

Third-order spin-wave theory for the Heisenberg antiferromagnet

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Spin-wave perturbation theory for the anisotropic Heisenberg antiferromagnet at zero temperature is carried to third order, using both the Dyson-Maleev and Holstein-Primakoff formalisms. Physical quantities calculated include the ground-state energy, staggered magnetization, staggered parallel susceptibility, transverse susceptibility, and energy gap. For the Holstein-Primakoff formalism, some terms diverge in the isotropic limit, but these divergences eventually cancel one another, and the final results are the same as for the Dyson-Maleev formalism. Applying these results to the square-lattice case, we find that the convergence of the spin-wave theory towards our recent series estimates is further improved if we promote the spin-wave theory to third order.

I. INTRODUCTION

There have been a large number of studies made recently of the Heisenberg antiferromagnet on a square lattice, motivated by the possible relevance of this model to high- T_c superconductors: for a review, see Barnes.¹ The general conclusion has been that at zero temperature the isotropic Heisenberg antiferromagnet is in an ordered state, with a nonzero staggered magnetization, corresponding to a spontaneously broken symmetry.

One fruitful method of numerical analysis has been to consider the anisotropic model first, and to perform a series expansion about the Ising limit.²⁻⁷ The series can then be extrapolated to the isotropic limit, using various means, with remarkable accuracy. In a recent paper,⁸ we extended these series by several terms, and showed that the results were in excellent agreement both with Monte Carlo (MC) simulations¹ and with the predictions of spin-wave theory. For each quantity calculated, second-order spin-wave theory provided a much more accurate representation than the first-order theory. It was natural, then, to ask whether the spin-wave calculations could be pushed to even higher order, and converge even closer to the exact results. This is the object of the present work.

Spin-wave theory for the Heisenberg antiferromagnet was first developed long ago. The original theory of Anderson⁹ was extended to second order by Kubo¹⁰ and Oguchi,¹¹ while the singular behavior of the anisotropic model was further discussed by Stinchcombe.¹² A fairly comprehensive treatment of the anisotropic model up to second order was presented by us in Refs. 8 and 13.

The spin-wave theory relies on a transformation from the original spin degrees of freedom to boson degrees of freedom. There are two different, but closely related, ways of doing this. The first, due to Holstein and Primakoff,¹⁴ involves the square root of an operator

$$f_l(S) = \left(1 - \frac{n_l}{2S}\right)^{1/2}, \quad (1.1)$$

where S is the spin per site, and n_l is the boson number operator, measuring the "spin deviation" at site l . The only way of dealing with this square root has been to perform a power-series expansion of $f_l(S)$, leading to an expansion in powers of $1/S$. The nature of this expansion has been discussed by Kubo:¹⁵ it is thought to be an asymptotic series only.

The second transformation, due to Dyson¹⁷ and Maleev,¹⁸ avoids the use of a square-root operator at the expense of a formalism in which the Hamiltonian is no longer manifestly Hermitian. The Dyson-Maleev formalism is easier to use in practice than the Holstein-Primakoff one in that the Hamiltonian takes a simple form, and matrix elements are less singular than in the latter case. If calculations are performed consistently to a given order in $1/S$, however, it appears that both transformations will eventually give the same final results – at least up to the order calculated so far.

Higher-order spin-wave calculations for the Heisenberg antiferromagnet have hitherto been carried out by Harris *et al.*¹⁹ and Kopietz,²⁰ who studied magnon damping at low temperature, by Castilla and Chakravarty,²¹ who calculated the staggered magnetization at zero temperature, and also by Igarashi and Watabe,²² who calculated the spin-wave velocity, the staggered magnetization, the transverse susceptibility, and the spin-stiffness constant at zero temperature. References 19–21 relied primarily on the Dyson-Maleev transformation, and Ref. 22 used the Holstein-Primakoff transformation. The result for the staggered magnetization of Castilla and Chakravarty²¹ disagrees with that of Igarashi and Watabe.²²

In the present work, we calculate the ground-state energy, staggered magnetization, energy gap, parallel staggered susceptibility, and transverse susceptibility to third order in the $1/S$ expansion, using both the Dyson-Maleev and Holstein-Primakoff transformations. The calculation involves some six-dimensional and four-dimensional integrations, which are carried out using two different methods: a series expansion via MATHEMATICA, and a Monte

Carlo integration. Although individual diagrams tend to be more divergent in the Holstein-Primakoff case, these divergences cancel exactly in the final results, which is the same for both transformations. We find that in general the third-order corrections are small, and show further convergence towards the "exact" results estimated from series expansions and Monte Carlo simulations.

The arrangement of the paper is as follows: In Sec. II we give the third-order spin wave theory for the Dyson-Maleev formalism and its application to the square lattice. In Sec. III we discuss the third-order spin-wave theory for the Holstein-Primakoff formalism, and make a careful comparison with the results of the Dyson-Maleev formalism. In Sec. IV our conclusions are summarized.

II. DYSON-MALEEV FORMALISM

The anisotropic Heisenberg antiferromagnet with magnetic field on a bipartite lattice can be described by the

following Hamiltonian:

$$H = \sum_{\langle lm \rangle} [S_l^z S_m^z + x(S_l^x S_m^x + S_l^y S_m^y)] + h_1 \sum_l S_l^z + h_2 \sum_m S_m^z, \quad (2.1)$$

where we have divided the lattice sites into even and odd sublattices, denoted by l and m respectively, and $x = 1$ corresponds to the isotropic Heisenberg model. The introduction of magnetic fields h_1 and h_2 is for convenience in the calculation of the magnetization and parallel susceptibility.

