

Elementary excitations for the two-dimensional quantum Heisenberg antiferromagnet

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The excitation spectrum of the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg Hamiltonian $H = \sum J \hat{S}_i \cdot \hat{S}_j$ on $L \times L$ lattices is evaluated by a projector quantum Monte Carlo method. These results suggest that the exact spectrum for the finite lattice is $\omega_k \simeq Z(L)\omega_k^{\text{SW}}$, for all \mathbf{k} , where $\omega_k^{\text{SW}} = 4JS\sqrt{1-\gamma_k^2}$ with $\gamma_k = (\cos k_x + \cos k_y)/2$ is from linear-spin-wave theory. We find $Z(L) = Z_E + B/L^3$, leading to $Z_E = 1.21 \pm 0.03$ for $L = \infty$. A comparison with experiments on La_2CuO_4 is discussed.

I. INTRODUCTION

Largely because of its relevance for high- T_c superconductors, the two-dimensional Heisenberg antiferromagnetic Hamiltonian

$$H = \sum_{\langle ij \rangle} J \hat{S}_i \cdot \hat{S}_j, \quad J > 0, \quad (1)$$

has been extensively studied recently.¹⁻¹³ However, there remains considerable uncertainty about the excitation spectrum for (1).

The most common approximation to (1) is linear-spin-wave (SW) theory,¹⁴ which for one dimension (1D) leads to

$$\omega_k^{\text{SW,1D}} = J |\sin(ka)| \quad (2)$$

and for two dimensions leads to

$$\omega_k^{\text{SW}} = 4JS(1 - \gamma_k^2)^{1/2}, \quad (3a)$$

where

$$\gamma_k = [\cos(k_x a) + \cos(k_y a)]/2. \quad (3b)$$

For the one-dimensional case, the exact spectrum is solved by using the Bethe ansatz,¹⁵ giving

$$\omega_k^{\text{1D}} = Z_E^{\text{1D}} \omega_k^{\text{SW,1D}}, \quad (4)$$

where

$$Z_E^{\text{1D}} = \frac{\pi}{2} = 1.57.$$

Thus spin-wave theory leads to results low by 36%, but the *shape* of the spectrum is exactly correct. Unfortunately, for 2D and higher, there has been no general solution of (1).

In this paper we calculate numerically the exact spectrum for 2D periodic $L \times L$ lattices ($L = 4, 6, 8, 12$). Extrapolated to $L = \infty$, these results lead to

$$\omega_k \simeq Z_E \omega_k^{\text{SW}} = Z_E [4JS(1 - \gamma_k^2)^{1/2}], \quad (5)$$

where $Z_E = 1.21 \pm 0.03$. Thus, for 2D, the shape of the lowest excitation spectrum is also the same as for spin-wave theory, but the renormalization factor is 1.21 rather than 1.57.

II. METHOD

To calculate the eigenstates of (1), we use the quantum projector Monte Carlo^{16,17} (PMC) method for finite $L \times L$ lattices and extrapolated to $L = \infty$. The basic idea of the PMC method is to start with trial functions ϕ, ψ (not orthogonal to the ground state) and to apply the *projector* $\exp(-\tau H)$ on ϕ for a sufficient time τ such that the wave function $\exp(-\tau H)\phi$ is a good approximation to the ground-state wave function. The ground-state energy is then computed as

$$E(0) = \langle \psi | H e^{-\tau H} | \phi \rangle / \langle \psi | e^{-\tau H} | \phi \rangle \quad (6a)$$

and the excitation energy is computed as

$$E(k) = \frac{\langle \psi | R(-\mathbf{k}) H e^{-\tau H} R(\mathbf{k}) | \phi \rangle}{\langle \psi | R(-\mathbf{k}) e^{-\tau H} R(\mathbf{k}) | \phi \rangle}, \quad (6b)$$

where the $R(\mathbf{k})$ operator projects out the states with definite momentum \mathbf{k} from a mixed wave function. Takahashi has used such a momentum operator in 1D.¹⁷ Here we extend it to the 2D case

$$R(\mathbf{k}) = \sum_r (\hat{S}_r^z - S) e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (7)$$

where \hat{S}_r^z is the spin- $\frac{1}{2}$ operator at site $\mathbf{r} = (r_x, r_y)$ and the sum is over the L^2 sites in the periodic lattice.

