Evidence for site-centered stripes from magnetic excitations in cuprate superconductors

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The success of models of coupled two-leg spin ladders in describing the magnetic excitation spectrum of $La_{2-x}Ba_xCuO_4$ has been widely interpreted as evidence for bond-centered stripes. Here, we determine the magnetic coupling induced by the charge stripes between bond- or site-centered spin stripe modeled by two- or three-leg ladder, respectively. We find that only the site-centered models order. We further report excellent agreement of a fully consistent analysis of coupled three-leg ladders using a spin-wave theory of bond operators with the experiment.

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I. INTRODUCTION

The mechanism of superconductivity in the presence of local antiferromagnetism in copper oxides is considered an outstanding problem in contemporary physics.[1,2] The materials are described by mobile charge carriers (holes) doped into a quasi-two-dimensional spin-1/2 antiferromagnet.[3] Inelastic neutron-scattering experiments have revealed a magnetic resonance peak[4,5] and, in some compounds, periodic modulations in the spin and charge density (stripes).[6–12] Tranquada *et al.*[13] found that the magnetic excitation spectrum of stripe-ordered $La_{1.875}Ba_{0.125}CuO_4$ looks similar to disordered $YBa_2Cu_3O_{6+x}$ (Ref. 5) or $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ref. 14) and observed that the data are consistent with bond-centered stripes modeled by two-leg ladders. This experiment, and its interpretation, is considered of key importance for the field of high-temperature superconductivity. The reason these findings are so vigorously discussed is that they may provide the decisive hint as to within which framework these conceptionally simple yet inscrutable systems are to be understood, and hence ultimately lead to a complete theory.

At present, there is no consensus with regard to such a framework, but instead a fierce competition among different schools of thought. One of these schools[8,9,11,12] attributes the unusual properties of the doped, two-dimensional antiferromagnets to their propensity to form stripes or their proximity to a quantum critical point (QCP) at which stripe order sets in. The resulting picture is highly appealing. Static stripes have been observed[7,10] only in certain compounds, most notably $La_{2-x}Sr_xCuO_4$ at a hole doping concentration $x=\frac{1}{8}$ and are known to suppress superconductivity. On the other hand, the mere existence of stripes would impose an effective one dimensionality and hence provide a framework to formulate fractionally quantized excitations. This one dimensionality would be roughly consistent with an enormous body of experimental data on the cuprates, including the electron spectral functions seen in angle-resolved photoemission spectroscopy. The charge carriers, the holons, would predominantly reside in the charge stripes, as they could maximize their kinetic energy in these antiferromagnetically disordered regions. In the spin stripes, by contrast, the antiferromagnetic exchange energy between the spins would be maximized, at the price of infringing on the mobility of the charge carriers. Most importantly, the spin stripes would impose a coupling between the charge stripes, which would yield an effective, pairwise confinement between the low-energy spinon and holon excitations residing predominantly in the charge stripes. The mechanism of confinement would be similar to that of coupled spin chains or spin ladders.[15–17] The holes would be described by spinon-holon bound states, and the dominant contribution to the magnetic response measured in Tranquada's as well as all other neutron-scattering experiments would come from spinon-spinon bound states.

The similarity of the "hour-glass" spectrum shown in Fig. 4b of Tranquada *et al.*[13] [which is reproduced for comparison in Fig. 1(b)] and the "elephants trousers" observed by Bourges *et al.*[5] (see Fig. 3 of their manuscript) provides the most striking evidence in favor of the picture advocated by this school, which attributes the anomalous properties of generic, disordered CuO superconductors to the formation of dynamic (rather than static) stripes, which fluctuate on time scales slow compared to the energy scales of most experi-

