Spin-wave theory and finite-size scaling for the Heisenberg antiferromagnet

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Spin-wave perturbation theory for the Heisenberg antiferromagnet at zero temperature is used to compute the finite-lattice corrections to the ground-state energy, the staggered magnetization, and the energy gap. The dispersion relation, the spin-wave velocity, and the bulk ground-state energy to order $O(1/S^2)$ are also computed for the square lattice. The results agree very well with the predictions of Neuberger and Ziman and the predictions of Fisher.

I. INTRODUCTION

The Heisenberg antiferromagnet on a square lattice has recently come under intensive study by a variety of methods, because of its possible relevance to high-T_c superconductors. Reviews of this work have been given by Barnes[1] and Manousakis.[2]

The finite-size scaling behavior of the system has been predicted by Neuberger and Ziman[3] and Fisher,[4] for use in the analysis of Monte Carlo results. These predictions are based on general arguments that the large-distance, low-energy behavior of the system will be dominated by massless, soft magnon modes, which can be described by a simple effective action involving just three unknown parameters, which can be taken as, for instance, the spin-wave velocity v, the helicity modulus or spin-wave stiffness ρ_s, and the staggered magnetization M^+. The values of these parameters are not predicted, but must be calculated from the microscopic Hamiltonian, or fitted to experiment.

Spin-wave perturbation theory has been found to give a comprehensive and surprisingly accurate description of the Heisenberg antiferromagnet on a square lattice. Our aim in this paper is to use spin-wave theory to compute the finite-size scaling behavior of the system, make comparison with the predictions of Neuberger and Ziman[3] and Fisher,[4] and determine the three parameters referred to above. We also present some higher-order spin-wave results for the bulk properties of the system.

The spin-wave theory for the Heisenberg antiferromagnet was originally developed by Anderson,[5] and then extended to second order by Kubo[6] and Oguchi.[7] The theory was extended to higher order first by Harris *et al.*,[8] and recently by Kopietz,[9] Castilla and Chakravarty,[10] Igarashi and Watabe,[11] Canali, Girvin, and Wallin,[12] Gochev,[13] and the present authors.[14] The works[8–10,12,13] relied on the Dyson-Maleev transformation, while Ref. 11 used the Holstein-Primakoff transformation. Harris *et al.*[8] and Kopietz[9] studied magnon damping at low temperature. Castilla and Chakravarty[10] calculated the staggered magnetization M^+ at zero temperature, and concluded that

$$M^+ = S - 0.196\,60 - 0.000\,68 S^{-2} + O(S^{-3}) . \tag{1.1}$$

Igarashi and Watabe[11] gave results for the renormalization factor of the spin-wave velocity Z_c, the staggered magnetization M^+, the transverse susceptibility $\chi_\perp$, and the spin-stiffness constant ρ_s at zero temperature as

$$\begin{aligned} &Z_c = 1 + \frac{0.158}{2S} - \frac{c_2}{(2S)^2}, \quad c_2 \geq 0.02 , \\ &M^+ = S - 0.197 - \frac{0.01}{(2S)^2} , \quad \chi_\perp = \frac{1}{8}\Big(1 - \frac{0.552}{2S} + \frac{0.04}{(2S)^2}\Big) , \\ &\rho_s = \begin{cases} S^2(1 - \frac{0.236}{2S} - \frac{0.15}{(2S)^2}), & \text{via relation } \rho_s = 8S^2 Z_c^2 \chi_\perp , \\ S^2(1 - \frac{0.236}{2S} - \frac{0.05}{(2S)^2}), & \text{direct calculation,} \end{cases} \end{aligned} \tag{1.2}$$

where they claimed the inconsistency in ρ_s was due to a rough estimate of Z_c.

Canali, Girvin, and Wallin[12] calculated the renormalization factor of the spin-wave velocity Z_c,

$$Z_c = 1 + \frac{0.157\,95}{2S} + \frac{0.0215(2)}{(2S)^2}. \tag{1.3}$$

Gochev[13] evaluated the ground-state energy,

$$\begin{aligned} E_0/N = &-2S^2 - 0.315\,88 S - 0.012\,46 \\ &-0.002\,10 S^{-1} + O(S^{-2}) . \end{aligned} \tag{1.4}$$

The present authors[14] used both the Dyson-Maleev and Holstein-Primakoff formalisms to investigate the anisotropic Heisenberg antiferromagnet, and obtained the consistent results for the isotropic model:

$$\begin{aligned} E_0/N = &-2S^2 - 0.315\,895 S - 0.012\,474 \\ &+0.000\,216(6)/S + O(S^{-2}) , \\ M^+ = &\ S - 0.196\,601\,9 + 0.000\,866(25) S^{-2} + O(S^{-3}) , \\ \chi_\perp = &\ 0.125 - 0.034\,447 S^{-1} \\ &+0.001\,701(3) S^{-2} + O(S^{-3}) . \end{aligned} \tag{1.5}$$

Obviously, there are substantial discrepancies between the different third-order spin-wave results. We believe this is probably due to the fact that works[10,11,13] used the following relation (in our notation[14]):

$$\sinh\theta_k = [(1-\gamma_k^2)^{-1/2}-1]^{1/2}/\sqrt{2}\ , \qquad (1.6)$$

which holds only if $\gamma_k \geq 0$. But because there is a δ function $\delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+\mathbf{4}}$ in the vertices $\mathcal{V}_i^{(0)}$, the momentum k cannot always be inside the first Brillouin zone, and γ_k can be less than 0: in this case, the above relation must be replaced by

$$\sinh\theta_k = -[(1-\gamma_k^2)^{-1/2}-1]^{1/2}/\sqrt{2}\ . \qquad (1.7)$$

In the present work, we calculate the finite-lattice corrections to the ground-state energy, the staggered magnetization and the mass gap for the cases of the one-dimensional linear chain and the two-dimensional square lattice. The results for the square lattice are in good agreement with the finite-size scaling predictions and Monte Carlo simulation. For the square lattice, we also present some further calculations for the third-order spin-wave velocity via both the Dyson-Maleev and Holstein-Primakoff formalisms, and the fourth-order ground-state energy via the Dyson-Maleev formalism. For the Holstein-Primakoff formalism, there are some divergent terms in the third-order spin-wave velocity, but they cancel each other, and the final results are the same as in the Dyson-Maleev formalism. We will not repeat the derivation of the general spin-wave theory, but the notations here have the same meanings as in our previous paper.[14]

The arrangement of the paper is as follows. In Sec. II we calculate the finite-lattice corrections. In Secs. III and IV, we calculate the third-order spin-wave velocity and the fourth-order ground-state energy, respectively. In Sec. V we make a comparison with the prediction of Neuberger and Ziman, and Fisher, and summarize our conclusions.