A. Phase convention

The Hamiltonian (1) has non-negative off-diagonal matrix elements, making the PMC method inapplicable. Thus we make a unitary transformation^{11,17}

$$U = \exp \left[i\pi \sum_r \hat{S}_r^z \right],$$

where the sum is over alternate sites. This flips the x, y components of spins on alternative sites,

$$U H U^{-1} = J \sum_{\langle ij \rangle} (-S_i^x S_j^x - S_i^y S_j^y + S_i^z S_j^z)$$

(i.e., the x, y terms change signs). Consequently, all off-diagonal elements become nonpositive and the PMC method is applicable. This does not change any observables, but the momentum of wave functions are shifted by

$$UT_x U^{-1} = e^{i\pi(L^2 S - M_z)} T_x,$$

$$UT_y U^{-1} = e^{i\pi(L^2 S - M_z)} T_y,$$

where $M_z = \sum_i S_i^z$ is a conserved quantity and $S = \frac{1}{2}$. Since L is an even number in our calculation and the lowest state is in $M_z = 0$ subspace, there is no momentum shift. In two dimensions all $L \times L$ (L even) antiferromagnetic system have $\mathbf{k} = (0, 0)$ as the ground states.

B. Partitioning of the Hamiltonian

The trial wave function ϕ is the sum

$$|\phi\rangle = \sum_{m=1}^C w_m |m\rangle, \quad (8)$$

where the spin state $|m\rangle$ is a product of L^2 one-spin eigenstates of \hat{S}_i^z for an $L \times L$ system and where $C \sim 10^6$ is the number of walkers which jumps from one-spin state to another in the calculation. The total number of spin states for the $L \times L$ system (with $M_z = 0$) is the binomial coefficient

$$C_{\max} = \binom{L^2}{\frac{1}{2}L^2} \simeq \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{L} 2^{L^2}$$

(for $L = 8$ this is 2×10^{18}). Thus C is much smaller than C_{\max} . Applying the projector, the ground-state wave function is approximated by

$$e^{-\tau H} |\phi\rangle = \sum_m w_m(\tau) |m(\tau)\rangle. \quad (9)$$

As the computation evolves from τ_n to τ_{n+1} , each walker m evolves from spin state $|m(\tau_n)\rangle$ to spin state $|m(\tau_{n+1})\rangle$ according to the propagator $e^{-\Delta\tau H}$.

A problem here is that the $2L^2$ terms in the Hamiltonian do not commute. To simplify the calculations, we decompose H into four sub-Hamiltonians¹¹

$$H = H_1 + H_2 + H_3 + H_4, \quad (10)$$

where each H_s has $L^2/2$ terms that commute among themselves (see Fig. 1):

$$H_1/J = \hat{S}_{11} \cdot \hat{S}_{21} + \hat{S}_{12} \cdot \hat{S}_{22} + \dots,$$

$$H_2/J = \hat{S}_{21} \cdot \hat{S}_{31} + \hat{S}_{22} \cdot \hat{S}_{32} + \dots.$$

Using (10), we can write $e^{-\Delta\tau H}$ as

$$e^{-\Delta\tau(H_1 + H_2 + H_3 + H_4)}$$

$$= e^{-\delta_4 H_1} e^{-\delta_2 H_2} e^{-\delta_4 H_1} e^{-\delta_4 H_3} e^{-\delta_2 H_4} e^{-\delta_4 H_3}$$

$$\times e^{-\delta_4 H_4} e^{-\delta_2 H_3} e^{-\delta_4 H_4} e^{-\delta_4 H_2} e^{-\delta_2 H_1} e^{-\delta_4 H_2}$$

$$+ O((\Delta\tau)^3), \quad (11)$$

where $\delta_2 = \Delta\tau/2$, $\delta_4 = \Delta\tau/4$. Because the $L^2/2$ terms in each H_s commute among themselves, the propagator $e^{-\delta H_s}$ factors into a product of $L^2/2$ two-spin transfer matrices, each of which can be further decomposed into a product of two matrices,^{16,17}

$$\langle S_{i,\tau_n}^z S_{j,\tau_n}^z | e^{-\delta S_i \cdot S_j} | S_{i,\tau_{n+1}}^z S_{j,\tau_{n+1}}^z \rangle = p_{\alpha\beta} q_{\beta}, \quad (12a)$$

