Letter

## Magnon spectra of cuprates beyond spin wave theory

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The usual starting point for understanding magnons in cuprate antiferromagnets such as  $La_2CuO_4$  is a spin model incorporating cyclic exchange, which descends from a one-band Hubbard model, and has parameters taken from fits based on non-interacting spin wave theory. Here we explore whether this provides a reliable description of experiment, using matrix product states (MPS) to calculate magnon spectra beyond spin wave theory. We find that analysis based on low orders of spin wave theory leads to systematic overestimates of exchange parameters, with corresponding errors in estimates of Hubbard t/U. Once these are corrected, the "standard" model provides a good account of magnon dispersion and lineshape in  $La_2CuO_4$ , but fails to fully capture the continuum observed at high energies. The extension of this analysis to CaCuO<sub>2</sub> and Sr<sub>2</sub>IrO<sub>4</sub> is also discussed.

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Introduction. Cuprate perovskites, typified by La<sub>2</sub>CuO<sub>4</sub>, are an important class of magnetic insulators, providing some of the best examples of quasi-two-dimensional antiferromagnets [1], as well as being parent materials for high-temperature superconductors [2,3]. Early attempts to understand magnon spectra in La<sub>2</sub>CuO<sub>4</sub> rested on the antiferromagnetic (AF) Heisenberg model on a square lattice [4], as derived from a one-band Hubbard model in the limit  $t/U \rightarrow 0$ [5]. More detailed measurements of magnon dispersion at high energy revealed a dispersion on the magnetic Brillouin zone boundary which could not be understood in terms of a simple Heisenberg AF [6]. This lead to the adoption of a more complicated model, including four-spin cyclic exchange [6-12], derived from the same one-band Hubbard model at finite t/U [13–16]. Variants of this model have been also used to analyze magnon spectra in CaCuO<sub>2</sub> [17,18], SrCuO<sub>2</sub> [19], and Sr<sub>2</sub>IrO<sub>4</sub> [20–24].

To date, where such models have been compared with experiment, the analysis has mostly rested on linear spin wave theory (LSWT) [6,8–12], or LSWT with leading 1/S corrections [7]. However, low-order spin-wave approximations can show significant deviations from quantum calculations [25]. In related work on the Heisenberg AF [26–33], and its material instantiation Cu(DCOO)<sub>2</sub> · 4D<sub>2</sub>O (CFTD) [34–36], quantum effects missing from these theories were found to have a significant impact on zone-boundary magnons. Moreover, estimates of Hubbard t/U taken from spin wave fits in La<sub>2</sub>CuO<sub>4</sub> [6–9,11] and CaCuO<sub>2</sub> [17,18] are consistently higher than *ab initio* values [37–39]. For this reason, it is important to understand whether the model currently used to understand magnetism in La<sub>2</sub>CuO<sub>4</sub> provides a reliable

description of experiment. This question is particularly significant in the light of the ongoing efforts to understand superconductivity in doped cuprates [40]. Magnon spectra can provide important information about electronic interactions [6]. But to access this, it is necessary to disentangle effects arising from the spin-wave approximation.

The goal of this Letter is to explore how well the model commonly used to describe magnetic excitations in cuprate antiferromagnets [6-12] fits experiment, once quantum effects beyond spin wave theory are taken into account. To this end, we use numerical simulation based on matrix product states (MPS) [41–47] to explore the magnon spectra of cuprate materials. We make explicit comparison with experimental results for La<sub>2</sub>CuO<sub>4</sub>, obtaining fits to magnon dispersion and intensity, and estimating the corresponding value of t/Uwithin a one-band Hubbard model. We explore the errors which arise in analysis of experiment based on LSWT, and introduce a method of estimating t/U directly from magnon energies at high-symmetry points. We find good agreement with magnon dispersion and lineshapes in La<sub>2</sub>CuO<sub>4</sub>, with the exception of the high-energy continuum observed near  $\mathbf{q}_{x}$  =  $(\pi, 0)$  [9,12]. The analysis of magnon dispersion is extended to CaCuO<sub>2</sub> and Sr<sub>2</sub>IrO<sub>4</sub>, with consistent findings. Key results are summarized in Fig. 1. We draw two main conclusions: (i) that fits to magnon spectra based on LSWT have lead to systematic errors in estimates of exchange parameters in cuprate AF's; and (ii) that the model provides a good description of spin-wave excitations in cuprate AF's, but not of the continuum at high energies.