II. FINITE-LATTICE CORRECTIONS

In our previous paper,[14] we discussed the bulk properties of the model. Here, we discuss the finite-lattice corrections for the isotropic case ($x=1$). The finite-size scaling corrections can give us a great deal of information about the model, using either finite-size scaling theory or the theory of conformal invariance at criticality in (1+1) dimensions.

A. Ground-state energy and staggered magnetization

The properties of the isotropic Heisenberg antiferromagnet such as the ground-state energy E_0 and the staggered magnetization M^+ are functions of $C_n(1)$ which is defined by

$$C_n(x) = \frac{2}{N}\sum_k [(1-x^2\gamma_k^2)^{n/2}-1]\ , \qquad (2.1)$$

where the sum over k denotes a sum over the first Brillouin zone of sublattice l. For a bulk system, the momentum k is continuous over the first Brillouin zone, but for a finite-lattice system, the momentum k is discrete. For the one-dimensional linear chain and two-dimensional square lattice, the structure factor γ_k, the first Brillouin zone for a bulk system, and the discrete momentum k for a finite-lattice system are the following:

(1) one-dimensional linear chain:

$$\gamma_k = \cos(k_x a)\ , \qquad (2.2)$$

momentum k: $0 < k_x a \leq \pi$ bulk system

$$k_x(i) = \frac{\pi i}{aL_l},\quad i=1,2,\ldots,L_l \quad \text{finite-lattice system}$$
$$L_l = L/2\ ,$$

(2) two-dimensional square lattice:

$$\gamma_k = \cos(\sqrt{2}k_x a/2)\cos(\sqrt{2}k_y a/2)\ , \qquad (2.3)$$

momentum k: $0 < \sqrt{2}k_x a/2, \sqrt{2}k_y a/2 \leq \pi$ bulk system

$$k_x(i) = \frac{2\pi i}{\sqrt{2}aL_l},\ k_y(i) = \frac{2\pi i}{\sqrt{2}aL_l},\quad i=1,2,\ldots,L_l \quad \text{finite-lattice system}$$
$$L_l = L/\sqrt{2}\ ,$$

where L and a are the lattice size and the lattice spacing for the whole system, respectively, and L_l is the lattice size for sublattice l. For convenience, we set the lattice spacing $a=1$ from now on.

The leading finite-size correction to C_i for the one-dimensional linear chain can be calculated exactly by using the Euler-Maclaurin formula.[15] For a two-dimensional square lattice, the finite-lattice corrections to C_i can be evaluated by a least-squares fit of $C_n(1,L)$ to the form $C_n(1,\infty)+a/L^{n+2}+b/L^{n+3}+c/L^{n+4}+\cdots$. The results are the following:

(1) one-dimensional linear chain:

$$C_1(1) = \frac{2}{\pi} - 1 - \frac{2\pi}{3L^2} + \cdots\ ,$$
$$C_{-1}(1) = -\frac{2}{\pi}\ln\left(\frac{2\pi}{L}\right) + \cdots\ . \qquad (2.4)$$

(2) two-dimensional square lattice:

$$C_1(1) = -0.157\,947\,420\,95 - 2.033\,28/L^3 + 0\times L^{-4} + O(L^{-5})\ ,$$
$$C_{-1}(1) = 0.393\,203\,929\,7 - 1.755\,736\,07/L + O(L^{-2})\ ,$$
$$C_{-3}(1) = 0.206\,014\,26L - 0.448\,848\,6 + O(L^{-1})\ . \qquad (2.5)$$

Note that the L^{-4} correction to C_1 is zero. From Eqs. (2.4) and (2.5) we derive the following results.

1. One-dimensional lattice

The ground-state energy, including finite-size correction, is found to be

$$\frac{E_0}{N} = -S^2 + S\left(\frac{2}{\pi}-1\right) - \frac{1}{4}\left(\frac{2}{\pi}-1\right)^2 - \frac{\pi}{3L^2}\left(2S-\frac{2}{\pi}+1\right) + O\left(\frac{1}{S}\right) . \tag{2.6}$$

Note that the energy $m(k)$ of a single-boson state with momentum $k \to 0$ is

$$m(k) = \left(2S - \frac{2}{\pi} + 1 + O(1/S)\right) k , \tag{2.7}$$

and the spin-wave velocity up to second order is

$$v = \left(2S - \frac{2}{\pi} + 1 + O(1/S)\right) . \tag{2.8}$$

Now according to the theory of conformal invariance, the leading finite-size correction at the isotropic limit is

$$\frac{E_0}{N} \sim \frac{E_0(\infty)}{N} - \frac{\pi v c}{6L^2} , \tag{2.9}$$

where c is the conformal anomaly, which characterizes the universality class of the critical point, and the allowed set of critical exponents. Comparing Eqs. (2.6) and (2.8), we see that the conformal anomaly is obtained as

$$c = 2 , \tag{2.10}$$

precisely through second order in spin-wave expansion. This disagrees with the known exact result[16] $c = 1$.

This failure of the spin-wave theory comes as no great surprise. It has long been known that spin-wave theory fails qualitatively to describe the one-dimensional Heisenberg antiferromagnet: the spin-wave expansion predicts a finite staggered magnetization, whereas the exact value[17] is zero; and for integer spin the expansion predicts a zero mass gap, whereas Haldane's conjecture,[18,19] supported by numerical analyses, predicts a finite mass gap.

2. Two-dimensional square lattice

The ground-state energy, including finite-size correction, is found to be

$$\frac{E_0}{N} = -2S^2 - 0.315\,894\,841\,9S - 0.012\,473\,693\,89 - \frac{4.066\,56S + 0.321\,151 + O(S^{-1})}{L^3} + \cdots , \tag{2.11}$$

while the staggered magnetization is

$$M^+ = S - 0.196\,602 + 0.000\,866(25)S^{-2} + O(S^{-3}) + \frac{0.877\,868\,0 + 0\times S^{-1} + O(S^{-2})}{L} + \cdots . \tag{2.12}$$

This last result must be interpreted with some care. Strictly speaking, the staggered magnetization at zero magnetic field on a finite lattice is zero (see later). Equation (2.12) describes the "bulk value" obtained either at a finite but very small field, or else, perhaps, by a measurement of the mean square magnetization.

A comparison of these results with the predictions of Neuberger and Ziman will be given in Sec. V.

B. Energy gap and zero modes

We now need to take careful consideration of the "zero modes" of the system, which have no special effect on the calculation of bulk properties or the finite-lattice corrections to the ground-state energy and bulk staggered magnetization, but which do play a crucial role in the finite-lattice behavior of the energy gap.