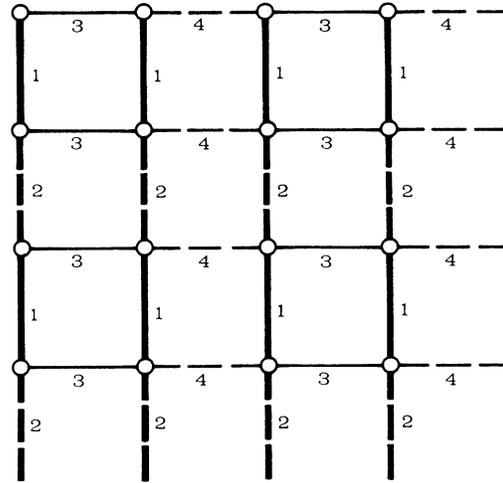


FIG. 1. Decomposition of H into $H_1 + H_2 + H_3 + H_4$. H_1 contains all the bonds denoted by 1 and similarly for H_2, H_3, H_4 .

where $\sum_{\alpha} p_{\alpha\beta} = 1$. The transition matrix \mathbf{p} changes the two-spin state from β to α with probability $p_{\alpha\beta}$. The diagonal matrix q contributes to the weight multiplicatively,

$$w_j(\tau_{n+1}) = \left[\prod_{j=1}^{12} \prod_{\beta=1}^{(1/2)L^2} q_{\beta} \right] w_j(\tau_n), \quad (12b)$$

where j is over the 12 factors in (11).

C. Redistribution

One application of $e^{-\Delta\tau H}$ contributes $6L^2$ factors to each weight [cf. Eq. (12b)]. Successive applications of $e^{-\Delta\tau H}$ thus lead to large increases in some w_m and large decreases in others, resulting in orders of magnitude differences in w_m for different walkers. As a result, the wave function ϕ_{τ} becomes quickly dominated by a few walkers having very large weights, leading to an effective reduction of the sampling space. To solve this problem, we periodically *redistribute* the weights to obtain a new set of C walkers equivalent to the existing set, but with equal weight.^{17,18} In this way walkers with very small weights are eliminated and those with large weights multiply in number. For the 8×8 lattice, we find it necessary to redistribute about every two applications of $e^{-\Delta\tau H}$.

D. Contraction

A second issue is the choice of the *contraction* function ψ in Eq. (6). One common choice¹⁶ is setting $\psi = \phi$. However, we find that it is important to use the *all-states* function

$$|\psi\rangle_{\text{all}} = \sum_{\text{all states}} |m\rangle. \quad (13)$$

The reason is that $\langle m_1 | H | m_2 \rangle$ is very sparse. Using $\psi = \phi$ would lead to very few nonzero off-diagonal contributions, resulting in large fluctuations in energies. The all-states function of (13) guarantees that each term of ϕ

will make nonzero off-diagonal contributions. In addition, since ψ has the same coefficient for all possible states, we need not store ψ , nor do we need to search ψ for the corresponding spin state once $H|m\rangle$ is generated.

Another significant advantage of the all-states choice is that with ψ independent of ϕ , we can *coherently* add the contributions from independent runs:

$$\frac{\langle \psi | H | \phi_1 + \phi_2 \rangle}{\langle \psi | \phi_1 + \phi_2 \rangle} = \frac{\langle \psi | H | \phi_1 \rangle + \langle \psi | H | \phi_2 \rangle}{\langle \psi | \phi_1 \rangle + \langle \psi | \phi_2 \rangle}. \quad (14)$$

Typically, we do 500 such independent runs. Thus, from each run ϕ_i , we need only accumulate the two numbers $\langle \psi | H | \phi_i \rangle$ and $\langle \psi | \phi_i \rangle$ from different runs until sufficient accuracy is obtained. With the other choice of $\psi = \phi$, the coherent average would require evaluation of cross terms $\langle \phi_1 | H | \phi_2 \rangle, \langle \phi_1 | \phi_2 \rangle$; this would require storing 500 wave functions each with 50 000 terms and would require evaluating 50 000² matrix elements.