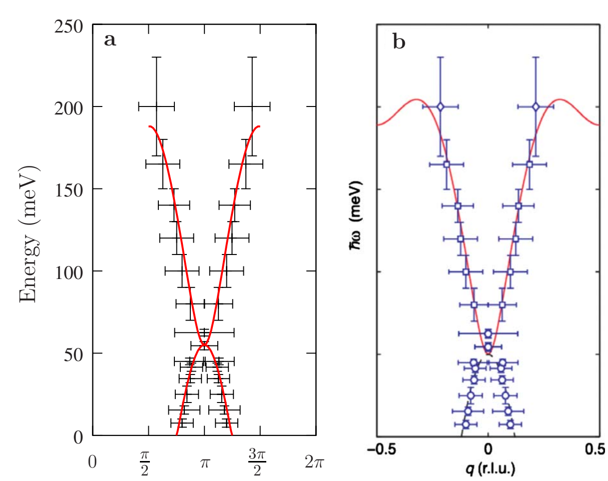

FIG. 1. (Color online) Comparison of dispersions resulting from different theories with experimental data. (a) Superpositions of cuts along (k_x,π) and (π,k_y) for the lowest mode of the SWT with $J=140$ meV and $J'=0.07J$ for site-centered stripes described in the text (red) superimposed with the experimental data obtained by inelastic neutron scattering (Ref. 13) (black). (b) The neutron data, with a triplon dispersion of a two-leg ladder superimposed (red line), reproduced from Tranquada *et al.* (Ref. 13). (Reprinted by permission from Macmillian Publishers Ltd: Nature 429: 534–538, ©2005.)

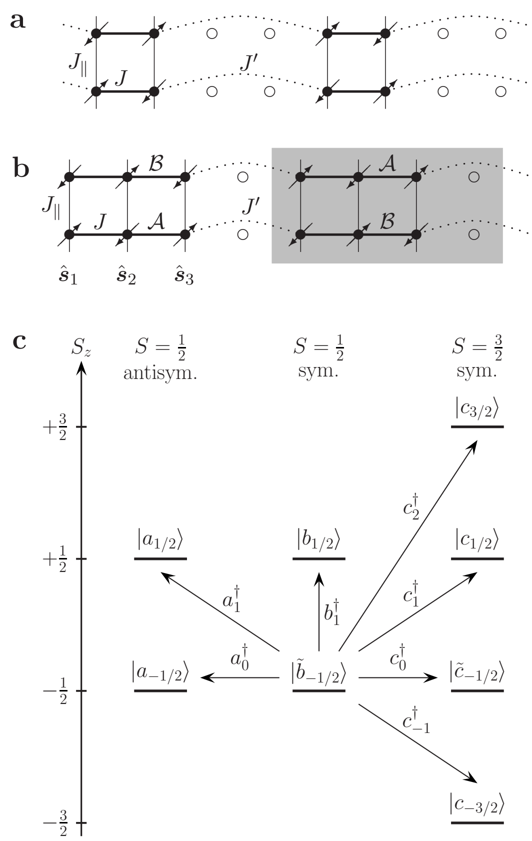

FIG. 2. Models of spin stripes: (a) bond-centered stripes modeled by two-leg ladders and (b) site-centered stripes modeled by three-leg ladders. (c) Definition of bosonic creation operators in the eight-dimensional Hilbert space spanned by a rung on sublattice $\mathcal{A}$ of the ladders shown in (b).

mental probes. This picture received additional support by Xu *et al.*,[18] who observed that the magnetic response of $La_{1.875}Ba_{0.125}CuO_4$ at higher energies is independent of temperature while the stripe order melts at about $T_{st} \sim 54$ K. Measurements on "untwinned" samples of $YBa_2Cu_3O_{6.6}$, where one would expect the dynamical stripes to orient themselves along one of the axis, however, exhibit a strong anisotropy in the response only at energies below the resonance[19] while the response is fourfold rotationally symmetric at higher energies.[20] This may indicate that the formation of stripe correlations, be it static or dynamic, is a low-energy phenomenon while the high-energy response probes itinerant antiferromagnets at length scales on which the stripes are essentially invisible. Another extremely appealing feature of the experiment by Tranquada *et al.*[13] is that it immediately suggests a model of ferromagnetically coupled two-leg ladders, as the upper part of the measured spectrum agrees strikingly well with the triplon (or spinon-spinon bound state) mode of isolated two-leg ladders [see Fig. 1(b)]. The experiment hence appears to point bond-centered rather than site-centered stripes [i.e., stripes as depicted in Fig. 2(a) rather than Fig. 2(b)] and thereby to resolve a long outstanding issue within the field of static stripes.