Using the Dyson-Maleev representation, one finds after a Fourier transformation that the terms in the Hamiltonian which involve only zero-momentum ($\mathbf{k} = 0$) modes are

$$H_{\mathbf{k}=0} = zS(a_0^\dagger a_0 + b_0^\dagger b_0 + a_0 b_0 + a_0^\dagger b_0^\dagger) - \frac{z}{N}(a_0^\dagger a_0 a_0 b_0 + a_0^\dagger b_0^\dagger b_0^\dagger b_0 + 2a_0^\dagger a_0 b_0^\dagger b_0) . \tag{2.13}$$

Now consider the operators corresponding to the total spin on the even (l) and odd (m) sublattices:

$$J_1^\pm = \sum_l S_l^\pm, \qquad J_1^z = \sum_l S_l^z , \qquad J_2^\pm = \sum_m S_m^\pm, \qquad J_2^z = \sum_m S_m^z . \tag{2.14}$$

If we carry out the same process, representing the spin operators in term of boson operators, Fourier transforming, and then dropping all terms which involve nonzero momentum, we find for the rotation-invariant combinations

$$(\mathbf{J}_1^2)_{\mathbf{k}=0} = \frac{NS}{2}\left(\frac{NS}{2}+1\right) , \qquad (\mathbf{J}_2^2)_{\mathbf{k}=0} = \frac{NS}{2}\left(\frac{NS}{2}+1\right) , \tag{2.15}$$

$$(\mathbf{J}_1 + \mathbf{J}_2)^2_{\mathbf{k}=0} = NS + NS(a_0^\dagger a_0 + b_0^\dagger b_0 + a_0 b_0 + a_0^\dagger b_0^\dagger) - (a_0^\dagger a_0 a_0 b_0 + a_0^\dagger b_0^\dagger b_0^\dagger b_0 + 2a_0^\dagger a_0 b_0^\dagger b_0) . \tag{2.16}$$

Comparing (2.13) with (2.14)–(2.16), we see that

$$H_{\mathbf{k}=0} = -zS + \frac{z}{N}(\mathbf{J}_1 + \mathbf{J}_2)^2_{\mathbf{k}=0} = -zS + \frac{z}{N}[2(\mathbf{J}_1^2 + \mathbf{J}_2^2) - (\mathbf{J}_1 - \mathbf{J}_2)^2]_{\mathbf{k}=0} . \tag{2.17}$$

Thus, if one restricts oneself entirely to the zero-mode sector, the situation is just that discussed by Neuberger and Ziman,[3] or more generally by Fisher and Privman:[20] the spins on each sublattice are aligned with each other, so that the total sublattice spins $\mathbf{J}_1^2$ and $\mathbf{J}_2^2$ are fixed at their maximum possible values, while the spins on different sublattices are antialigned, such that in the ground state the total spin $(\mathbf{J}_1+\mathbf{J}_2)^2$ is zero. The Hamiltonian is rotationally symmetric, of course, and the zero-mode spectrum provides a Wigner representation of this symmetry. In particular, the ground-state eigenvector on the finite lattice is also rotationally symmetric, so that the order parameter in any particular direction is zero. The relative energy eigenvalues in the zero-mode sector are

$$\Delta E_{\mathbf{k}=0} = zj(j+1)/N, \qquad j=0,1,2,\ldots \tag{2.18}$$

so that the energy gap to the first excited state is

$$m_N = 2z/N\ . \tag{2.19}$$

The staggered magnetic field operator is

$$\begin{aligned} V &= h\left(\sum_l S_l^z - \sum_m S_m^z\right) \\ &= h(J_1^z - J_2^z)\ . \end{aligned} \tag{2.20}$$

If $h=0$, the Hamiltonian is rotationally symmetric, and the spontaneous magnetization vanishes, as noted above. If h is large enough, then V will dominate over $H_{\mathbf{k}=0}$, and the ground state will be the eigenstate with $\mathbf{J}_1^2 = \mathbf{J}_2^2 = NS/2$, $J_1^z - J_2^z = -NS$, so that the staggered magnetization will take its bulk value

$$M^+ = -\frac{1}{N}\frac{\partial E_0}{\partial h} = S \tag{2.21}$$

to leading order. The condition on the field strength required for this to happen is

$$NhS \gg z/N\ , \tag{2.22}$$

i.e.,

$$N^2 h \gg z/S\ , \tag{2.23}$$

in agreement with the arguments of Fisher and Privman.[20]

A little consideration shows that the neglected terms involving nonzero-momentum modes will modify these results, producing corrections of higher order in spin-wave perturbation theory, which we have not explicitly calculated. The basic scenario will remain the same, however. We have also checked that the same results hold in the Holstein-Primakoff representation, to leading order.

III. DISPERSION RELATION AND SPIN-WAVE VELOCITY

In our previous paper,[14] we calculated the spin-wave energy of a single-boson state with momentum $k=0$ for the anisotropic Heisenberg antiferromagnet. Here we calculate the spin-wave energy $m(k)$ of a single-boson state with nonzero momentum k, and then estimate the spin-wave velocity Z_c and the stiffness constant ρ_s. For the anisotropic Heisenberg antiferromagnet ($x\neq 1$), the spin-wave velocity is zero, so in this section we only consider the isotropic model ($x=1$), using both the Dyson-Maleev and Holstein-Primakoff formalisms.

A. Dyson-Maleev formalism

As before,[14] the spin-wave energy of a single-boson state with momentum k up to order $O(1/S)$ can be derived as

$$m(k) = m^{(1)}(k) + m^{(0)}(k) + m^{(-1)}(k) + O(1/S^2)\ , \tag{3.1}$$

where

$$\begin{aligned} m^{(1)}(k) &= zS(1-x^2\gamma_k^2)^{1/2}\ ,\\ m^{(0)}(k) &= -\frac{z}{2}\left[(1-x^2\gamma_k^2)^{1/2}C_1 + (1-x^2)(C_{-1}-C_1)\gamma_k^2(1-x^2\gamma_k^2)^{-1/2}\right]\ ,\\ m^{(-1)}(k) &= \Delta m_a^{(-1)}(k) + \Delta m_b^{(-1)}(k) + \Delta m_c^{(-1)}(k) + \Delta m_d^{(-1)}(k) + \Delta m_e^{(-1)}(k)\ , \end{aligned} \tag{3.2}$$

and $\Delta m_a^{(-1)}(k)$ is the contribution from Fig. 2(a) in the previous paper,[14] etc.:

$$\begin{aligned} \Delta m_a^{(-1)}(k) &= -\frac{z}{8x^2S}(1-x^2)^2(C_{-1}-C_1)^2\gamma_k^2(1-x^2\gamma_k^2)^{-3/2}\ ,\\ \Delta m_b^{(-1)}(k) &= -\frac{z}{2S}\left(\frac{2}{N}\right)^2\sum_{i=1}^{3}\delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+k}\frac{V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},k)V_5^{(0)}(\mathbf{3},k,\mathbf{1},\mathbf{2})}{\sum_{i=1}^{3}(1-x^2\gamma_i^2)^{1/2}+(1-x^2\gamma_k^2)^{1/2}}\ ,\\ \Delta m_c^{(-1)}(k) &= -\frac{z}{2S}\left(\frac{2}{N}\right)^2\sum_{i=1}^{3}\delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+k}\frac{V_2^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},k)V_3^{(0)}(\mathbf{3},k,\mathbf{1},\mathbf{2})}{\sum_{i=1}^{3}(1-x^2\gamma_i^2)^{1/2}-(1-x^2\gamma_k^2)^{1/2}}\ ,\\ \Delta m_d^{(-1)}(k) &= -\frac{z}{8xS}\left(\frac{2}{N}\right)\sum_{k'}(1-x^2)(C_{-1}-C_1)\gamma_{k'}(1-x^2\gamma_{k'}^2)^{-1}[V_2^{(0)}(k',k,k,k')+V_2^{(0)}(k,k',k,k')]\ ,\\ \Delta m_e^{(-1)}(k) &= -\frac{z}{8xS}\left(\frac{2}{N}\right)\sum_{k'}(1-x^2)(C_{-1}-C_1)\gamma_{k'}(1-x^2\gamma_{k'}^2)^{-1}[V_3^{(0)}(k',k,k,k')+V_3^{(0)}(k',k,k',k)]\ , \end{aligned} \tag{3.3}$$

with

$$\Delta m_d^{(-1)}(k) + \Delta m_e^{(-1)}(k) = \frac{z}{4x^2 S}(1-x^2)^2 (C_{-1} - C_1)\gamma_k^2 (1 - x^2\gamma_k^2)^{-1/2} \; . \tag{3.4}$$

In the isotropic limit ($x = 1$),

$$\Delta m_a^{(-1)}(k) = \Delta m_d^{(-1)}(k) + \Delta m_e^{(-1)}(k) = 0 \tag{3.5}$$

and

$$\Delta m_b^{(-1)}(k) + \Delta m_c^{(-1)}(k) = -\frac{z}{2S}(1-\gamma_k^2)^{1/2} m_{bc}(k) \; , \tag{3.6}$$

where

$$m_{bc}(k) = \left(\frac{2}{N}\right)^2 \sum_{k_1,k_2,k_3} \frac{\delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+k}}{[\sum_{i=1}^3 (1-\gamma_i^2)^{1/2}]^2 - [(1-\gamma_k^2)^{1/2}]^2} \times \left(\frac{[V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},k)V_5^{(0)}(\mathbf{3},k,\mathbf{1},\mathbf{2}) + V_2^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},k)V_3^{(0)}(\mathbf{3},k,\mathbf{1},\mathbf{2})]\sum_{i=1}^3(1-\gamma_i^2)^{1/2}}{(1-\gamma_k^2)^{1/2}} + [V_2^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},k)V_3^{(0)}(\mathbf{3},k,\mathbf{1},\mathbf{2}) - V_5^{(0)}(\mathbf{1},\mathbf{2},\mathbf{3},k)V_5^{(0)}(\mathbf{3},k,\mathbf{1},\mathbf{2})] \right) \; . \tag{3.7}$$

For the square lattice, the integration of $m_{bc}(k)$ can be evaluated for finite lattices up to lattice size $L_l = 120$, then extrapolated to the infinite lattice by the form $m_{bc}(k,\infty) + \frac{a}{L^2} + \frac{b}{L^3} + \frac{c}{L^4}$. Figure 1 shows the dispersion relation along the line $k_x = k_y$. The third-order results here disagree with those of Igarashi and Watabe.[11]

In the limit $k \to 0$, using MATHEMATICA, $m_{bc}(k)$ can be found to have two integration parts:

$$m_{bc}(k) = \left(\frac{2}{N}\right)^2 \sum_{i=1}^{3} \delta_{\mathbf{1}+\mathbf{2},\mathbf{3}+k} [2\tilde{m}_{bc}^{(-1)}/k + \tilde{m}_{bc}^{(0)}] \; , \quad k \to 0 \; , \tag{3.8}$$

where the expressions for $\tilde{m}_{bc}^{(-1)}$ and $\tilde{m}_{bc}^{(0)}$ are too complicated to be given here. The integral of the divergent part is found to be zero. Replacing all $(1-\gamma_i^2)^{1/2}$ ($i = 1,2,3$) by $(1 - t^2\gamma_i^2)^{1/2}$ in the second integration part, and using the series expansion technique in our previous paper,[14] we can obtain a series in t for the integral of $m_{bc}(0)$ for the infinite lattice. This series can be supplied on request. Extrapolating[14] the series to the limit $t \to 1$, we get

$$m_{bc}(0) = -0.010\,76(1) \; . \tag{3.9}$$

Therefore, the energy gap of the isotropic Heisenberg antiferromagnet at the small k limit is

$$m(k) = 4S\left(1 + \frac{0.157\,947\,421}{2S} + \frac{0.021\,52(2)}{(2S)^2} + O(1/S^3) \right)(\sqrt{2}k/2) \; , \tag{3.10}$$

and the renormalization factor of the spin-wave velocity is

$$Z_c = \frac{v}{v_0} = 1 + \frac{0.157\,947\,421}{2S} + \frac{0.021\,52(2)}{(2S)^2} + O(1/S^3) \; , \tag{3.11}$$

where v_0 is the "bare" spin-wave velocity of the linear spin-wave approximation, namely, $v_0 = 2\sqrt{2}S$. The stiffness constant ρ_s can be estimated by using the hydrodynamic relation

$$\rho_s = v^2\chi_\perp = S^2 \left(1 - \frac{0.235\,25}{2S} - \frac{0.0517(2)}{(2S)^2} + O(1/S^3) \right), \tag{3.12}$$

where $\chi_\perp$ is the uniform perpendicular susceptibility.[14]

Here the result for the spin-wave velocity is different from that of Igarashi and Watabe[11] but agrees with that of Canali, Girvin, and Wallin,[12] and the stiffness constant