We firstly introduce boson operators a_l and b_m via the Dyson-Maleev transformation on the l and m sublattices, respectively:

$$S_l^z = S - a_l^\dagger a_l, \quad S_l^+ = (2S)^{1/2} a_l - (2S)^{-1/2} a_l^\dagger a_l a_l, \quad S_l^- = (2S)^{1/2} a_l^\dagger, \quad (2.2)$$

$$S_m^z = b_m^\dagger b_m - S, \quad S_m^+ = (2S)^{1/2} b_m^\dagger - (2S)^{-1/2} b_m^\dagger b_m^\dagger b_m, \quad S_m^- = (2S)^{1/2} b_m.$$

Note that this transformation is not Hermitian. In terms of the boson operators, the Hamiltonian can be expressed as:

$$H = -SN(Sz - h_1 + h_2)/2 + (zS - h_1) \sum_l a_l^\dagger a_l + (zS + h_2) \sum_m b_m^\dagger b_m + xS \sum_{\langle lm \rangle} (a_l b_m + a_l^\dagger b_m^\dagger) - \sum_{\langle lm \rangle} a_l^\dagger a_l b_m^\dagger b_m - \frac{x}{2} \sum_{\langle lm \rangle} (a_l^\dagger a_l a_l b_m + a_l^\dagger b_m^\dagger b_m^\dagger b_m). \quad (2.3)$$

Then, as in Ref. 8, we can introduce the Bloch-type boson operators a_k, b_k by a Fourier transformation:

$$a_k = \left(\frac{2}{N}\right)^{1/2} \sum_l e^{ikl} a_l, \quad b_k = \left(\frac{2}{N}\right)^{1/2} \sum_m e^{-ikm} b_m, \quad (2.4)$$

where N is the total number of lattice sites. The quadratic part of H can be diagonalized by a Bogoliubov transformation:

$$a_k = \alpha_k \cosh \theta_k - \beta_k^\dagger \sinh \theta_k, \quad b_k = -\alpha_k^\dagger \sinh \theta_k + \beta_k \cosh \theta_k, \quad (2.5)$$

where $\tanh 2\theta_k = x\gamma_k/D$, $D = 1 - (h_1 - h_2)/(2zS)$, z is the coordination number of the lattice (i.e., 4 for the square lattice), and γ_k is the structure factor:

$$\gamma_k = \frac{1}{z} \sum_\rho e^{ik\rho}. \quad (2.6)$$

The Hamiltonian now can be expressed as

$$H = \mathcal{E}_h + \sum_k (\mathcal{A}_k^- n_k + \mathcal{A}_k^+ n'_k) + \sum_{k_1, k_2} [\mathcal{B}^{(1)}(n_1 n_2 + n'_1 n'_2) + \mathcal{B}^{(2)} n_1 n'_2] + \sum_k \mathcal{V}_0^{(0)} (\alpha_k \beta_k + \alpha_k^\dagger \beta_k^\dagger) - \frac{z}{2N} \sum_{k_i} \delta_{1+2,3+4} [\mathcal{V}_1^{(0)} (\beta_1^\dagger \beta_2^\dagger \beta_3 \beta_4 + \alpha_3^\dagger \alpha_4^\dagger \alpha_1 \alpha_2) - 2\mathcal{V}_2^{(0)} (\alpha_3^\dagger \beta_4 \alpha_1 \alpha_2 + \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger \beta_3) - 2\mathcal{V}_3^{(0)} (\alpha_3^\dagger \alpha_4^\dagger \alpha_2 \beta_1^\dagger + \alpha_1 \beta_2^\dagger \beta_3 \beta_4) + 2\mathcal{V}_4^{(0)} (\alpha_3^\dagger \alpha_1 \beta_2^\dagger \beta_4 + \alpha_4^\dagger \alpha_2 \beta_1^\dagger \beta_3) + \mathcal{V}_5^{(0)} (\alpha_3^\dagger \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger + \alpha_1 \alpha_2 \beta_3 \beta_4)], \quad (2.7)$$

where we have adopted the convention of writing $\mathbf{1}$ instead of \mathbf{k}_1 , and \sum' sums over the purely off-diagonal momentum space. The definitions of n_k , n'_k , \mathcal{E}_h , \mathcal{A}_k^\pm , and $\mathcal{B}^{(i)}$ are as follows:

$$\begin{aligned} n_k &= \alpha_k^\dagger \alpha_k, \quad n'_k = \beta_k^\dagger \beta_k, \\ \frac{\mathcal{E}_h}{N} &= -S^2 z (D - \frac{1}{2}) + \frac{z D S C_1}{2} - \frac{z}{8} \left\{ [(1-D)C_{-1} + D C_1]^2 + D^2 (C_{-1} - C_1)^2 \frac{(1-x^2)}{x^2} \right\}, \end{aligned} \quad (2.8)$$

$$\begin{aligned} \mathcal{A}_k^\pm &= z S \left[(D^2 - x^2 \gamma_k^2)^{1/2} \pm \frac{1}{2zS} (h_1 + h_2) \right] - \frac{z}{N} \left\{ \frac{D - x^2 \gamma_k^2}{(D^2 - x^2 \gamma_k^2)^{1/2}} \sum_{k_2} \left(\frac{D - x^2 \gamma_{k_2}^2}{(D^2 - x^2 \gamma_{k_2}^2)^{1/2}} - 1 \right) \right. \\ &\quad \left. + \frac{x^2 (1-x^2) \gamma_k^2}{(D^2 - x^2 \gamma_k^2)^{1/2}} \sum_{k_2} \frac{\gamma_{k_2}^2}{(D^2 - x^2 \gamma_{k_2}^2)^{1/2}} \right\}, \end{aligned} \quad (2.9)$$