This interpretation received support by theoretical studies.[21–23] Vojta and Ulbricht[21] used a bond operator formalism[24] to study a spin-only model of coupled two-leg ladders [as depicted in Fig. 2(a)] with $J_{\|}=J$, took into account a bond-boson renormalization of J, and assumed a value J' for the ferromagnetic (FM) coupling between the ladders which is large enough to close the spin gap of the ladders, i.e., to induce long-range magnetic order. Within their approximations, a value of $J'=-0.06J$ is sufficient. This value is not consistent with previous studies,[25–27] but as no method to calculate or even estimate the true J' induced by charge stripes was available, it did not seem a problem at the time. The spectrum they obtained agrees well with experimental data measured by Tranquada *et al.*[13] and hence appeared to justify their assumptions *a posteriori*. They concluded in favor of bond-centered stripes. This conclusion was independently strengthened by Uhrig *et al.*,[22] who used the method of continuous unitary transformations to study a model of ferromagnetically coupled two-leg ladders and observed that the critical value of J'_c can be significantly reduced if a cyclic exchange term J_{cyc} on the ladders is included.[28] They likewise fine-tuned J' to the QCP where the gap closes and long-range magnetic order ensues and reported good agreement with experiment. Seibold and Lorenzana[29,30] calculated the magnetic response for a range of dopings within the time-dependent Gutzwiller approximation and found good agreement with the measured data for both bond- and site-centered stripe models.

II. NUMERICAL EVALUATION OF INTERLADDER COUPLINGS

The first question we wish to address here is whether the key assumption that J' is large enough to induce order is valid. There exist several estimates for the critical value J'_c required if the coupling between isotropic ladders is antiferromagnetic. Gopalan *et al.*[25] found $J'_c \approx 0.25J$ in a simple mean-field treatment of bond bosons. Quantum Monte Carlo (QMC) calculations by Tworzydło *et al.*[26] yielded $J'_c = 0.30(2)J$, a value subsequently confirmed by Dalosto and Riera.[27] We have redone the mean-field calculation of Gopalan *et al.*[25] for FM couplings $J'_c < 0$ and find that within this approximation, the absolute value of J'_c is independent of the sign of the coupling. QMC calculations by Dalosto and Riera,[27] however, indicate that the true value is at least $J_c = -0.4J$ [see Fig. 6b of their article]. The physical reason why a significant coupling between the ladders is required to induce magnetic order is that the individual two-leg ladders possess a gap of order $\Delta \approx J/2$. As a cyclic exchange term $J_{cyc} \approx 0.25J$ reduces this gap by a factor of two,[28] we would expect that J'_c would likewise be reduced by a factor of two. We hence conclude that a FM coupling of at least somewhere between $J'_c = -0.2J$ and $-0.4J$ is required, depending on the strength of a possible cyclic exchange term.

The explicit calculation of the ferromagnetic coupling induced by the charge stripes between the spin stripes we describe below, however, yields $J' = -0.05J$. The coupling is hence insufficient to induce order in a model of bond-centered stripes.

For a model of site-centered stripes described by antiferromagnetically coupled three-leg ladders, as shown in

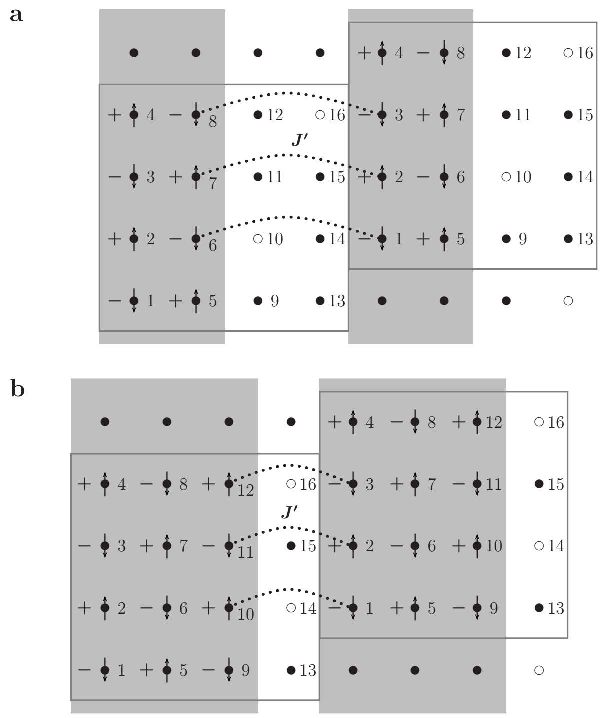

FIG. 3. Finite-size geometries with unfrustrated periodic boundaries for (a) bond-centered and (b) site-centered stripe models. The spin stripes are localized by a staggered magnetic field B as indicated by the signs in the gray shaded areas.