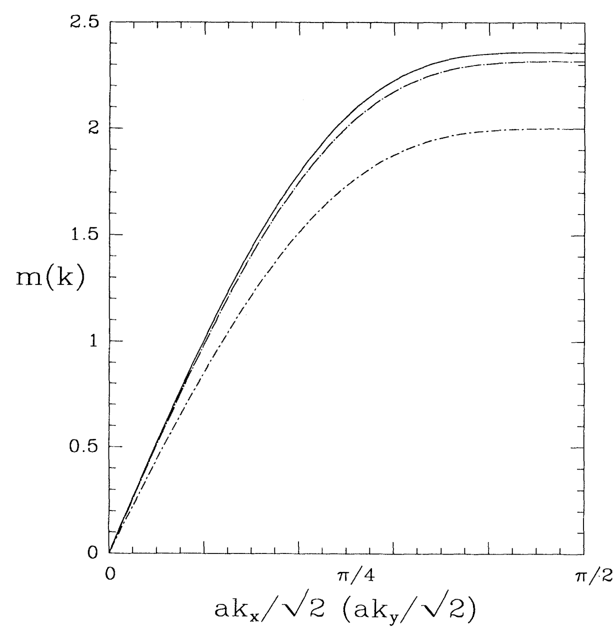

FIG. 1. The spin-wave energy $m(k)$ as a function of momentum $ak_x/\sqrt{2}$ along a line $k_x = k_y$. The three curves shown are the first-, second-, and third-order spin-wave predictions, corresponding to short-dashed, long-dashed , and solid lines, respectively.

ρ_s is consistent with the direct calculation of Igarashi and Watabe.

B. Holstein-Primakoff formalism

The energy gap $m(k)$ can be calculated using the same method as in the Dyson-Maleev formalism, and the result is

$$m(k) = m^{(1)}(k) + m^{(0)}(k) + m^{(-1)}(k) + O(1/S^2), \tag{3.13}$$

where $m^{(1)}(k)$ and $m^{(0)}(k)$ are the same as in the Dyson-Maleev formalism, and $m^{(-1)}(k)$ is

$$m^{(-1)}(k) = \Delta m_0^{(-1)}(k) + \Delta m_a^{(-1)}(k) + \Delta m_b^{(-1)}(k) + \Delta m_c^{(-1)}(k) + \Delta m_d^{(-1)}(k) + \Delta m_e^{(-1)}(k) , \tag{3.14}$$

where

$$\Delta m_0^{(-1)}(k) = \frac{z}{32S}\left[2(C_{-1}-C_1)(C_{-1}+1) + x^2\gamma_k^2\left(C_{-1}(C_{-1}+2) - \frac{3}{x^2}(C_{-1}-C_1)^2\right)\right](1-x^2\gamma_k^2)^{-1/2} , \tag{3.15}$$

while the results for $\Delta m_a^{(-1)}(k)$ and $\Delta m_d^{(-1)}(k) + \Delta m_e^{(-1)}(k)$ are the same as in the Dyson-Maleev formalism for all bipartite lattices. The terms $\Delta m_b^{(-1)}(k)$, $\Delta m_c^{(-1)}(k)$, and $m_{bc}(k)$ have the same expression as in the Dyson-Maleev formalism except that the vertices $V_i^{(0)}$ are the Holstein-Primakoff vertices.

In the isotropic limit $x = 1$,

$$\Delta m_0^{(-1)}(k) = \frac{z}{32S}\Big\{ [2(C_{-1}-C_1)(C_{-1}+1) + C_{-1}(C_{-1}+2) - 3(C_{-1}-C_1)^2](1-\gamma_k^2)^{-1/2} + [3(C_{-1}-C_1)^2 - C_{-1}(C_{-1}+2)](1-\gamma_k^2)^{1/2}\Big\} . \tag{3.16}$$

For the square lattice, the integration $m_{bc}(k)$ can also be evaluated for a finite-lattice up to lattice $L_l = 120$, while here the finite lattice correction is $\frac{a}{L} + \frac{b}{L^2} + \cdots$. The calculation gives the same dispersion relation as Fig. 1.

In the limit $k \to 0$,

$$\begin{aligned}\Delta m_0^{(-1)}(k) &= \frac{z}{32S}\bigg([2(C_{-1}-C_1)(C_{-1}+1) + C_{-1}(C_{-1}+2) - 3(C_{-1}-C_1)^2]\frac{2}{\sqrt{2}k} \\ &\quad + [3(C_{-1}-C_1)^2 - C_{-1}(C_{-1}+2)]\sqrt{2}k/2\bigg) \\ &= \frac{2}{\sqrt{2}S}[0.195\,68/k - 0.001\,857k], \quad k \to 0 .\end{aligned} \tag{3.17}$$

Note that $\Delta m_0^{(-1)}(k)$ is divergent in the limit $k \to 0$, and $m_{bc}(k)$ is found, via MATHEMATICA, to have three integration parts in the small k limit:

$$m_{bc}(k) = \left(\frac{2}{N}\right)^2 \sum_{i=1}^{3} \delta_{1+2,3+k}\left[4\tilde{m}_{bc}^{(-2)}/k^2 + 2\tilde{m}_{bc}^{(-1)}/k + \tilde{m}_{bc}^{(0)}\right], \quad k \to 0 . \tag{3.18}$$

Let

$$m_{bc}^{(i)} = \left(\frac{2}{N}\right)^2 \sum_{i=1}^{3} \delta_{1+2,3+k}\tilde{m}_{bc}^{(i)}, \quad (i = -2, -1, 0) , \tag{3.19}$$

the integration $m_{bc}^{(-1)}$ is found to be zero, and the integration for $m_{bc}^{(-2)}$ and $m_{bc}^{(0)}$ can be carried out in the same way as before:

$$\begin{aligned} m_{bc}^{(-2)} &= 0.049(2) , \\ m_{bc}^{(0)} &= -0.012(2) . \end{aligned} \tag{3.20}$$

Therefore, in the limit $k \to 0$, the divergent parts of $\Delta m_0^{(-1)}(0)$ and $\Delta m_b^{(-1)}(0) + \Delta m_c^{(-1)}(0)$ cancel each other, and the final result for $m(0)$ is finite, agreeing with that obtained via the Dyson-Maleev formalism.

IV. FOURTH-ORDER SPIN-WAVE RESULTS

In this section, we present the fourth-order spin-wave expansion for the ground-state energy within the Dyson-Maleev formalism. We only consider the case without an external magnetic field, that is, $h_1 = h_2 = 0$.