$$\mathcal{B}^{(1)} = -\frac{z}{2N} \left\{ \frac{D^2 - 2x^2 D \gamma_2^2 + x^2 \gamma_1 \gamma_2 \gamma_{1-2}}{(D^2 - x^2 \gamma_1^2)^{1/2} (D^2 - x^2 \gamma_2^2)^{1/2}} - 1 \right\}, \quad \mathcal{B}^{(2)} = -\frac{z}{N} \left\{ \frac{D^2 - 2x^2 D \gamma_2^2 + x^2 \gamma_1 \gamma_2 \gamma_{1-2}}{(D^2 - x^2 \gamma_1^2)^{1/2} (D^2 - x^2 \gamma_2^2)^{1/2}} + 1 \right\}, \quad (2.10)$$

where C_n is defined by

$$C_n = \frac{2}{N} \sum_k [(1 - x^2 \gamma_k^2 D^{-2})^{n/2} - 1]. \quad (2.11)$$

The two-particle vertex factor $\mathcal{V}_0^{(0)}(k)$ and four-particle vertex factors $\mathcal{V}_i^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4})$ ($i = 1, \dots, 5$) are the Dyson-Maleev vertices, their symmetrized form being (where s_i and c_i denote $\sinh \theta_{k_i}$ and $\cosh \theta_{k_i}$, respectively)

$$\begin{aligned} \mathcal{V}_0^{(0)} &= \frac{z}{2x} [C_{-1}(D - 2x^2 + x^2 D^{-1}) + C_1(x^2 - D)] \gamma_k (1 - x^2 \gamma_k^2 D^{-2})^{-1/2}, \\ \mathcal{V}_1^{(0)} &= \gamma_{3-2} c_1 s_2 s_3 c_4 + \gamma_{3-1} s_1 c_2 s_3 c_4 + \gamma_{4-2} c_1 s_2 c_3 s_4 + \gamma_{4-1} s_1 c_2 c_3 s_4 \\ &\quad - x(\gamma_3 s_1 s_2 c_3 s_4 + \gamma_4 s_1 s_2 s_3 c_4 + \gamma_4 c_1 c_2 c_3 s_4 + \gamma_3 c_1 c_2 s_3 c_4), \\ \mathcal{V}_2^{(0)} &= \gamma_{4-2} c_1 s_2 c_3 c_4 + \gamma_{4-1} s_1 c_2 c_3 c_4 + \gamma_{3-2} c_1 s_2 s_3 s_4 + \gamma_{3-1} s_1 c_2 s_3 s_4 \\ &\quad - x(\gamma_3 s_1 s_2 c_3 c_4 + \gamma_4 s_1 s_2 s_3 s_4 + \gamma_4 c_1 c_2 c_3 c_4 + \gamma_3 c_1 c_2 s_3 s_4), \\ \mathcal{V}_3^{(0)} &= \gamma_{4-1} c_1 c_2 c_3 s_4 + \gamma_{3-1} c_1 c_2 s_3 c_4 + \gamma_{3-2} s_1 s_2 s_3 c_4 + \gamma_{4-2} s_1 s_2 c_3 s_4 \\ &\quad - x(\gamma_3 c_1 s_2 c_3 s_4 + \gamma_4 c_1 s_2 s_3 c_4 + \gamma_4 s_1 c_2 c_3 s_4 + \gamma_3 s_1 c_2 s_3 c_4), \\ \mathcal{V}_4^{(0)} &= \gamma_{4-2} c_1 c_2 c_3 c_4 + \gamma_{3-2} c_1 c_2 s_3 s_4 + \gamma_{4-1} s_1 s_2 c_3 c_4 + \gamma_{3-1} s_1 s_2 s_3 s_4 \\ &\quad - x(\gamma_3 s_1 c_2 c_3 c_4 + \gamma_4 s_1 c_2 s_3 s_4 + \gamma_4 c_1 s_2 c_3 c_4 + \gamma_3 c_1 s_2 s_3 s_4), \\ \mathcal{V}_5^{(0)} &= \gamma_{4-2} s_1 c_2 c_3 s_4 + \gamma_{4-1} c_1 s_2 c_3 s_4 + \gamma_{4-1} s_1 c_2 s_3 c_4 + \gamma_{3-1} c_1 s_2 s_3 c_4 \\ &\quad - x(\gamma_3 s_1 s_2 s_3 c_4 + \gamma_4 s_1 s_2 c_3 s_4 + \gamma_4 c_1 c_2 s_3 c_4 + \gamma_3 c_1 c_2 s_3 c_4). \end{aligned} \quad (2.12)$$

For convenience in later calculations, we also define that, in zero magnetic field,

$$V_i^{(0)} = \mathcal{V}_i^{(0)}(h_1 = h_2 = 0) \quad (i = 0, \dots, 5), \quad C_n = C_n(h_1 = h_2 = 0). \quad (2.13)$$

Asymptotic expansions for C_n near $x = 1$ can be found in Ref. 8 for the square lattice and Ref. 13 for other lattices.