*Model.* The model we consider is the one commonly used to analyze magnon spectra in  $La_2CuO_4$  [6–10,12],

$$\mathcal{H}_{\sigma} = J_1 \sum_{\langle ij \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle ij \rangle_2} \mathbf{S}_i \cdot \mathbf{S}_j + J_3 \sum_{\langle ij \rangle_3} \mathbf{S}_i \cdot \mathbf{S}_j + J_c \sum_{\langle ijlk \rangle} [(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_j \cdot \mathbf{S}_k)(\mathbf{S}_l \cdot \mathbf{S}_i) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)], \qquad (1)$$

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FIG. 1. Magnon spectra of cuprate and iridate magnets, compared with predictions descended from a one-band Hubbard model. (a) Dispersion and intensity of excitations in La<sub>2</sub>CuO<sub>4</sub>, as found in calculations of  $S_{\perp}(\mathbf{q}, \omega)$  for the effective spin model  $\mathcal{H}_{\sigma}$  [Eq. (1)], using matrix product states (MPS), linear spin wave theory (LSWT), and interacting spin wave theory (LSWT + 1/S). Points show the results of inelastic neutron scattering (INS) experiments [9], with energy measured in units of the first-neighbor interaction  $J_1$ . (b) Equivalent results for CaCuO<sub>2</sub>, compared with results of resonant inelastic x-ray scattering (RIXS) [17]. (c) Results for Sr<sub>2</sub>IrO<sub>4</sub>, characterized using RIXS [22]. (d) Ratio of excitation energies at  $\mathbf{q}_{\Sigma} = (\pi/2, \pi/2)$  and  $\mathbf{q}_X = (\pi, 0)$ , showing scaling with  $J_c/J_1 \sim t^2/U^2$  [Eq. (5)]. (e) Parameters for La<sub>2</sub>CuO<sub>4</sub> reported in the experimental literature [6,8,9], and subsequent analysis using self-consistent spin wave theory (sc-SWT) [7] and modified spin wave theory (m-SWT) [11]. Results from this study are indicated with (\*). Where fits have been characterized using the one-band Hubbard model, values are quoted for t/U.

where exchange interactions on first, second, and thirdneighbor bonds, compete with four-spin terms originating in cyclic exchange [15,48,49]. The relevant interactions are illustrated in Fig. 2(a).

This spin model can in turn be derived from the one-band Hubbard model which provides the minimal description of  $La_2CuO_4$  [3]:

$$\mathcal{H}_{\mathsf{U}} = -t \sum_{\langle ij \rangle_1 \sigma} [c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{H.c.}] + U \sum_i c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} , \quad (2)$$

cf., Fig. 2(b). Within an expansion about half-filling [13–16], the corresponding exchange parameters are  $J_1 = 4t^2/U(1 - 6t^2/U^2)$ ,  $J_c = 20J_2 = 20J_3 = 80(t^4/U^3)$ .

Further details of this mapping are given [50]. In La<sub>2</sub>CuO<sub>4</sub>, *ab initio* estimates suggest that  $t/U \approx 0.1$  [37,38], and the four-spin interaction  $J_c$  is therefore a significant fraction of the first-neighbor exchange  $J_1$ . We use  $\mathcal{H}_{\sigma}$  [Eq. (1)], with parameters appropriate to the one-band Hubbard model  $\mathcal{H}_U$ , as the basis for all of the calculations in this Letter. Except where comparing to experimental data, we set  $\hbar = 1$ .

*Methods*. Matrix product states [42] provide a means of calculating ground-state and dynamical properties of quantum

systems, which is equally capable of describing the magnons associated with conventional magnetic order [33], and the fractionalized excitations found in quantum spin chains [52] and quantum spin liquids [45]. The calculations in this Letter were carried out for a square lattice wrapped onto a cylinder, and are not subject to any intrinsic bias, but are subject to corrections coming from from finite cylinder circumference and MPS bond dimension. Technical details, including an analysis of convergence, are provided in the Supplemental Material [50].