E. Procedure

The calculation of E_0 and $E(\mathbf{k})$ is done simultaneously for all values of \mathbf{k} . We start with an initial function ϕ randomly chosen and propagate according to (9), (11), and (12) to approximate the ground-state wave function ϕ_0 . We allow this relaxation of the initial ϕ for 100 time steps ($\tau_0 = 100\Delta\tau$), during which the redistribution is applied every 5 steps (for a 8×8 lattice).

Next, we apply the following process of $\tau_1 + \tau_2$ steps many times until convergence is reached. During the τ_1 process ($\approx 50\Delta\tau$ steps), the function ϕ_0 is relaxed with a more frequent redistribution of every two steps. At the beginning of the next τ_2 process ($\approx 20\Delta\tau$ steps), we compute the phase factors

$$R(\mathbf{k}, m) = \langle m(\tau') | R(\mathbf{k}) | m(\tau') \rangle.$$

$R(\mathbf{k}, m)$ remains associated with the m th walker, although the walker may well possibly walk into different spin state $|m(\tau)\rangle$. With each set of the phase factors $\{R(\mathbf{k}, m), m = 1, 2, \dots, C\}$ for a momentum \mathbf{k} , the corresponding wave function is constructed as

$$\phi(\mathbf{k}) \equiv e^{\tau H} R(\mathbf{k}) | \phi \rangle = \sum_m w_m(\tau) R(\mathbf{k}, m) | m(\tau) \rangle, \quad (15a)$$

and $E(\mathbf{k})$ is evaluated every two steps. (This is very similar to the *forward walking* in the Green-function Monte Carlo method.¹⁹) At the end of the τ_2 process, we take the current wave function as the starting wave function of the next $\tau_1 + \tau_2$ process. We found that τ_2 cannot be too large because ϕ_0 is not exact ground-state wave function at the beginning of the τ_2 process when $R(\mathbf{k}, m)$ is calculated. The τ_1 process separates the τ_2 process so that the consecutive measurements of E_0 and $E(\mathbf{k})$ are less correlated.

We calculated the excited states for $L = 4, 6,$ and 8 using $C = 4000, 64\,000,$ and $128\,000$, respectively. In each case the ϕ was chosen to have a total spin projection component (M_z) of zero. We found that $\Delta\tau = 0.1$ leads to accurate results (e.g., tests on $L = 4$ and 6 using $\Delta\tau = 0.05$ lead to energies differing by less than 0.5%). In

TABLE I. $E(k_x, k_y)/J$ for all momentum on the 4×4 lattice. The exact results are from Ref. 4. The statistical uncertainties are indicated in parentheses.

k_x, k_y	Exact	PMC
0,0	-11.2285	-11.228(11)
$0, \frac{\pi}{2}$	-8.7944	-8.749(12)
$0, \pi$	-8.5183	-8.510(20)
$\frac{\pi}{2}, \frac{\pi}{2}$	-8.5183	-8.506(17)
$\frac{\pi}{2}, \pi$	-8.8864	-8.909(17)
π, π	-10.6499	-10.63(4)

all cases the coherent averages were carried out on the $\tau_1 + \tau_2$ process for 500 repetitions. As a test, we computed the spectrum on a 4×4 lattice and compared with the exact results from direct diagonalization⁴ in Table I. The agreement is excellent.

We found that the ground-state energy converges quickly, leading to accurate results up to $L = 12$. [This is a singlet spin state ($\hat{S}^2\Psi = 0$) for the L^2 spin system.] The excited-states energies are much more difficult to calculate for large lattices, and the excited-state spectrum for $L \geq 10$ did not converge well. [In each case the excited state is a triplet spin state $\hat{S}^2\Psi = 2\Psi$.] Probably, the large configuration space ($\sim 10^{42}$ for $L = 12$) requires a substantially larger number of walkers or a larger number of runs in the coherent average. Another difficulty in obtaining the spectrum $\omega_k = E(k) - E_0$ is the subtraction of two large numbers. Both $E(k)$ and E_0 are extensive quantities proportional to the area of the system L^2 , whereas their difference remains a constant (very weakly dependent on the sizes). For an 8×8 lattice, $E_0 = -43.03 \pm 0.05J$, while ω_k is about $1J$. Consequently, to obtain an accuracy of 5% error in ω_k requires an accuracy of 0.1% error in $E(k)$ and E_0 . Considering the Monte Carlo (MC) nature of our method, this is a rather stringent requirement. The coherent addition mentioned above [cf. Eq. (14)] is critical to obtain reasonably accurate results.