A. Ground-state energy

Using Rayleigh-Schrodinger perturbation theory, we can treat the terms containing $\mathcal{V}_i^{(0)}$ in the Hamiltonian Eq. (2.7) as perturbation terms, which are purely off-diagonal. Up to $O(1/S)$, there are only two extra terms contributing to the ground-state energy E_0 from these perturbations. They may be represented diagrammatically as in Fig. 1. The contribution from Fig. 1(a) is

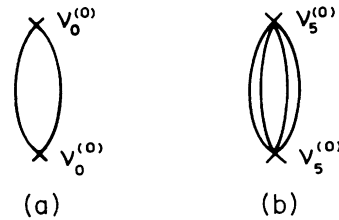


FIG. 1. The perturbation diagrams that contribute to the ground-state energy E_0/N . The crosses represent the interaction vertices as indicated; the lines represent boson excitations in the intermediate states. To save space, we have not differentiated between α and β bosons.

$$\Delta\mathcal{E}_a^{(-1)} = \sum_k \frac{[\mathcal{V}_0^{(0)}]^2}{-2zSD(1-x^2\gamma_k^2 D^{-2})^{1/2}} = -\frac{zDN}{16x^4 S} [C_{-1}(D-2x^2+x^2 D^{-1}) + C_1(x^2-D)]^2 (C_{-3} - C_{-1}); \quad (2.14)$$

the contribution from Fig. 1(b) is

$$\Delta\mathcal{E}_b^{(-1)} = -\frac{zN}{8SD} \left(\frac{2}{N}\right)^3 \sum_{k_i} \delta_{1+2,3+4} \frac{\mathcal{V}_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}) \mathcal{V}_5^{(0)}(\mathbf{3}, \mathbf{4}, \mathbf{1}, \mathbf{2})}{\sum_i (1-x^2\gamma_i^2 D^{-2})^{1/2}}. \quad (2.15)$$

Therefore, the ground-state energy per site \mathcal{E}_0/N for the Heisenberg antiferromagnet with external magnetic field is

$$\begin{aligned} \mathcal{E}_0/N = & -S^2 z(D-1/2) + zDSC_1/2 \\ & -\frac{z}{8} \{[(1-D)C_{-1} + DC_1]^2 + D^2(C_{-1} - C_1)^2(1-x^2)/x^2\} + \Delta\mathcal{E}_a^{(-1)}/N + \Delta\mathcal{E}_b^{(-1)}/N. \end{aligned} \quad (2.16)$$

In zero external magnetic field (i.e. $h_1 = h_2 = 0$), the ground-state energy E_0 is

$$\begin{aligned} E_0/N = & -\frac{zS}{2} \left[S - C_1 + \frac{1}{4S} \left(C_1^2 + \frac{1-x^2}{x^2} (C_{-1} - C_1)^2 \right) \right] \\ & -\frac{z}{16x^4 S} (1-x^2)^2 (C_{-1} - C_1)^2 (C_{-3} - C_{-1}) + \Delta E_b^{(-1)}/N, \end{aligned} \quad (2.17)$$

where

$$\Delta E_b^{(-1)} = \Delta\mathcal{E}_b^{(-1)}(h_1 = h_2 = 0). \quad (2.18)$$

$\Delta\mathcal{E}_b^{(-1)}$ is a six-dimensional integral over the first Brillouin zone of the sublattice l , the integrand being singular at $x = 1$. It has been calculated using two different methods. The first one is a series expansion in x : via MATHEMATICA, we can expand $\Delta E_b^{(-1)}$ into a power series about $x = 0$, where the expansion coefficients are of the form

$$\sum_{i,j,k,l,m,n} a_{i,j,k,l,m,n} \gamma_1^i \gamma_2^j \gamma_3^k \gamma_4^l \gamma_5^m \gamma_6^n, \quad (2.19)$$

which is integrable analytically (where $a_{i,j,k,l,m,n}$ is a constant). The second method is a Monte Carlo integration. For the square lattice, the results of the series expansion are

$$\begin{aligned} \Delta E_b^{(-1)} = & \frac{N}{2S} [0.00128173828125x^4 + 0.000324249267578125x^6 + 0.000012166798114777x^8 \\ & -0.000082444283179939x^{10} - 0.00010488787211216x^{12} - 0.00010292760305219x^{14} \\ & -0.000093275871366177x^{16} - 0.000081998597367727x^{18} - 0.000071262011849609x^{20} \\ & -0.000061745507075153x^{22} - 0.000053558412862410x^{24} - 0.000046602384643213x^{26} \\ & -0.000040716885275295x^{28} - 0.000035736530468971x^{30} + O(x^{32})]. \end{aligned} \quad (2.20)$$

For the spin- $\frac{1}{2}$ model, the series for E_0/N in x from second-order and third-order spin-wave theory, and the exact series⁸ for E_0/N are, respectively,

$$\begin{aligned} \frac{E_0^{2\text{nd}}}{N} = & -\frac{1}{2} - \frac{5x^2}{32} - \frac{3x^4}{256} - 0.00234985x^6 - 0.000627041x^8 - 0.000165582x^{10} + O(x^{12}), \\ \frac{E_0^{3\text{rd}}}{N} = & -\frac{1}{2} - \frac{21x^2}{128} - \frac{95x^4}{16384} - 0.000202179x^6 + 0.000185855x^8 + 0.000137933x^{10} + O(x^{12}), \\ \frac{E_0^{\text{exact}}}{N} = & -\frac{1}{2} - \frac{x^2}{6} + \frac{x^4}{1080} - 0.00158157x^6 - 0.000825213x^8 - 0.00031185x^{10} + O(x^{12}). \end{aligned} \quad (2.21)$$

Clearly, the series for third-order spin-wave theory is closer to the exact series than that for second-order spin-wave theory.