*Ground states.* We first use density matrix renormalization group (DMRG) [41,53] to determine the ground state of the effective spin model [Eq. (1)]. The Néel order found in La<sub>2</sub>CuO<sub>4</sub> has ordering vector  $\mathbf{q}_M = (\pi, \pi)$ , and is characterized by a staggered magnetization

$$m_s^2(\pi,\pi) = \frac{1}{N^2} \sum_{ij} e^{i(\pi,\pi) \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle .$$
(3)

In Fig. 2(c) we show results for  $m_s^2(\pi, \pi)$  as a function of t/U for infinite cylinders with circumference  $L_y = 4, 6, 8$ .



FIG. 2. Interactions and ground-state properties of model for magnetism in cuprate antiferromagnets. (a) Parameters of effective spin model  $\mathcal{H}_{\sigma}$  [Eq. (1)]. (b) Parameters of parent one-band Hubbard model  $\mathcal{H}_{U}$ . (c) Staggered magnetization squared,  $m_s^2(\pi, \pi)$ , found in calculations based on matrix product states (MPS), as a function of t/U, (and equivalently,  $J_c/J_1$ ). The corresponding Néel order is shown in an inset. (d) Equivalent results for  $m_s^2(\pi, \pi)$  in thermodynamic limit,  $L_y \to \infty$ . MPS results for the spin model are shown using triangles. Predictions  $\tilde{m}_s^2(\pi, \pi)$ , taking into account charge fluctuations [51], are denoted with squares. All calculations were carried out for  $\mathcal{H}_{\sigma}$  [Eq. (1)], on cylinders of circumference  $L_y$ .

Interpolating  $L_y \to \infty$  by  $m_s^2(\mathbf{q})|_L = m_s^2(\mathbf{q})|_\infty + a/L + b/L^2 + \mathcal{O}(1/L^3)$  (cf., e.g., [54]), we find that  $m_s(\pi, \pi)$  takes on a finite value for  $t/U \leq 0.2$ , and vanishes for larger values of t/U [Fig. 2(d)], consistent with published results [55]. Where comparing with experiment, it is also necessary to take into account charge fluctuations at  $\mathcal{O}(t^4/U^3)$  [51], which turns the magnetization into  $\tilde{m}_s = (1 - 2zt^2/U^2)m_s$ , where z = 4is the coordination number. Allowing for these, the staggered magnetization for  $t/U \leq 0.15$  is largely independent of t/U, and takes on a value of  $\tilde{m}_s(\pi, \pi) \approx 0.3$  [Fig. 2(d)]. Assuming isotropic  $g \approx 2$ , this translates into an ordered moment of ~0.6  $\mu_B$ , consistent with earlier theory for the Heisenberg AF [56,57], but somewhat higher than experimental estimates for La<sub>2</sub>CuO<sub>4</sub> [58].

*Excitation spectra.* We now turn to spin dynamics, which we calculate within the same MPS framework, using the time-dependent variational principle (TDVP) [43,44]. Since we are principally interested in magnon excitations, we concentrate on the transverse structure factor [59]

$$S_{\perp}(\mathbf{q},\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \sum_{\mathbf{r}_i} e^{i(\omega t - \mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j))} \\ \times \langle S_i^+(t) S_i^-(0) + S_i^-(t) S_i^+(0) \rangle.$$
(4)

In Fig. 1 we present results obtained for t/U = 0.102[Fig. 1(a)], t/U = 0.141 [Fig. 1(b)], and t/U = 0.154[Fig. 1(c)]. In all cases, energy is measured in units of  $J_1$ , and  $S_{\perp}(\mathbf{q}, \omega)$  has been convoluted with Gaussian envelope with  $\sigma_{\omega} \approx 0.072 J_1$ , such that an infinitely sharp excitation is rendered as Gaussian with FWHM = 0.17  $J_1$ . For comparison, we also show the results of linear spin-wave theory (LSWT), and a spin wave theory with leading interaction corrections (LSWT + 1/S) [50], calculated for the same parameter set.

TABLE I. Estimates of model parameters for square-lattice antiferromagnets, obtained using empirical scaling relation Eq. (5). Corresponding predictions for magnon spectra in La<sub>2</sub>CuO<sub>4</sub>, CaCuO<sub>2</sub>, and Sr<sub>2</sub>IrO<sub>4</sub> are shown in Figs. 1(a)-1(c).