The program was developed on a parallel supercomputer, the 64-node Caltech/JPL MarkIIIIfp Hypercube.²⁰ Each node contains a fixed number ($C/64$) of spin states. Application of $e^{-\Delta\tau H}$ is carried out locally on each node. However, redistribution must be done globally because the weights on one processor will influence the redistribution of walkers on other processors. We have devised an efficient algorithm for this redistribution which for $C = 64\,000$ takes only 15% of the total time. For $C = 64\,000$ the total time for one $\Delta\tau$ step in the 64-node hypercube is 4 sec. In comparison, the same code (written in C) running on a one-processor Cray XMP (at JPL) is 20 sec. Thus the hypercube is about 5 times faster.

III. RESULTS AND ANALYSIS

The calculated ground-state energy density (energy per atom) $E(0, L)/L^2$ is shown in Fig. 2(a) for $L = 4 - 12$. We find that $E(0, L)/L^2$ is very accurately fitted by

$$E(0,L)/L^2 = e_0 + B/L^3,$$

as indicated in Fig. 2(a). This fit ($B = -2.17 \pm 0.04$) gives the ground-state energy per site of the infinite system,

$$e_0 = (-0.668 \pm 0.001)J, \quad (15b)$$

in good agreement with other calculations. The Green-function MC results^{6,7} are $e_0 = -0.6692(2)$ and the world-line MC results are $e_0 = -0.670(1)$,⁵ $-0.6661(2)$,¹⁰ and $-0.6693(2)$.¹² (See Ref. 13 for more complete review.)

The point $\mathbf{k}a = (\pi, \pi)$, is of special interest. This state is a spin-triplet state, whereas the ground state $(0,0)$ is a spin-singlet state. In spin-wave theory the (π, π) and $(0,0)$ states are degenerate. Similarly in 1D the state $\mathbf{k}a = \pi$ is degenerate, with $\mathbf{k} = 0$ for both spin-wave theory and the exact energy. However, for finite L , $\mathbf{k} = (\pi, \pi)$ has an energy higher than $\mathbf{k} = (0,0)$ by

$$\Delta = E(\pi, \pi) - E_0 > 0. \quad (16)$$

This gap decreases with L , and we find that the gap goes to zero^{7,10,21} as

$$\Delta \approx \frac{A}{L^2}, \quad (17)$$

where $A = 9.26$ [see Fig. 2(b)]. The triplet state (π, π) is difficult to calculate directly in $M_z = 0$ subspace. We instead obtain $E(\pi, \pi)$ as the lowest energy for in the $M_z = 1$ subspace.

Our goal is to obtain an analytical expression of the spectrum for $\omega_{\mathbf{k}}$ for the infinite lattice. In principle, for each fixed (k_x, k_y) , one could compute $\omega_{\mathbf{k}}$ on a series of lattices and then extrapolate to the infinite lattice. However, this is difficult to implement because each $L \times L$ lattice leads to a different set of discrete momenta (k_x, k_y) with few in common. Here we use the alternative approach of finding an analytical expression which fits the data for each finite lattice and then extrapolating the fitting parameter to the infinite lattice.

As discussed in the Introduction, for 1D the linear-spin-wave spectrum has the same analytical form as the exact spectrum except for a scaling or renormalization constant $Z_E^{1D} = 1.57$. Motivated by this result, we factor the finite-size dependence for the 2D system into the form