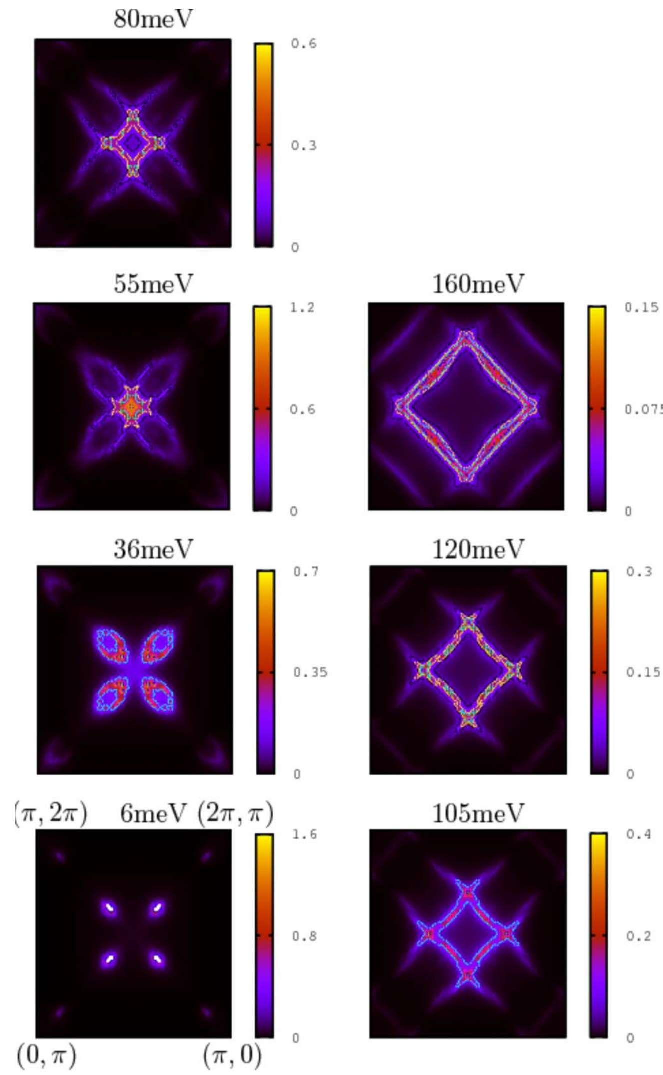

FIG. 4. (Color online) Constant energy slices of the neutron-scattering intensity $\chi^{+-}(\boldsymbol{k},\omega)$ for the lowest mode of the SWT with $J=140$ meV and $J'=0.07J$. We have replaced the δ functions in frequency by Lorentzians with half width $\Delta=0.05J$ and averaged over both stripe orientations (i.e., horizontal and vertical).

Fig. 2(b), the critical coupling required for long-range ordering to set in is by contrast $J'_c=0$. The reason is simply that there is no need to close a gap, as the three-leg ladders are individually gapless.[15] A conventional spin-wave analysis for such a spin-only model of three- and four-leg ladders was performed by Yao *et al.*,[31] who found that their approximation agrees reasonable well with the experimental data if they take $J'=0.05J$ and $J'=-0.09J$ for coupled three- and four-leg ladders, respectively. The calculation we present in the following, however, singles out $J'=0.07J$ for the antiferromagnetic coupling between spin stripes modeled by three-leg ladders.