Extrapolating the series $\Delta E_b^{(-1)}$ using integrated Dlog Padé approximants²³ in $\delta = 1 - (1-x^2)^{1/2}$, one can obtain an estimate at the isotropic limit $x = 1$:

$$\Delta E_b^{(-1)}/N = \frac{0.000432(12)}{2S}; \quad (2.22)$$

The extrapolation of the full series for E_0/N [that is, Eq. (2.17)] in δ gives

$$E_0/N = \begin{cases} -0.669989(16), & S = \frac{1}{2}; \\ -2.328153(10), & S = 1. \end{cases} \quad (2.23)$$

Extracting the integrable part, we get

$$\Delta E_b^{(-1)}/N = \begin{cases} 0.000433(16), & S = \frac{1}{2}; \\ 0.000216(10), & S = 1. \end{cases} \quad (2.24)$$

The above series estimates are consistent with the results of a numerical integration:

$$\Delta E_b^{(-1)}/N = \frac{0.00045(2)}{2S} \quad (x = 1). \quad (2.25)$$

Therefore, we conclude that for the square lattice

$$E_0/N = -2S^2 - 0.315895S - 0.012474 + 0.000216(6)/S + O(S^{-2}). \quad (2.26)$$

B. Staggered magnetization and parallel staggered susceptibility

Let $h_1 = -h_2 = h$, and differentiate Eq. (2.16) with respect to h , then one finds the staggered magnetization M^+ and parallel staggered susceptibility $\chi_{//}^S$:

$$M^+ = \frac{1}{N} \frac{\partial \mathcal{E}_0}{\partial h} \Big|_{h=0} = S - \frac{C_{-1}}{2} - \frac{1-x^2}{4Sx^2} (C_{-1} - C_1)(C_{-3} - C_{-1}) + \Delta M_a^{(-2)} + \Delta M_b^{(-2)}, \quad (2.27)$$

$$\chi_{//}^S = -\frac{1}{N} \frac{\partial^2 \mathcal{E}_0}{\partial h^2} \Big|_{h=0} = \frac{1}{2zS} (C_{-3} - C_{-1}) + \frac{1}{4zS^2} \left\{ \frac{1-x^2}{x^2} [(C_{-1} - C_1)(C_{-1} + 3C_{-5} - 4C_{-3}) + (C_{-3} - C_{-1})^2] \right. \\ \left. + C_1(C_{-3} - C_{-1}) \right\} + \Delta \chi_a^{(-3)} + \Delta \chi_b^{(-3)}, \quad (2.28)$$

where

$$\Delta M_a^{(-2)} = \frac{1}{N} \frac{\partial \Delta \mathcal{E}_a^{(-1)}}{\partial h} \Big|_{h=0} \\ = -\frac{1}{16x^4 S^2} (1-x^2)(C_{-1} - C_1) \\ \times \{ (1-x^2)[3C_{-5}(C_{-1} - C_1) + 4C_{-1}^2 - 9C_{-1}C_{-3} + 2C_{-3}^2 - 3C_{-3}C_1] + 2C_1(C_{-3} - C_{-1}) \}, \quad (2.29)$$

$$\Delta M_b^{(-2)} = \frac{1}{N} \frac{\partial \Delta \mathcal{E}_b^{(-1)}}{\partial h} \Big|_{h=0}; \\ \Delta \chi_a^{(-3)} = -\frac{1}{N} \frac{\partial^2 \Delta \mathcal{E}_a^{(-1)}}{\partial h^2} \Big|_{h=0} \\ = \frac{1}{16S^3 z x^4} [2C_{-3}C_1^2 - 2C_{-1}C_1^2 \\ + (1-x^2)^2 (2C_{-3}^3 + 18C_{-5}C_{-3}C_{-1} - 34C_{-3}^2C_{-1} + 15C_{-7}C_{-1}^2 - 48C_{-5}C_{-1}^2 + 61C_{-3}C_{-1}^2 \\ - 14C_{-1}^3 - 18C_{-5}C_{-3}C_1 + 24C_{-3}^2C_1 - 30C_{-7}C_{-1}C_1 + 66C_{-5}C_{-1}C_1 \\ - 48C_{-3}C_{-1}C_1 + 6C_{-1}^2C_1 + 15C_{-7}C_1^2 - 18C_{-5}C_1^2 + 3C_{-3}C_1^2) \\ + (1-x^2)(4C_{-3}^2C_1 + 12C_{-5}C_{-1}C_1 - 24C_{-3}C_{-1}C_1 + 8C_{-1}^2C_1 - 12C_{-5}C_1^2 + 12C_{-3}C_1^2)], \\ \Delta \chi_b^{(-3)} = -\frac{1}{N} \frac{\partial^2 \Delta \mathcal{E}_b^{(-1)}}{\partial h^2} \Big|_{h=0}. \quad (2.30)$$

Although these expressions are quite complicated, the above derivatives can be easily carried out via MATHEMATICA. Via MATHEMATICA, we also can prove that

$$\Delta M_b^{(-2)} = -\frac{1}{16S^2} \left(\frac{2}{N} \right)^3 \sum_{k_i} \delta_{1+\mathbf{2},\mathbf{3}+\mathbf{4}} \left\{ 2[V_5^{(0)}]^2 \left[\sum_{i=1}^4 \frac{1}{(1-x^2\gamma_i^2)^{1/2}} \right] \left[\sum_{i=1}^4 (1-x^2\gamma_i^2)^{1/2} \right]^{-2} \right. \\ \left. + V_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}) [V_2^{(0)}(\mathbf{3}, \mathbf{4}, \mathbf{1}, \mathbf{2}) + V_3^{(0)}(\mathbf{4}, \mathbf{3}, \mathbf{1}, \mathbf{2})] \frac{\sum_i \frac{x\gamma_i}{(1-x^2\gamma_i^2)}}{\sum_i (1-x^2\gamma_i^2)^{1/2}} \right\}. \quad (2.31)$$

In the limit $x = 1$, the above formula for the staggered magnetization agrees with that of Castilla and Chakravarty²¹ (note that there is a sign difference in the definition of some vertices $V_i^{(0)}$).