According to the Hamiltonian H in Eq. (2.7) of our previous paper,[14] there are seven perturbation diagrams shown in Fig. 2 contributing to the order $O(S^{-2})$ for ground-state energy E_0; the first two diagrams also contribute to the order $O(S^{-1})$ of E_0, and the $O(S^{-1})$ part has been considered in our previous paper. The contributions from each diagram are

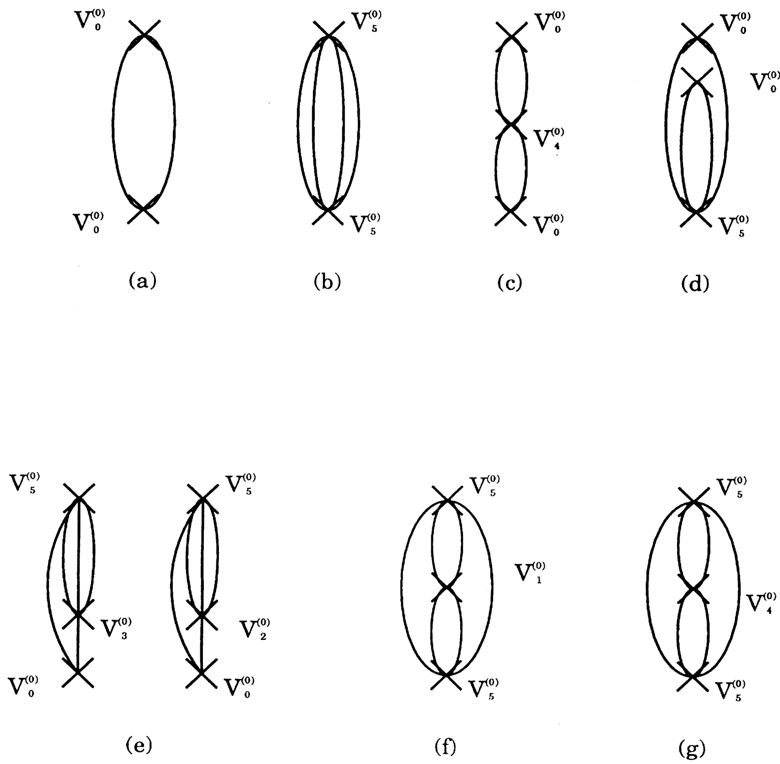

FIG. 2. The perturbation diagrams that contribute to the ground-state energy E_0/N. The crosses represent the interaction vertices as indicated; the lines represent boson excitations in the intermediate states. To save space, we have not differentiated between the α and β bosons and possible time ordering of the vertices in the diagrams.

$$
\begin{aligned}
\Delta E_a &= \sum_k \frac{[V_0^{(0)}]^2}{2\{-zSq_k - \frac{z}{2}[q_k C_1 + (1-x^2)\gamma_k^2 q_k^{-1}(C_{-1}-C_1)]\}} \\
&\equiv \Delta E_a^{(-1)} + \Delta E_a^{(-2)} + O(S^{-3}) \ , \\
\Delta E_b &= -\frac{z^2 N}{8}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{1+2,3+4} \frac{V_5^{(0)}(1,2,3,4)V_5^{(0)}(3,4,1,2)}{\sum_i\{zSq_i + \frac{z}{2}[q_i C_1 + (1-x^2)\gamma_i^2 q_i^{-1}(C_{-1}-C_1)]\}} \\
&\equiv \Delta E_b^{(-1)} + \Delta E_b^{(-2)} + O(S^{-3}) \ , \\
\Delta E_c^{(-2)} &= -\frac{N}{16zS^2}\left(\frac{2}{N}\right)^2 \sum_{k_1,k_2} [V_4^{(0)}(1,2,2,1) + V_4^{(0)}(2,1,1,2)]V_0^{(0)}(1)V_0^{(0)}(2)/(q_1 q_2) \ , \\
\Delta E_d^{(-2)} &= -\frac{N}{16zS^2}\left(\frac{2}{N}\right)^2 \sum_{k_1,k_2} [V_5^{(0)}(1,2,1,2) + V_5^{(0)}(1,2,2,1)]V_0^{(0)}(1)V_0^{(0)}(2)/(q_1 q_2) \ , \\
\Delta E_e^{(-2)} &= -\frac{N}{4S^2}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{1+2,3+4} \frac{V_0^{(0)}(1)[V_3^{(0)}(2,1,3,4)V_5^{(0)}(3,4,1,2) + V_2^{(0)}(3,4,1,2)V_5^{(0)}(1,2,3,4)]}{q_1(q_1+q_2+q_3+q_4)} \ , \\
\Delta E_f^{(-2)} &= -\frac{zN}{8S^2}\left(\frac{2}{N}\right)^4 \sum_{k_i} \delta_{1+2,3+4}\delta_{1+2,5+6} \frac{V_5^{(0)}(1,2,3,4)V_1^{(0)}(3,4,5,6)V_5^{(0)}(5,6,1,2)}{(q_1+q_2+q_3+q_4)(q_1+q_2+q_5+q_6)} \ , \\
\Delta E_g^{(-2)} &= -\frac{zN}{4S^2}\left(\frac{2}{N}\right)^4 \sum_{k_i} \delta_{1+2,3+4}\delta_{4+6,5+1} \frac{V_5^{(0)}(1,2,3,4)V_4^{(0)}(4,6,5,1)V_5^{(0)}(3,5,2,6)}{(q_1+q_2+q_3+q_4)(q_2+q_3+q_5+q_6)} \ ,
\end{aligned}
\tag{4.1}
$$

where

$$
\begin{aligned}
q_k &= (1 - x^2\gamma_k^2)^{1/2} \ , \\
\Delta E_a^{(-1)} &= -\frac{zN}{16x^4 S}(1-x^2)^2(C_{-1}-C_1)^2(C_{-3}-C_{-1})
\end{aligned}
$$

$$\Delta E_a^{(-2)} = \frac{zN}{32x^6S^2}(1-x^2)^2(C_{-1}-C_1)^2\{C_1(C_{-1}-C_{-3}) +(1-x^2)[C_{-1}(C_{-3}-C_{-1})+(C_{-3}-C_{-5})(C_{-1}-C_1)]\} , \tag{4.2}$$

$$\Delta E_b^{(-1)} = -\frac{zN}{8S}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{\mathbf{1+2,3+4}} \frac{V_5^{(0)}(\mathbf{1,2,3,4})V_5^{(0)}(\mathbf{3,4,1,2})}{q_1+q_2+q_3+q_4} ,$$

$$\Delta E_b^{(-2)} = -\frac{zN}{16S^2}\left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{\mathbf{1+2,3+4}} \frac{V_5^{(0)}(\mathbf{1,2,3,4})V_5^{(0)}(\mathbf{3,4,1,2})\{\sum_i[q_iC_1+(1-x^2)\gamma_k^2 q_i^{-1}(C_{-1}-C_1)]\}}{(q_1+q_2+q_3+q_4)^2} .$$