	$E_{\Sigma}$ [meV]	$E_X$ [meV]	$J_c/J_1$ [Eq. (1)]	<i>t/U</i> [Eq. (2)]
CFTD [36]	13.3	14.5	0.0	0.0
$La_2CuO_4$ [9]	281	323	0.22	0.102
CaCuO <sub>2</sub> [17]	240	375	0.45	0.141
$Sr_2IrO_4$ [22]	110	205	0.55	0.154
SrCuO <sub>2</sub> [19]	191	362	0.56	0.155

The magnon dispersion found in MPS calculations shows clearly defined, linearly dispersing magnons approaching the ordering vector,  $\mathbf{q}_M = (\pi, \pi)$ . At higher energies, the dispersion is more complicated, and shows a progressive evolution as a function of t/U. Two trends stand out. The first of these is a reduction in the spin-wave velocity characterizing Goldstone modes for  $\mathbf{q} \rightarrow \mathbf{q}_M$ . The second is a softening of excitations at  $\mathbf{q}_{\Sigma} = (\pi/2, \pi/2)$ , relative to  $\mathbf{q}_X = (\pi, 0)$ . This effect is particularly marked for t/U = 0.154 [Fig. 1(c)]. For small t/U, LSWT + 1/S gives a reasonable account of magnon dispersion [Fig. 1(a)]. However, it fails to capture the softening at  $\Sigma$ , leading to significant deviations from MPS results at larger t/U [Fig. 1(c)].

These findings motivate us to introduce an empirical scaling relation for ratio of magnon energies,  $E_{\Sigma}/E_X$ . Expressing this in terms of the dominant interactions  $J_1$  and  $J_c$ , we find that the results of MPS calculations are well described by

$$J_c/J_1 \approx -E_{\Sigma}/E_X + 1.09 , \qquad (5)$$

as illustrated in Fig. 1(d). This result can easily be reexpressed in terms of t/U, and used to extract Hubbard model parameters from experimental measurements of  $E_{\Sigma}$  and  $E_X$ . The resulting estimates for CFTD [36], La<sub>2</sub>CuO<sub>4</sub> [9], CaCuO<sub>2</sub> [17], Sr<sub>2</sub>IrO<sub>4</sub> [22], and SrCuO<sub>2</sub> [19] are listed in Table I.

Application to La<sub>2</sub>CuO<sub>4</sub>. In Fig. 1(a) we present a comparison of the magnon spectra found in MPS calculations for t/U = 0.102, and inelastic neutron scattering experiments on La<sub>2</sub>CuO<sub>4</sub> [9]. Results are shown for both the dispersion, characterized by  $S_{\perp}(\mathbf{q}, \omega)$ , and the intensity of the magnon peak  $I(\mathbf{q}) = S_{\perp}(\mathbf{q}, E_{\mathbf{q}})$ , where  $E_{\mathbf{q}}$  is the associated magnon energy. We find excellent agreement for both quantities across the vast majority of the Brillouin zone. Nonetheless, for  $\mathbf{q} \approx$  $(\pi, 0)$ , the intensity measured in experiment shows a small, but systematic, reduction relative to simulation.

Turning to the magnon lineshape, in Fig. 3 we show a comparison between dynamical structure factor measured in INS and RIXS experiments, and calculated using MPS. In this case, results are shown for  $S(\mathbf{q}, \omega)$ , defined as

$$S(\mathbf{q},\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \sum_{\mathbf{r}_i} e^{i(\omega t - \mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j))} \langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle.$$
(6)

For  $\mathbf{q}_{\Sigma} = (\pi/2, \pi/2)$  [Fig. 3(a)], the majority of spectral weight is found in the magnon peak, and MPS results provide a good account of experiment. However, for  $\mathbf{q}_X = (\pi, 0)$  [Fig. 3(b)], a significant fraction of the spectral weight measured in experiment is found in a broad



FIG. 3. Comparison of excitations on the magnetic Brillouin Zone boundary, as found in simulations using matrix product state (MPS), and experiments on La<sub>2</sub>CuO<sub>4</sub>. (a) Dynamical structure factor  $S(\mathbf{q}, \omega)$  for  $\mathbf{q}_{\Sigma} = (\pi/2, \pi/2)$ , showing good agreement between MPS results for t/U = 0.102, inelastic neutron scattering (INS), and resonant inelastic x-ray scattering (RIXS) [12]. (b) Equivalent results for  $\mathbf{q}_X = (\pi, 0)$ , showing agreement on peak position and amplitude, but significant differences at high energy. (c) Evolution of  $S(\mathbf{q}_X, \omega)$  with increasing t/U, showing how spectral weight is redistributed from the high-energy tail found in the Heisenberg model [t/U = 0], to lower energies. All MPS simulations were carried out for Eq. (1), with maximum bond dimension  $\chi = 800$ , and energy resolution 0.13  $J_1$ , comparable to experiment.