The series results for $\Delta M_b^{(-2)}$ and $\Delta \chi_b^{(-3)}$ are

$$\begin{aligned} \Delta M_b^{(-2)} = \frac{1}{8S^2} [& 0.00640869140625x^4 + 0.0046501159667969x^6 + 0.0029826834797859x^8 \\ & + 0.0018767764559016x^{10} + 0.0011732400171240x^{12} + 0.00072314925716910x^{14} \\ & + 0.00043070786120816x^{16} + 0.00023760905449608x^{18} + 0.00010833363513788x^{20} \\ & + 0.000020892898846470x^{22} - 0.000038605089915444x^{24} - 0.000079121460409459x^{26} \\ & - 0.00010655268617341x^{28} - 0.00012485066948381x^{30} - 0.00013670867820712x^{32} \\ & - 0.00014398999285620x^{34} + O(x^{36})], \end{aligned} \tag{2.32}$$

$$\begin{aligned} \Delta \chi_b^{(-3)} = \frac{1}{16S^3} [& -0.01531982421875x^4 - 0.0193939208984375x^6 - 0.0195425525307655x^8 \\ & - 0.018459238344803x^{10} - 0.017114416566994x^{12} - 0.015738031119135x^{14} \\ & - 0.014474118591607x^{16} - 0.013386613963396x^{18} - 0.012440583026018x^{20} + O(x^{22})]. \end{aligned} \tag{2.33}$$

For the spin- $\frac{1}{2}$ model, the series for M^+ in x from second-order and third-order spin-wave theory, and the exact series⁸ for M^+ are

$$\begin{aligned} M_{2nd}^+ &= \frac{1}{2} - \frac{3x^2}{32} - \frac{31x^4}{1024} - 0.0149841x^6 - 0.00900531x^8 - 0.00605425x^{10} + O(x^{12}), \\ M_{3rd}^+ &= \frac{1}{2} - \frac{27x^2}{256} - \frac{891x^4}{32768} - 0.0115871x^6 - 0.00638643x^8 - 0.00413427x^{10} + O(x^{12}), \\ M_{exact}^+ &= \frac{1}{2} - \frac{x^2}{9} - \frac{4x^4}{225} - 0.00947129x^6 - 0.00744292x^8 - 0.00437691x^{10} + O(x^{12}). \end{aligned} \tag{2.34}$$

Again, the series for third-order spin-wave theory is closer to the exact series than that for second-order spin-wave theory.

Analyzing the series $\Delta M_b^{(-2)}$ and $\Delta \chi_b^{(-3)}$, we get at $x = 1$

$$\Delta M_b^{(-2)} = \frac{0.00696(8)}{8S^2}, \tag{2.35}$$

$$(1 - x^2)^{1/2} \Delta \chi_b^{(-3)} = -\frac{0.052(3)}{16S^3}.$$

Note that at the limit of $x \rightarrow 1$,

$$(1 - x^2)^{1/2} \Delta \chi_a^{(-3)} = 0.0060975S^{-3}, \tag{2.36}$$

so

$$(1 - x^2)^{1/2} (\Delta \chi_a^{(-3)} + \Delta \chi_b^{(-3)}) = 0.0028(2)S^{-3}. \tag{2.37}$$

The analysis of the full series M^+ and $\chi_{//}^S$ gives at $x = 1$:

$$M^+ = \begin{cases} 0.3069(2), & S = \frac{1}{2}; \\ 0.80428(4), & S = 1, \end{cases} \tag{2.38}$$

$$(1 - x^2)^{1/2} \chi_{//}^S = \begin{cases} 0.239(3), & S = \frac{1}{2}; \\ 0.098(2), & S = 1, \end{cases} \tag{2.39}$$

which means that,

$$\Delta M_b^{(-2)} = \begin{cases} 0.00088(6)S^{-2}, & S = \frac{1}{2}; \\ 0.00088(4)S^{-2}, & S = 1, \end{cases} \tag{2.40}$$

$$(1 - x^2)^{1/2} (\Delta \chi_a^{(-3)} + \Delta \chi_b^{(-3)}) = \begin{cases} 0.0022(4)S^{-3}, & S = \frac{1}{2}; \\ 0.003(2)S^{-3}, & S = 1. \end{cases} \tag{2.41}$$

The above estimate for $\Delta M_b^{(-2)}$ at $x = 1$ is consistent with the results of numerical integration, although the numerical integrations are not very accurate. We have not carried out the numerical integration for $\Delta \chi_b^{(-3)}$ because it is too complicated, and also divergent. We conclude that for a square lattice

$$\begin{aligned} M^+ &= S - 0.1966019 + 0.00087(1)S^{-2} + O(S^{-3}), \\ (1 - x^2)^{1/2} \chi_{//}^S &= [0.07957747S^{-1} + 0.0156451S^{-2} + 0.0026(4)S^{-3} + O(S^{-4})]. \end{aligned} \tag{2.42}$$