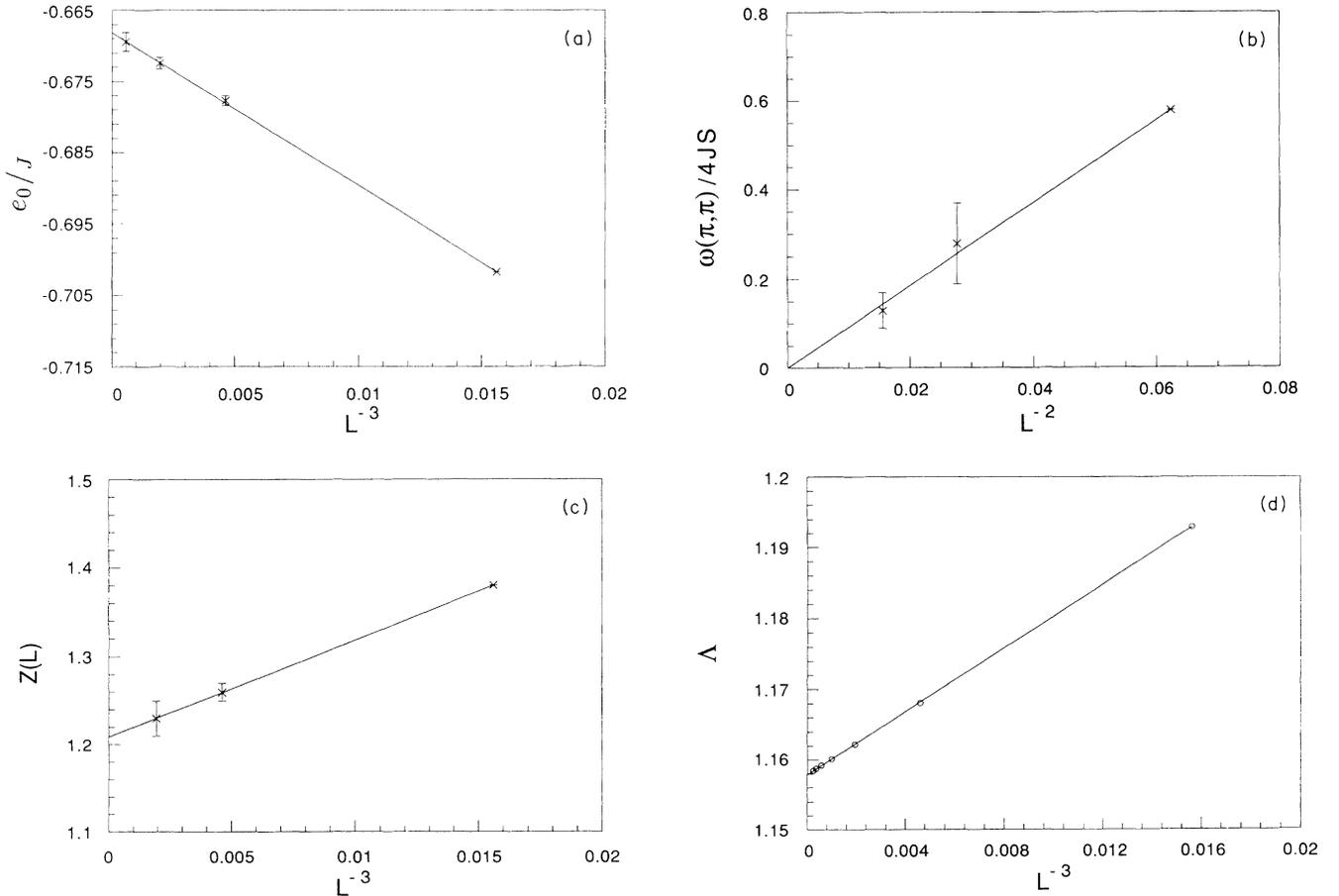


FIG. 2. Size dependencies of various quantities: (a) the ground-state energy (in units of J), and the line is $e_0 + B/L^3$ fit; (b) the energy gap $\omega(\pi, \pi) = E_{(\pi, \pi)} - E_{(0,0)}$, and the line is $\omega(\pi, \pi) = A/L^2$; (c) the spectrum renormalization factor $Z(L)$; and (d) $\Lambda(L)$ from Schwinger boson MF theory.

$$\omega_k^{2D}(L) = Z(L, k) [4JS(1 - \gamma_k^2 + A_k^2/L^4)^{1/2}], \quad (18a)$$

where $Z(L, k) = 1$ and $A_k = 0$ would lead to the ω_k^{SW} of Eq. (3a). Here the term A_k^2/L^4 accounts for the finite-size effects,²¹ which break the symmetry of $1 - \gamma_k^2$ between $(0,0)$ and (π, π) and thus generate the gap. A_k changes smoothly with \mathbf{k} ; the exact form is not important, as shown below. At $\mathbf{k} = (\pi, \pi)$ this form leads to a gap that scales as $1/L^2$. For all other momenta, except $(0,0)$, of course, the A_k^2/L^4 term is very small compared with $1 - \gamma_k^2$, so that this correction can be neglected. [Even in the most extreme case of $\mathbf{k} \rightarrow 0$,

$$1 - \gamma_k^2 \simeq (k_x^2 + k_y^2)/2 = 2\pi^2(n_x^2 + n_y^2)/L^2,$$

where $n_x, n_y \ll L$ are integers. This is still much larger than A_k^2/L^4 .]