high-energy continuum [9,10,12,60,61], which has been discussed as potential evidence for spinon excitations [10,31,62]. While MPS calculations for the effective spin model, Eq. (1), correctly reproduce the dispersion for  $\mathbf{q} \approx \mathbf{q}_X$ , they do not reproduce the lineshape seen in experiment. What distinguishes them is the continuum at high energies, which manifests as a broad, highly asymmetric peak in experiment, and as a weaker, high–energy tail in simulation.

Calculations of  $S(\mathbf{q}, \omega)$  for the Heisenberg AF [Eq. (1),  $\lim t/U \to 0$ ], find a "roton minimum" in the magnon dispersion at  $\mathbf{q}_X = (\pi, 0)$  [27,28,30], accompanied by significant spectral weight at high energies [31,33,36,63]. We have confirmed that our calculations are consistent with published MPS results for the Heisenberg AF [33]. However, with increasing t/U, we find that  $S(\mathbf{q}_X, \omega)$  exhibits a transfer of spectral weight from high to lower energies [Fig. 3(c)], leading to the result shown in Fig. 3(b). These calculations do not, by themselves, resolve whether the high-energy continua observed in La<sub>2</sub>CuO<sub>4</sub>, CaCuO<sub>2</sub>, and CFTD originates in fractionalized excitations. However, since MPS results are robust against changes in bond dimension, cylinder circumference, and cylinder geometry [50], we infer that the disagreement between experiment and simulation for  $\mathbf{q} \approx \mathbf{q}_X$  [Fig. 3(b)] cannot be explained using Eq. (1). We return to this point below.

Application to CaCuO<sub>2</sub>. The infinite-layer cuprate CaCuO<sub>2</sub> is believed to exhibit particularly large cyclic exchange [17,18,64]. In Fig. 1(b) we show magnon spectra found in MPS calculations for t/U = 0.141, as compared with RIXS experiments on the CaCuO<sub>2</sub> [17]. Setting  $J_1 = 172$  meV, we find reasonable agreement for the dispersion at high energies. At low energies, the RIXS spectra show a gap at  $\mathbf{q} = \Gamma$ , which has been attributed to interlayer coupling [17]. Since this is not included in our model, comparison is difficult. However, the overall distribution of intensity  $I(\mathbf{q})$  shows good agreement with experiment, except near  $\mathbf{q}_X = (\pi, 0)$ , where experiment shows a significant high-energy continuum, similar to that found in La<sub>2</sub>CuO<sub>4</sub>. RIXS data for CaCuO<sub>2</sub> have previously been fitted using LSWT [17], leading to an estimate t/U = 0.194, which places CaCuO<sub>2</sub> near the limits of stability of  $(\pi, \pi)$  Néel order [Fig. 2(d)]. As in La<sub>2</sub>CuO<sub>4</sub>, MPS results suggest that this is a significant overestimate, cf., Fig. 1(d).

Application to Sr<sub>2</sub>IrO<sub>4</sub>. The quasi-two-dimensional antiferromagnet Sr<sub>2</sub>IrO<sub>4</sub> provides an interesting counterpoint to La<sub>2</sub>CuO<sub>4</sub>, since it has a similar phenomenology [22,65], but is known to exhibit strong spin-orbit coupling, with Ir<sup>4+</sup> moments having the character j = 1/2 [66,67]. In Fig. 1(c) we show comparison of RIXS data for Sr<sub>2</sub>IrO<sub>4</sub> [22] with MPS calculations for t/U = 0.154, setting  $J_1 = 96$  meV [65]. We find excellent agreement for dispersion and intensity of magnon excitations across the entire Brillouin zone, consistent with the idea that Sr<sub>2</sub>IrO<sub>4</sub> can be described by a one-band Hubbard model [68]. However, it should be noted the RIXS data shown in Fig. 1(c) does not have sufficiently high resolution to probe any gap at  $\mathbf{q}_M = (\pi, \pi)$  coming from terms breaking spin-rotation symmetry [24].