At the isotropic limit $x=1$, we can easily prove that

$$\Delta E_b^{(-2)} = \frac{C_1}{2S}\Delta E_b^{(-1)} ,$$
$$\Delta E_a^{(-1)} = \Delta E_a^{(-2)} = \Delta E_c^{(-2)} = \Delta E_d^{(-2)} = \Delta E_e^{(-2)} = 0 . \tag{4.3}$$

Therefore, the ground-state energy per site E_0/N is

$$E_0/N = -\frac{zS}{2}\left[S - C_1 + \frac{1}{4S}\left(C_1^2 + \frac{1-x^2}{x^2}(C_{-1}-C_1)^2\right)\right] -\frac{z}{16x^4S}(1-x^2)^2(C_{-1}-C_1)^2(C_{-3}-C_{-1}) + \Delta E_b^{(-1)}/N +(\Delta E_a^{(-2)}+\Delta E_b^{(-2)}+\Delta E_c^{(-2)}+\Delta E_d^{(-2)}+\Delta E_e^{(-2)}+\Delta E_f^{(-2)}+\Delta E_g^{(-2)})/N+O(S^{-3}) . \tag{4.4}$$

Hitherto, the results have been applicable to all bipartite lattices. We now restrict ourselves to the two-dimensional square lattice, where $\Delta E_c^{(-2)}$ and $\Delta E_d^{(-2)}$ are four-dimensional integrals over the first Brillouin zone: the integrations can be carried out analytically, and the results are

$$\Delta E_c^{(-2)} + \Delta E_d^{(-2)} = -\frac{N}{8x^6S^2}(1-x^2)^3(C_{-1}-C_1)^2(C_{-3}-C_{-1})^2 . \tag{4.5}$$

$\Delta E_b^{(-2)}$ and $\Delta E_e^{(-2)}$ are both six-dimensional integrals over the first Brillouin zone, while $\Delta E_f^{(-2)}$ and $\Delta E_g^{(-2)}$ are eight-dimensional integrals. They have been calculated using two different methods. The first one is a series expansion in x; the results can be supplied on request. Thus, for the spin-$\frac{1}{2}$ model, the series for E_0/N in x from the fourth-order spin-wave theory is

$$\frac{E_0^{\text{fourth}}}{N} = -\frac{1}{2} - \frac{85x^2}{512} - 0.002\,974\,955\,0x^4 +0.000\,653\,517\,49x^6 + 0.000\,270\,572\,6x^8 +0.000\,010\,691x^{10} + O(x^{12}) , \tag{4.6}$$

clearly, this series is closer to the exact series than that for third-order spin-wave theory.[14]

The most interesting thing here is the ground-state energy at the isotropic limit ($x=1$). The series obtained seems to be too short to give a reliable extrapolation to $x=1$, but we can also use another technique: the finite-lattice technique discussed in the first section. We evaluate numerically Eq. (4.1) by dividing the first Brillouin zone into a finite number of meshes, $L_l \times L_l$, and extrapolate the sum to $L_l \to \infty$. For small x, this technique confirms the results of the above series expansion. For x close to 1, the results for $\Delta E_f^{(-2)}$ are shown in Fig. 3 as an example. Extrapolating to $x=1$ and $L_l \to \infty$, we can get

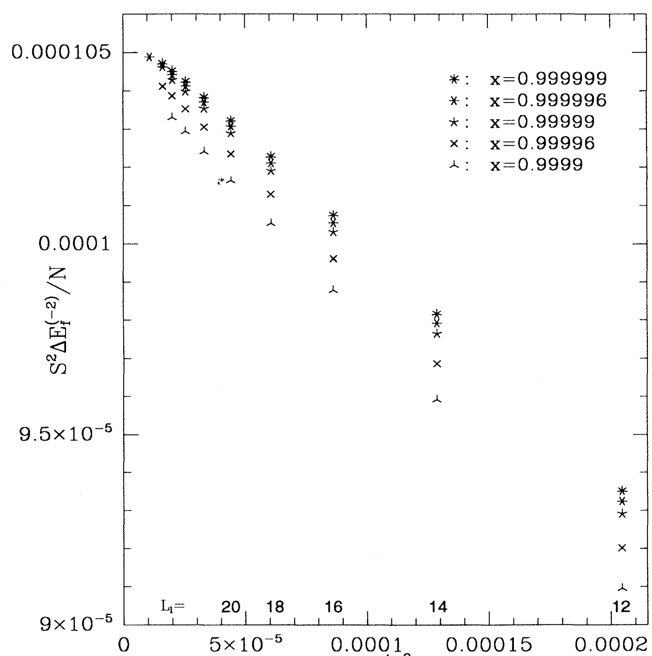

FIG. 3. The estimates of $S^2\Delta E_f^{(-2)}/N$ as a function of the lattice size L and anisotropy parameter x.

$$\Delta E_b^{(-1)}/N = \frac{0.000\,428\,5(4)}{2S}\,,$$
$$\Delta E_f^{(-2)}/N = \frac{0.000\,105\,4(4)}{S^2}\,, \tag{4.7}$$
$$\Delta E_g^{(-2)}/N = \frac{3.61(4)\times 10^{-5}}{S^2}\,,$$

where the results for $\Delta E_b^{(-1)}/N$ are consistent with our previous results,[14] but substantially more accurate. The results for $\Delta E_b^{(-2)}$ can be found by using relation (4.3):

$$\Delta E_b^{(-2)}/N = -\frac{6.768(6)\times 10^{-5}}{(2S)^2}\,. \tag{4.8}$$

Therefore, we conclude that for the square lattice

$$E_0/N = -2S^2 - 0.315\,894\,842S - 0.012\,473\,693\,9 + 0.000\,214\,2(2)/S + 1.246(9)\times 10^{-4}/S^2 + O(S^{-3}). \tag{4.9}$$

If we use Padé approximants[21] to analyze the above series, we get

$$E_0/N = \begin{cases} -0.6693(2), & S=\frac{1}{2}, \\ -2.328\,01(4), & S=1. \end{cases} \tag{4.10}$$

V. SUMMARY AND CONCLUSIONS

As further results of spin-wave perturbation theory for the Heisenberg antiferromagnet, we have calculated the finite-lattice corrections to the ground-state energy and the staggered magnetization, and also the finite-lattice energy gap, for both the one-dimensional linear chain and two-dimensional square lattice. We have also calculated the spin-wave velocity, and the ground-state energy to order $O(1/S^2)$ for the square lattice.