To determine the effective coupling J' between the two- and three-leg ladders representing bond- or site-centered stripe, respectively, we have exactly diagonalized 16-site clusters of itinerant spin-1/2 antiferromagnets described by the (nearest-neighbor) *t-J* model[3] with $J=0.4t$, two holes, and periodic boundary conditions (PBCs), in which the stripes are localized through a staggered magnetic field B in the gray shaded areas shown in Figs. 3(a) and 3(b). We then compare the ground-state energies we obtain for clusters with the unfrustrated PBCs shown in Fig. 3 with the ground-state energies we obtain for clusters with frustrated PBCs, in which the 16-site unit cells shown on the right are shifted by one lattice spacing to the top, such that sites 15 and 1, 16 and 2, etc., are nearest neighbors. We then consider spin-only Heisenberg models of two- and three-leg ladders [consisting of only the sites in the shaded areas in Figs. 3(a) and 3(b)] subject to the same staggered field B and couple them ferromagnetically or antiferromagnetically by J', respectively, as indicated. We again compare the ground-state energies for unfrustrated PBCs, where J' couples sites 6 and 1, 7 and 2, etc., for the two-leg ladders shown in Fig. 3(a), with frustrated PBCs, where J' couples sites 7 and 1, 8 and 2, etc. Finally, we determine J' such that the difference in the ground-state energies between frustrated and unfrustrated PBCs in the *t-J* clusters matches this difference in the spin-only ladder models.

With $B=0.225J$ and $B=0.170J$ for the bond- or site-centered stripe models we obtain $J'=-0.051J$ and $J'=0.071J$, respectively. The values for B are chosen such that the magnetic localization energy $E_{\text{mag}}=-B\Sigma_i(-1)^i S_i^z$ is equal for both types of stripes, and such that the mean value of the staggered magnetization $\langle -S_1^z+S_5^z\rangle$ in the *t-J* cluster for the site-centered stripe matches the value we obtain in the spin-wave theory (SWT) of three-leg ladders described below. We estimate the error resulting from finite-size corrections and the use of a nearest-neighbor *t-J* model to be of order $\pm 0.01J$.

III. SPIN-WAVE THEORY OF THREE-SITE RUNGS

In the remainder of this paper, we will show, albeit not in full detail, that a fully consistent SWT of bond operators representing the eight-dimensional Hilbert spaces on each rung of the three-leg ladders agrees perfectly with the experimental data if and only if the correct, calculated value $J'=0.07J$ is used for the coupling. This discussion will complete our argument showing that the experiment by Tranquada *et al.*[13] provides evidence for site-centered, and not bond-centered, stripes.

To begin with, consider a single rung on sublattice $\mathcal{A}$ with three spins $\boldsymbol{s}_1$, $\boldsymbol{s}_2$, and $\boldsymbol{s}_3$, as indicated in Fig. 2(b). Diagonalization of the Hamiltonian $\hat{H}^{\mathcal{A}}=J(\hat{\boldsymbol{s}}_1\hat{\boldsymbol{s}}_2+\hat{\boldsymbol{s}}_2\hat{\boldsymbol{s}}_3)$ yields a spin doublet $\{|b_{-1/2}\rangle,|b_{1/2}\rangle\}$ with energy $E=-J$ and a quadruplet $\{|c_{-3/2}\rangle,|c_{-1/2}\rangle,|c_{1/2}\rangle,|c_{3/2}\rangle\}$ with $E=\frac{J}{2}$, both of which are symmetric under mirror reflection (interchange of sites 1 and 3), and another doublet $\{|a_{-1/2}\rangle,|a_{1/2}\rangle\}$ with $E=0$, which is antisymmetric under this mirror reflection. The subscripts in the kets label the eigenvalues of $\hat{s}^z_{\text{tot}}$. We define a fiducial state $|\tilde{b}_{-1/2}\rangle$ for sublattice $\mathcal{A}$ via $|\tilde{b}_{-1/2}\rangle\equiv|b_{-1/2}\rangle\cos\phi+|c_{-1/2}\rangle\sin\phi$, which interpolates between the $s^z_{\text{tot}}=-\frac{1}{2}$ quantum ground state $|b_{-1/2}\rangle$ of the isolated rung for $\phi=0$ and the classically Néel ordered state $|\downarrow\uparrow\downarrow\rangle$ for $\phi=\arctan(\frac{1}{\sqrt{2}})=0.6155$. We then introduce bosonic operators $a_0^\dagger\equiv|a_{-1/2}\rangle\langle\tilde{b}_{-1/2}|$, etc., as indicated in Fig. 2(c). Written in terms of these operators, the Hamiltonian $H^{\mathcal{A}}$ of a single rung will contain a linear term $\frac{3}{4}(c_0^\dagger+c_0)\sin 2\phi$. Finally, we introduce a similar formalism with operators $A_0^\dagger\equiv|a_{1/2}\rangle\langle\tilde{b}_{1/2}|$, etc., and a fiducial state $|\tilde{b}_{1/2}\rangle$ with $S^z_{\text{tot}}=+\frac{1}{2}$ for the rungs on sublattice $\mathcal{B}$ and express all the spin operators on all the individual sites in terms of the bosonic operators.