*Limitations of LSWT*. Spin wave theory (SWT) remains an important tool for interpreting magnon spectra in experiment [6,7,9,10,12,17,22]. Relative to MPS, fits based on low orders of spin wave theory lead to systematic overestimates in values of parameters [Fig. 1(e)]. This follows from two effects: first that the spin model, Eq. (1), is underconstrained, and second that corrections to LSWT from quantum fluctuations are of the same scale as those coming from subleading interactions.

While Eq. (1) has four parameters  $(J_1, J_2, J_3, J_c)$ , magnon spectra for La<sub>2</sub>CuO<sub>4</sub> are well described by LSWT calculations for an effective model with only two parameters: an AF interaction  $J_1^{\text{eff}}$  on first-neighbor bonds, and a FM interaction  $J_2^{\text{eff}}$  on second-neighbor bonds [8]. In [50] we show how such a two-parameter model can be derived from Eq. (1), and parametrized from a one-band Hubbard model, within the lowest order of interacting SWT (LSWT + 1/S). However, in order to mimic the softening of magnon dispersion at  $\mathbf{q}_{\Sigma} = (\pi/2, \pi/2)$  by quantum fluctuations, t/U must be made artificially large. And this in turn leads to significant errors in estimates of  $(J_2, J_3, J_c)$  [Fig. 1(e)].

In the case of La<sub>2</sub>CuO<sub>4</sub>, fits based on LSWT overestimate  $J_2$ ,  $J_3$ , and  $J_c$  by ~100% [Fig. 1(e)]. Including 1/S corrections reduces this error to  $\gtrsim$ 40%. Systematic calculations of higher-order corrections [57,69–72] are currently lacking for any realistic model of La<sub>2</sub>CuO<sub>4</sub>. However, recent calculations for Eq. (1) within a modified spin wave theory, compare

well with MPS results, at the expense of a more complicated formalism [11].

What is missing from the spin model? If we take the disagreement between experiment and simulations at face value [Fig. 3(b)], we are obliged to ask what is missing from our model of magnetism in La<sub>2</sub>CuO<sub>4</sub>? One possibility is that the one-band Hubbard model [Eq. (2)] remains valid, but that charge fluctuations at high order in t/U modify the spin dynamics. To rule this out, it would be necessary to calculate directly from the Hubbard model, which is beyond the scope of the present work. Alternatively, the Hubbard model itself might need modification. The simplest extension would be hopping t' on second-neighbor bonds [73], a term which has been argued to play an important role in superconductivity [74,75]. Further refinements include spin-orbit coupling [76–79], generalization to a three-band model [40,80,81], or coupling to phonons. To distinguish between these alternatives, it may also be necessary to revisit experiment. We leave these as questions for future work.

Summary and conclusions. In this Letter, we have used calculations based on matrix product states (MPS) to characterize the magnon spectra of cuprate materials, starting from the model commonly used to fit experiments: an effective spin model with four-spin exchange [Eq. (1)], which descends from a one-band Hubbard model [Eq. (2)]. We have made explicit comparison with experimental results for La<sub>2</sub>CuO<sub>4</sub> [Fig. 1(a)], CaCuO<sub>2</sub> [Fig. 1(b)], and Sr<sub>2</sub>IrO<sub>4</sub> [Fig. 1(c)], finding generally good agreement with the measured magnon dispersion throughout the Brillouin zone. We also find good agreement for magnon lineshape, except near  $\mathbf{q}_X = (\pi, 0)$ , where experiment reveals a high-energy continuum which is not well described by simulations [Fig. 3(b)]. We estimate

the ratio t/U that characterizes a one-band Hubbard in each case (Table I), finding values which are systematically lower than those obtained in published fits to linear spin wave theory (LSWT). We also introduce a method of estimating t/U directly from measured magnon energies at  $\mathbf{q}_X = (\pi, 0)$  and  $\mathbf{q}_{\Sigma} = (\pi/2, \pi/2)$  [Fig. 1(d)].

These results suggest two main conclusions. First, that fitting the magnon dispersion using linear spin-wave theory leads to systematic errors in estimates of in values of exchange parameters, and corresponding overestimates of t/U. And second, that, suitably parametrized, the "standard" model describes some, but not all of the properties of the magnon spectrum in cuprate antiferrimagents, providing a good overall account of dispersion, but failing to capture the continuum observed at high energies.

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