For the one-dimensional linear chain, spin-wave theory gives the conformal anomaly as

$$c = 2 \tag{5.1}$$

precisely, through second order in the expansion, whereas the true value[16] is $c=1$. This is no great surprise, since it is already well known that spin-wave theory fails to describe the one-dimensional chain, incorrectly predicting a nonzero staggered magnetization, and a mass gap which vanishes for all spins.

For the square lattice of size $N=L^2$, our results may be summarized as follows

Bulk ground-state energy per site,

$$e_\infty = \lim_{N\to\infty}\frac{E_0}{N} = -2S^2 - 0.315\,894\,842S - 0.012\,473\,693\,9 + \frac{0.000\,214\,2(2)}{S} + \frac{0.000\,124\,6(9)}{S^2} + O(S^{-3})\,, \tag{5.2}$$

with finite-lattice correction

$$\frac{E_0}{N} - e_\infty = -\frac{4.066\,56S + 0.321\,151 + O(S^{-1})}{L^3} + \cdots\,. \tag{5.3}$$

Bulk staggered magnetization,

$$M_\infty^+ = S - 0.196\,601\,9 + 0.000\,866(25)S^{-2} + O(S^{-3})\,, \tag{5.4}$$

with "finite-lattice correction"

$$M_N^+ - M_\infty^+ = \frac{0.877\,868\,0 + 0\times S^{-1} + O(S^{-2})}{L} + \cdots\,. \tag{5.5}$$

Transverse susceptibility[14],

$$\chi_\perp = \frac{1}{8} - 0.034\,447S^{-1} + 0.001\,701(3)S^{-2} + O(S^{-3})\,. \tag{5.6}$$

Dispersion relation in the small k limit

$$E(k) = 2\sqrt{2}S\left(1 + \frac{0.157\,947\,421}{2S} + \frac{0.021\,52(2)}{(2S)^2} + O(S^{-3})\right)k\,. \tag{5.7}$$

Finite-lattice energy gap,

$$m_N = [8 + O(S^{-1})]/L^2\,. \tag{5.8}$$

Spin-wave velocity renormalization factor,

$$Z_c = E(k)/(2\sqrt{2}Sk) = 1 + \frac{0.157\,947\,421}{2S} + \frac{0.021\,52(2)}{(2S)^2} + O(S^{-3})\,. \tag{5.9}$$

Spin-stiffness constant ρ_s,

$$\rho_s = v^2\chi_\perp = S^2\left[1 - \frac{0.235\,25}{2S} - \frac{0.0517(2)}{(2S)^2} + O(S^{-3})\right]\,. \tag{5.10}$$

The spin-wave velocity Z_c was calculated through both the Dyson-Maleev and Holstein-Primakoff transformations, and the fourth-order ground-state energy via the Dyson-Maleev formalism. As before,[14] in the Holstein-Primakoff formalism there are some divergent terms, but the divergences eventually cancel one another. Our result for the spin-wave velocity is different from that of Igarashi and Watabe,[11] but agrees with that of Canali, Girvin, and Wallin,[12] and the spin-stiffness constant is consistent with the direct calculation of Igarashi and Watabe.[11] Obviously, the corrections of high orders are pretty small, and the spin-wave theory continues to give consistent results, and improved convergence towards the exact values. These results should be compared with other estimates: for the spin-$\frac{1}{2}$ model, Runge[22] finds that $E_0/N = -0.669\,34(3)$ and $Z_c = 1.10(3)$ using a Green's function Monte Carlo method, while Singh[23] predicts that $Z_c = 1.18(2)$ and $\rho_s = 0.73(4)$ using a series expansion.

The finite-lattice predictions from the effective theory of Neuberger and Ziman[3], and Fisher[4] amount to six relations, which are

$$\frac{E_0}{N} - e_\infty = \frac{2\beta v}{L^3} \ , \tag{5.11}$$

$$M_\infty^+ = 2\kappa_1\kappa_2 \ , \tag{5.12}$$

$$M_N^+ - M_\infty^+ = -\frac{\kappa_1\alpha}{2\kappa_2 L} \ , \tag{5.13}$$

$$\chi_\perp = 2\kappa_2^2/v \ , \tag{5.14}$$

$$E(k) = vk \ , \tag{5.15}$$

$$m_N = \frac{1}{\chi_\perp L^2} \ , \tag{5.16}$$

involving two calculable structure constants $\alpha = -0.6208$, $\beta = -0.7186$, and three unknown microscopic parameters κ_1, κ_2, and v. Comparing (5.11)–(5.16) with (5.3)–(5.8), we find these predictions are exactly satisfied, order by order in spin-wave perturbation theory as far as we have calculated, with $\alpha = -0.620\,746\,4$, $\beta = -0.718\,87$, the velocity v given by

$$v = \frac{E(k)}{k} = 2\sqrt{2}S\left(1 + \frac{0.157\,947\,421}{2S} + \frac{0.021\,52(2)}{(2S)^2} + O(S^{-3})\right) , \tag{5.17}$$

and

$$\kappa_1 = S^{1/2}\left(2^{1/4} - \frac{0.116\,900}{S} - \frac{0.004\,10(2)}{S^2} + O(S^{-3})\right) , \tag{5.18}$$

$$\kappa_2 = S^{1/2}\left(2^{-5/4} - \frac{0.041\,330\,5}{S} - \frac{0.002\,615(8)}{S^2} + O(S^{-3})\right) .$$

This agreement is very satisfying, and helps to give us confidence that the spin-wave results are correct.

The finite-lattice energy gap has been measured by Carlson[24] using a Green's function Monte Carlo method, with the result

$$\begin{aligned} \Delta E(j=1) &\simeq 10/L^2 \qquad \text{for total spin}-1, \\ \Delta E(j=2) &\simeq 29/L^2 \qquad \text{for total spin}-2, \end{aligned} \tag{5.19}$$

while from the data of Runge[22] we obtain

$$\begin{aligned} \Delta E &\simeq 5.2j(j+1)/L^2 \qquad \text{for} \quad L=6, \\ \Delta E &\simeq 5.4j(j+1)/L^2 \qquad \text{for} \quad L=8. \end{aligned} \tag{5.20}$$

Similar results can be found in the paper by Gross *et al.*[25] The leading order spin-wave result (2.18) is

$$\Delta E = \frac{4j(j+1)}{L^2} \ . \tag{5.21}$$

If we use the relation (5.16) together with (5.6), the higher-order result is predicted to be

$$\begin{aligned} \Delta E = {} & [4 + 1.102\,304/S \\ & + 0.2493(1)/S^2 + O(S^{-3})]\frac{j(j+1)}{L^2}, \\ \simeq {} & 7.202j(j+1)/L^2 \ , \end{aligned} \tag{5.22}$$

although this has not been confirmed by direct calculation. The result is at least in the same ballpark as the "experiment."

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