agreement with the LCO spin-weight spectrum and distribution can be obtained for $U/t \in (6, 8)$. For $U/t$ values smaller than 6 (and larger than 8), the spin-wave dispersion between $[\pi/2, 0]$ and $[\pi/2, \pi/2]$ has too large energy bandwidth (and is too flat) for any reasonable value of $t$. From the residue of the spin-wave pole the susceptibility coherent part reads

$$\chi_{\nu \nu'}^{RPA}(\vec{k}, i\omega) = Z_{\nu \nu'}^{exp} \sum_{l=0,1} \frac{\text{Res} [\chi^{-}(\vec{k}, l \omega(\vec{k}))]}{i\omega - l \omega(\vec{k})}.$$

The measured intensity is $I_{SW}(\vec{k}) = \pi [S^{xy}(\vec{k}) + S^{yx}(\vec{k})] = \pi S^{-\dagger}(\vec{k})$ [17]. In fig. 2 lower panel, we plot the corresponding RPA spin-wave intensity, $I_{SW}(\vec{k}) = -[\pi/2] Z_{\nu \nu'}^{exp} \text{Res} [\chi^{-}(\vec{k}, \omega(\vec{k}))]$. The good agreement with the experimental data, specially near the point $M$, reproduces the theoretical results of ref. [6]. It is here obtained for the value $Z_{\nu \nu'}^{exp} \approx 0.49$, which corresponds to the choice $m_{AF} = m_{AF}^{GB} = m_{AF}^{0}(1 - 2d)$ such that $\delta S \approx d$. As in ref. [6], it shows disagreement around the $X$ point, which here probably stems from the RPA.

To derive the spectrum of the spin $S = 1$ excited states producing the inelastic form factor spectral weight, we use the spinon operator representation of ref. [5]. The ground-state spin degrees of freedom are described by a full s1 fermion band, which coincides with an antiferromagnetic reduced Brillouin zone. Each s1 fermion is a spin-singlet two-spinon composite object. The spin $S = 1$ excited states of momentum $\vec{k} = [\pi, \pi] - \vec{q} - \vec{q}'$ are generated upon breaking one s1 fermion spinon pair, which leads to the emergence of two holes of momenta $\vec{q}$ and $\vec{q}'$ in the otherwise full s1 band. The inelastic coherent spin-wave spectrum is generated by processes where $\vec{q}$ points in the nodal direction and $\vec{q}'$ belongs to the boundary of the s1 band.
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Fig. 3: (Colour on-line) The energy-momentum space limits of the spin $S = 1$ excited-states spectrum for $U/t = 6.1$, $t = 295$ meV, and $k_x$ and $k_y$ in units of $2\pi$. States whose energy is for a given $\vec{k}$ lower than that of the intermediate spin-wave sheet as well as those of any energy and equivalent momenta $[0, 0] = [0, 2\pi] = [2\pi, 0] = [2\pi, 2\pi]$ do not contribute to the spin spectral weight.

band reduced zone [5]. The remaining choices of $\vec{q}$ and $\vec{q}'$ either generate the inelastic incoherent continuum spectral weight or vanishing weight, respectively. The studies of ref. [5] are limited to the spin-wave spectrum. Here we consider the energy-momentum space domain of all above spin $S = 1$ excited states, which is represented in fig. 3. (A similar spectrum is obtained for the values $U/t = 8.0$ and $t = 335$ meV of ref. [4].) The intermediate sheet refers to the spin-wave spectrum. For each $\vec{k}$, states of energy lower than the latter spectrum do not contribute to the form-factor weigh. Furthermore and consistent with the first-moment sum rules of an isotropic antiferromagnet, no and nearly no weight is generated by states of any energy and momentum $[0, 0]$ near $[0, 0]$, respectively. Unfortunately, the method of ref. [5] does not provide the detailed continuum weight distribution. However, it is expected that, similarly to the Heisenberg model case [4], its energy-integrated intensity follows the same trend as the spin-wave intensity. Analysis of fig. 3 reveals that for momentum $[\pi, 0]$ there are no excited states of energy higher than the spin waves. Thus, at momentum $[\pi, 0]$, the continuum weight distribution energy-integrated intensity vanishes or is extremely small, due to $sl$ band four-hole processes. Given the expected common trend of both intensities, this is consistent with a damping of the spin-wave intensity at momentum $[\pi, 0]$, as observed [6] but not captured by the fig. 2 RPA intensity.