The above analysis also suggest that $Z(L, k)$ has little dependence on k , i.e., $Z(L, k) \approx Z(L)$. Thus we have

$$\omega_k^{2D} \approx Z(L) 4JS(1 - \gamma_k^2)^{1/2} = Z(L) \omega_k^{SW, 2D}. \quad (18b)$$

Indeed, using the only parameter $Z(L)$ for a given $L \times L$ lattice, one can fit the obtained $\omega(k)$ to Eq. (18b) for all \mathbf{k} , as shown in Fig. 2. Plotted in units of $8JSZ(L)$, all data points on the three lattices ($L = 4, 6, 8$) collapse into a single curve [except at $\mathbf{k} = (\pi, \pi)$ because of the gap term A_k^2/L^4], giving clear evidence that the exact spectrum has the same shape as the spin-wave spectrum $(1 - \gamma_k^2)^{1/2}$. The fact that one parameter $Z(L)$ fits all data points on each lattice confirms the usefulness of Eqs. (18).

These data fits to theoretical form give $Z(L) = 1.38 \pm 0.002$, 1.26 ± 0.01 , and 1.22 ± 0.02 for $L = 4, 6$, and 8 , respectively. [For 4×4 we used the exact spectrum at $(\pi/2, 0)$ and $(\pi, 0)$ in the fit.] To estimate the limit for $L \rightarrow \infty$, we fit $Z(L)$ to L^{-n} and find a size dependence of $Z(L)$ as

$$Z_E(L) = Z_E + B/L^3, \quad (19)$$

as shown in Fig. 2(c); the result is $Z_E = 1.21 \pm 0.03$ and $B = 11.1 \pm 0.8$. [Here we use Z_E to distinguish from Z_c , the renormalization of the spin-wave form at the $\mathbf{k} \rightarrow 0$ limit.]

To give some further understanding of the $1/L^3$ extrapolation found in our data fit, we examined $E(k, L)$ within the framework of the Schwinger boson mean-field (MF) theory.² This theory is an approach different from spin-wave theory, and it gives improved results on a number of aspects, such as the correlation length, uniform susceptibility, etc. The theory leads to a spectrum very close to the spin-wave result: For a $L \times L$ square lattice, the spectrum is given by

$$\omega_k^{MF} = 2\Lambda(L) [1 - \eta^2(L) \gamma_k^2]^{1/2}, \quad (20a)$$

where γ_k is given in (3b). Λ and η are determined by minimizing the free energy, leading to

$$1 = \sum_k \frac{2}{L^2} |\gamma_k|^2 \omega_k^{-1} \coth(\frac{1}{2}\beta\omega_k), \quad (20b)$$

subject to the condition

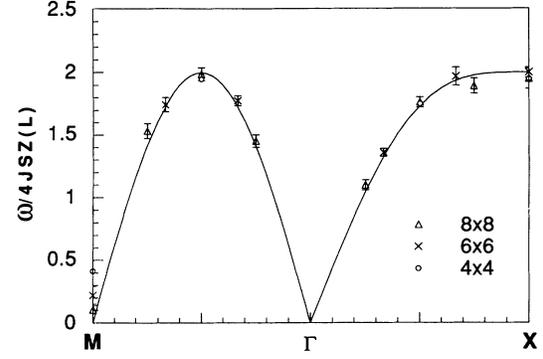


FIG. 3. Comparison of results from PMC calculations for $L \times L$ lattices with $L = 4, 6, 8$ to the spin-wave spectrum [see Eq. (18)]. In each case the results have been scaled as $\omega(\mathbf{k})/8JSZ(L)$ with $Z(4) = 1.38$, $Z(6) = 1.26$, and $Z(8) = 1.22$, which are obtained by fitting the spectrum in the branch Γ [$\mathbf{k} = (0,0)$] to X [$\mathbf{k} = (0,\pi)$]. Except the gap at M [$\mathbf{k} = (\pi,\pi)$], all other data points fall along the curve $(1 - \gamma_k^2)^{1/2}$.