C. Energy gap

Here we only consider the case without external magnetic field (i.e., $h_1 = h_2 = 0$). According to the Rayleigh-Schrödinger perturbation theory, up to order $O(1/S)$, there are five diagrams in Fig. 2 contributing to the energy gap m . We denote the contribution from Fig. 2(a) as $\Delta m_a^{(-1)}$ etc, as before:

$$\begin{aligned}
 \Delta m_a^{(-1)} &= -\frac{z}{8x^2S}(1-x^2)^{1/2}(C_{-1}-C_1)^2, \\
 \Delta m_b^{(-1)} &= -\frac{z}{2S}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{1+2,3} \frac{V_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, 0)V_5^{(0)}(\mathbf{3}, 0, \mathbf{1}, \mathbf{2})}{\sum_{i=1}^3(1-x^2\gamma_i^2)^{1/2} + (1-x^2)^{1/2}}, \\
 \Delta m_c^{(-1)} &= -\frac{z}{2S}\left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{1+2,3} \frac{V_3^{(0)}(\mathbf{3}, 0, \mathbf{1}, \mathbf{2})V_2^{(0)}(\mathbf{1}, \mathbf{2}, 0, \mathbf{3})}{\sum_{i=1}^3(1-x^2\gamma_i^2)^{1/2} - (1-x^2)^{1/2}}, \\
 \Delta m_d^{(-1)} &= -\frac{z(1-x^2)(C_{-1}-C_1)}{4xS}\left(\frac{2}{N}\right) \sum_k \frac{\gamma_k V_2^{(0)}(\mathbf{k}, 0, 0, \mathbf{k})}{(1-x^2\gamma_k^2)^{1/2}}, \\
 \Delta m_e^{(-1)} &= -\frac{z(1-x^2)(C_{-1}-C_1)}{4xS}\left(\frac{2}{N}\right) \sum_k \frac{\gamma_k V_3^{(0)}(\mathbf{k}, 0, 0, \mathbf{k})}{(1-x^2\gamma_k^2)^{1/2}},
 \end{aligned}
 \tag{2.43}$$

and

$$\Delta m_d^{(-1)} + \Delta m_e^{(-1)} = -\frac{z}{4x^2S}(1-x^2)^{3/2}(C_{-1}-C_1)(C_{-3}-C_{-1}).
 \tag{2.44}$$

Therefore, the energy gap m is

$$m = m^{(1)} + m^{(0)} + m^{(-1)},
 \tag{2.45}$$

where

$$\begin{aligned}
 m^{(1)} &= zS(1-x^2)^{1/2}, \\
 m^{(0)} &= -zC_{-1}(1-x^2)^{1/2}/2, \\
 m^{(-1)} &= -\frac{z}{8x^2S}(1-x^2)^{1/2}(C_{-1}-C_1)[C_{-1}-C_1 + 2(1-x^2)(C_{-3}-C_{-1})] + \Delta m_b^{(-1)} + \Delta m_c^{(-1)}.
 \end{aligned}
 \tag{2.46}$$

Note that $\Delta m_b^{(-1)}$ and $\Delta m_c^{(-1)}$ are each finite at the isotropic limit $x \rightarrow 1$, but using MATHEMATICA, we can prove that

$$\Delta m_b^{(-1)} + \Delta m_c^{(-1)} = -\frac{z}{2S}(1-x^2)^{1/2}\Delta m_{bc},
 \tag{2.47}$$

where

$$\begin{aligned}
 \Delta m_{bc} &= \left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{1+2,3} [(q_1 + q_2 + q_3)^2 - (1-x^2)]^{-1} \\
 &\quad \times \left\{ x^4 \frac{\gamma_1^2 \gamma_3^2 - \gamma_1 \gamma_2 \gamma_3}{2q_1 q_3} + \gamma_1^2 \left[-1 + \frac{1}{q_1 q_2} + \frac{1}{q_2 q_3} - \frac{q_2 + q_3}{2q_1} + \frac{q_1 + q_3}{2q_2} - \frac{q_1 + q_2}{2q_3} \right] \right. \\
 &\quad \left. + x^2 \gamma_1^2 \left[\frac{1}{2} - \frac{1}{q_1 q_2} - \frac{1}{2q_2 q_3} + \frac{\gamma_2^2}{q_1 q_2} + \frac{\gamma_2^2}{q_1 q_3} + \frac{q_2 + q_3}{2q_1} \right] \right. \\
 &\quad \left. - x^2 \gamma_1 \gamma_2 \gamma_3 \left[\frac{1}{2} + \frac{1}{q_1 q_2} + \frac{q_1}{2q_2} + \frac{3}{2q_1 q_3} + \frac{q_3}{2q_1} \right] \right\},
 \end{aligned}
 \tag{2.48}$$

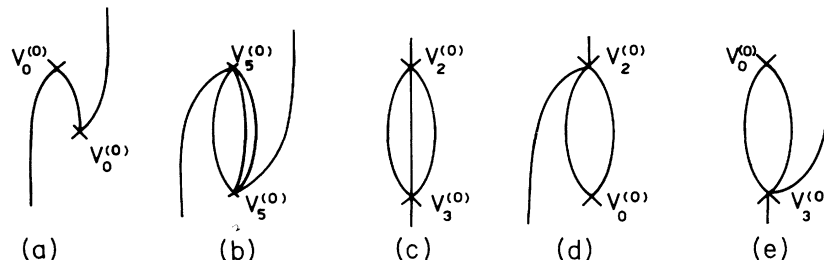


FIG. 2. The perturbation diagrams that contribute to the energy gap m .

$$q_i = (1 - x^2 \gamma_i^2)^{1/2} \quad (i = 1, 2, 3).$$

At $x = 1$, the summation in Eq. (2.48) is finite and $\Delta m_b^{(-1)} + \Delta m_c^{(-1)}$ vanishes.