When we couple the rungs with intraladder couplings $J_\parallel=J$ and interladder couplings J' [see Fig. 2(b)], we keep terms up to quadratic order in the bosonic operators and adjust the angle ϕ introduced above such that the terms linear in the operators vanish. This yields $\phi=0.341$ for $J'=0.07J$. We introduce Fourier transforms of our bosonic operators into momentum space using the unit cell indicated by the gray area in Fig. 2(b) and rewrite the total Hamiltonian in terms of those. As the linear SWT preserves both the mirror-reflection symmetry and the total spin quantum number S^z, the Hamiltonian separates into several terms, $\hat{H}=\tilde{E}_0+\hat{H}_{a0}+\hat{H}_{c0}+\hat{H}_{a1}+\hat{H}_{c2}+\hat{H}_{b1,c1,c-1}$, where $\tilde{E}_0$ is a contribution to the ground-state energy, $\hat{H}_{a0}$ contains only the operators $a_0^\dagger$, a_0, $A_0^\dagger$, and A_0, and so on. The low-energy spectrum we are interested in is exclusively contained in

$$\hat{H}_{b1,c1,c-1}=\sum_{\boldsymbol{k}}\left[\hat{\Psi}_{\boldsymbol{k}}^\dagger H_{\boldsymbol{k}}\hat{\Psi}_{\boldsymbol{k}}-\frac{1}{2}\text{tr}(H_{\boldsymbol{k}})\right],$$

where $\hat{\Psi}_{\boldsymbol{k}}\equiv(B_{-1,\boldsymbol{k}},b_{1,\boldsymbol{k}}^\dagger,C_{-1,\boldsymbol{k}},c_{1,\boldsymbol{k}}^\dagger,C_{1,-\boldsymbol{k}}^\dagger,c_{-1,-\boldsymbol{k}})^{\text{T}}$ and $H_{\boldsymbol{k}}$ is a 6×6 matrix. We diagonalize $\hat{H}_{b1,c1,c-1}$ via a six-dimensional Bogoliubov transformation at each point in $\boldsymbol{k}$ space.

Cuts of the dispersion of the lowest mode we find are shown in Fig. 1(a). They agree strikingly well with the superimposed experimental data by Tranquada *et al.*[13] Constant energy slices of the neutron-scattering intensity $\chi^{+-}(\boldsymbol{k},\omega)$ of this mode, which may be compared to the data reported in Fig. 2 of Tranquada *et al.*,[13] are shown in Fig. 4. The other two modes of $H_{b1,c1,c-1}$, as well as all modes from the other terms in $\hat{H}$, are only weakly dispersing and start at energies of order $2J$, i.e., in a regime where we would no longer expect our spin-wave theory to yield reliable results.

Finally, let us remark that for $J'\lesssim 0.5J$, the saddle-point energy in our model is given to a highly accurate approximation by $\omega(\pi,\pi)\approx 1.47\sqrt{J'J}$. Since we expect J' to decrease with decreasing doping, we would expect a similar doping dependence for the saddle-point energy.[29,30]

IV. CONCLUSION

In conclusion, we have shown that models of coupled two-leg ladders describing bond-centered stripes cannot explain the magnetic spectrum of $La_{2-x}Ba_xCuO_4$ (Ref. 13) as the coupling induced by the charge stripes between the ladders is insufficient to induce long-range magnetic order. We have further shown that a model of coupled three-leg ladders describing site-centered stripes accounts accurately for the experimental data. The experiment hence provides evidence for site-centered, and not bond-centered, stripes.

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