In table 1 we provide the sublattice magnetization magnitudes along with our calculations of the following integrated spectral weights (in units of $\mu_B^2$): the total weight, $W_T = 2(1 - 2d)$; the spin-wave weight, $W_{SW} = 2Z_{dp} Z_{dp} (1 - 2d)$; the weight for energy $\hbar \omega \leq 450$ meV, $W_{<450} = W_{SW}/0.71 + 4(m_{GB}^2)^2$; and the weight $W_{<450} = [W_T - W_{<450}]$ for energy $\hbar \omega > 450$ meV. $W_{<450}$ is derived by combining our theoretical expressions with the observations of ref. [6] that for the energy range up to about 450 meV, 71% and 29% of the weight corresponding to the inelastic spin-wave weight and incoherent continuum weight, respectively. Our prediction for $W_{<450}$ varies between 1.6 $\mu_B^2$ for $U/t \approx 6.1$ and 1.7 $\mu_B^2$ for $U/t \approx 8.0$, in agreement with the experimental value $1.9 \pm 0.3$ $\mu_B^2$ reported in ref. [6]. From our above analysis, the small weight $W_{<450} \approx 0.1 \mu_B^2$ is expected to extend to about 566 meV (see fig. 3), mostly at and around the momentum $[\pi, \pi]$.

Finally, we have checked the consistency of our results by confirming that for $U/t \in (6, 8)$ the single-particle gap $\Delta_{MH}$ of the Hubbard model on the square lattice is of the order of that observed experimentally for LCO. Within the operator representation used above to derive the spin spectrum, the approximate studies of ref. [5] found $\Delta_{MH} \approx 566$ meV at $U/t = 6.1$. Furthermore, we have performed DMRG calculations both for $10 \times 4$ and $10 \times 6$ Hubbard cylinders. (From those, the magnitude $\Delta_{MH} \approx 566$ meV is rather reached at $U/t \approx 7.1$, still within our range $U/t \in (6, 8)$.) The chemical potential was set to $U/2$ and two states were targeted, one with $N$ particles and the other with $N - 1$. (Targeting $N + 1$ electrons would have given the same results.) Both states were put into the same density matrix in the traditional multi-state targetting DMRG approach. Thus, the same truncation error applied to both states, leading to significant error cancelation. The resulting gap at each sweep was plotted $vs$. the maximum truncation error in the sweep, yielding approximately linear behavior, and allowing the extrapolation to zero truncation error. The error estimate is roughly the size of the extrapolation from the last point. From 1800 ($10 \times 4$ Hubbard cylinder) to 6000 ($10 \times 6$ Hubbard cylinder) states were kept. We find $\Delta_{MH} \approx 1.39(2) t$ for $U/t = 6$ and $\Delta_{MH} \approx 2.15(2) t$ for $U/t = 8$. This leads to a range $\Delta_{MH} \in (408$ meV, 721 meV) for $U/t \in (6, 8)$. Here we used the $t$ magnitudes $t \approx 293$ meV and $t \approx 335$ meV for which the model describes the LCO neutron scattering for $U/t = 6$ and $U/t = 8$, respectively. For the $U/t = 6.1$ value used in some of our calculations, we find $\Delta_{MH} \approx 1.40(5) t$ from the DMRG analysis, so that $\Delta_{MH} \approx 414$ meV for $t \approx 295$ meV.

Optical experiments overestimate the charge-transfer gap magnitudes of the parent insulating compounds [18]. On the other hand, by measuring the Hall coefficient $R_H$ in LCO, the studies of ref. [19] have estimated the energy gap over which the electron and hole carriers are thermally activated to be $\approx 890$ meV. Such a gap refers to the full Mott-Hubbard gap, so that its magnitude is twice that of the single-particle gap. Hence such experimental results are consistent with a single-particle
gap of $\Delta_{MH} \approx 445$ meV. Remarkably, this magnitude is within the range $\Delta_{MH} \in (408 \text{ meV}, 721 \text{ meV})$ of our above theoretical predictions for $U/t \in (6, 8)$. (Our theoretical approach based on the combination of our DMRG results with the $U$ and $t$ values for which agreement with the LCO neutron-scattering agreement is reached leads to $\Delta_{MH} \approx 445$ meV for $U/t \approx 6.3$.)

In summary, we have studied several open issues raised by the recent LCO neutron scattering data reported in ref. [6]. Our result that at momentum $[\pi, 0]$ the continuum weight energy-integrated intensity vanishes or is very small is consistent with a corresponding damping of the spin-wave intensity at $[\pi, 0]$, as observed in the recent experiments of ref. [6]. We suggest that future LCO neutron scattering experiments scan the energies between 450 meV and 566 meV and momenta around $[\pi, \pi]$.

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