$$\frac{1}{\Lambda(L)} = \sum_k \frac{1}{L^2} \omega_k^{-1} \coth(\frac{1}{2}\beta\omega_k), \quad (20c)$$

where $\beta = 1/T$. Clearly, $\Lambda(L)$ is very similar to $Z(L)$ in Eq. (18) and we are interested in the size scaling of $\Lambda(L)$. For this purpose we solved Eq. (20) for $L = 4 - 24$ at the $T \rightarrow 0$ limit. [We used $T = 0.02J$ and verified with $T = 0.01J$.] First, $\eta(L)$ is found to be very close to 1 (η increases from 0.993 for $L = 4$ to 0.999 for $L = 16$ and becomes indistinguishable from 1 for larger lattices). Second, the $\Lambda(L)$ can be well fitted by

$$\Lambda(L) = \Lambda_\infty + D/L^3,$$

as shown in Fig. 2(d). We find $\Lambda_\infty = 1.158 \pm 0.001$ and $D = 2.24 \pm 0.01$, in good agreement with the original calculation.² This is a theoretical justification to our empirical scaling.

IV. DISCUSSION

At the long-wavelength limit $\mathbf{k} \rightarrow 0$, the spin-wave spectrum is simplified to

$$\omega_k^{SW} = \sqrt{8}JSka, \quad k^2 = k_x^2 + k_y^2. \quad (21)$$

The linear coefficient $\sqrt{8}JSa$ is the usual spin velocity. The correction to this linear coefficient, the spin-velocity renormalization factor Z_c has been calculated by a number of authors.^{6, 8-10, 22} On the other hand, our results suggest an overall renormalization Z_E for all \mathbf{k} . Thus $Z_E = Z_c$. Oguchi²² obtained $Z_c = 1.16$ using a $1/2S$ expansion of higher-order spin-wave theory. Singh⁸ obtained $Z_c = 1.18 \pm 0.02$ by a series expansion around the Ising limit. The Green-function MC simulation of Trevedi and Ceperly⁶ gave an estimate $Z_c = 1.14 \pm 0.05$ from a variational method. Gross, Sanchez-Velasco, and Siggia¹⁰ measured ground-state energies of various size square lattices by a projector Monte Carlo technique and compared them with those of spin-wave theory, giving $Z_c \approx 1.18 \pm 0.10$. Our result $Z_E = 1.21 \pm 0.03$ is in reason-

able agreement with these calculations.

The linear dispersion relation at small \mathbf{k} has been observed in inelastic neutron-scattering experiments.²³ For La_2CuO_4 , experiment gives a spin-wave velocity of $\hbar c_s = 0.85 \pm 0.03$ eV Å. Using a lattice parameter of $a = 3.80$ Å (determined by x-ray diffraction²⁴) and an exchange coupling value of $J = 1450 \pm 30\text{K} = 0.125 \pm 0.003$ eV (obtained by fitting the Monte Carlo results¹¹ to the observed spin-correlation length²⁴), our result $Z_E = 1.21 \pm 0.03$ leads to $\hbar c_s = Z_E \sqrt{8JSa} = 0.80 \pm 0.03$ eV Å, quite close the experimental value. (Using $Z_c = 1.16$ leads to $\hbar c_s = 0.77$ eV Å.) This indicates that the simple Heisenberg model describes well the magnetic interactions in La_2CuO_4 .

In conclusion, our numerical calculation of the excitation spectrum and finite-size analysis suggests that the exact spectrum of the 2D Heisenberg Hamiltonian has the

same form as linear-spin-wave theory, except for an overall renormalization constant of $Z_E = 1.21 \pm 0.03$. This justifies the use of the spin-wave spectrum for a wide variety of calculations, including the Schwinger boson mean-field theory and modified spin-wave theory. Our numerical value on spin velocity agrees with both the previous calculations and neutron-scattering experiment.

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