For the square lattice, the series results for $\Delta m_b^{(-1)}$ and $\Delta m_c^{(-1)}$ are

$$\begin{aligned} \Delta m_b^{(-1)} &= \frac{2}{S} [0.002044677734375x^4 + 0.00072956085205078x^6 + 0.00015844218432903x^8 \\ &\quad - 0.00008217465074267x^{10} - 0.00018331177739128x^{12} - 0.00022252277285162x^{14} \\ &\quad - 0.00023307646341684x^{16} - 0.00023014596432591x^{18} + O(x^{20})], \\ \Delta m_c^{(-1)} &= \frac{2}{S} [0.006103515625x^4 + 0.002391815185546875x^6 + 0.0010838806629181x^8 \\ &\quad + 0.0005122232250869x^{10} + 0.00023472870816477x^{12} + 0.0000893833246209x^{14} \\ &\quad + 0.0000094244732853x^{16} - 0.00003582112473023x^{18} + O(x^{20})]. \end{aligned} \quad (2.49)$$

By analyzing the above series, one can see that $\Delta m_b^{(-1)}$ and $\Delta m_c^{(-1)}$ do not vanish at the isotropic limit $x = 1$; and the numerical integration also confirms that at $x = 1$

$$\Delta m_b^{(-1)} = -0.0051(2) \frac{2}{S}, \quad \Delta m_c^{(-1)} = 0.0051(2) \frac{2}{S}. \quad (2.50)$$

Longer series can be calculated using Eq. (2.48):

$$\begin{aligned} \Delta m_b^{(-1)} + \Delta m_c^{(-1)} &= \frac{2}{S} (1 - x^2)^{1/2} [0.008148193359375x^4 + 0.0071954727172852x^6 \\ &\quad + 0.0058585833758116x^8 + 0.0047680364368716x^{10} + 0.0039357639191167x^{12} \\ &\quad + 0.0033007838421142x^{14} + 0.0028094164399784x^{16} + 0.0024226289552537x^{18} \\ &\quad + 0.0021130430983801x^{20} + 0.0018614244153671x^{22} + 0.0016540820830473x^{24} \\ &\quad + 0.0014811092879290x^{26} + 0.0013352148677443x^{28} \\ &\quad + 0.0012109445784598x^{30} + O(x^{32})]. \end{aligned} \quad (2.51)$$

The Monte Carlo integration gives in the isotropic limit ($x \rightarrow 1$)

$$\Delta m_b^{(-1)} + \Delta m_c^{(-1)} = 0.08137(4)(1 - x^2)^{1/2} \frac{2}{S}, \quad (2.52)$$

which is consistent with the series estimates. Therefore, the energy gap near the isotropic limit $x \rightarrow 1$ is

$$m = (1 - x^2)^{1/2} [4S - 0.78641 + 0.01086(8)S^{-1} + O(S^{-2})]. \quad (2.53)$$

D. Perpendicular susceptibility

Consider the Heisenberg antiferromagnet with an external magnetic field directed along the x axis:

$$H = \sum_{\langle lm \rangle} [S_l^z S_m^z + x(S_l^x S_m^x + S_l^y S_m^y)] + p \sum_i S_i^x. \quad (2.54)$$

Performing the same Dyson-Maleev transformation, Fourier transformation and Bogoliubov transformation as before, the above Hamiltonian becomes

$$\begin{aligned} H &= -S^2 N z / 2 + z N S C_1 / 2 - \frac{z N}{8} [C_1^2 + (C_{-1} - C_1)^2 (1 - x^2) / x^2] \\ &\quad + \sum_k A_k (n_k + n'_k) + \sum_{k_1, k_2} [B^{(1)}(n_1 n_2 + n'_1 n'_2) + B^{(2)} n_1 n'_2] \\ &\quad + \sum_k V_0^{(0)} (\alpha_k \beta_k + \alpha_k^\dagger \beta_k^\dagger) - \frac{z}{2N} \sum_{k_i} ' \delta_{1+2,3+4} [V_1^{(0)} (\beta_1^\dagger \beta_2^\dagger \beta_3 \beta_4 + \alpha_3^\dagger \alpha_4^\dagger \alpha_1 \alpha_2) - 2V_2^{(0)} (\alpha_3^\dagger \beta_4 \alpha_1 \alpha_2 + \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger \beta_3) \\ &\quad - 2V_3^{(0)} (\alpha_3^\dagger \alpha_4^\dagger \alpha_2 \beta_1^\dagger + \alpha_1 \beta_2^\dagger \beta_3 \beta_4) + 2V_4^{(0)} (\alpha_3^\dagger \alpha_1 \beta_2^\dagger \beta_4 + \alpha_4^\dagger \alpha_2 \beta_1^\dagger \beta_3) \\ &\quad + V_5^{(0)} (\alpha_3^\dagger \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger + \alpha_1 \alpha_2 \beta_3 \beta_4)] \\ &\quad + V_0^{(\frac{1}{2})} (\alpha_0 + \alpha_0^\dagger + \beta_0 + \beta_0^\dagger) + V_0^{(-\frac{1}{2})} (\alpha_0 + \beta_0^\dagger) \\ &\quad - \frac{p}{2\sqrt{NS}} \sum_{k_i} \delta_{1,2+3} [V_1^{(-\frac{1}{2})} (\alpha_1^\dagger \alpha_2 \alpha_3 + \beta_3^\dagger \beta_2^\dagger \beta_1) + 2V_2^{(-\frac{1}{2})} (\alpha_1^\dagger \beta_2^\dagger \alpha_3 + \beta_3^\dagger \alpha_2 \beta_1) + V_3^{(-\frac{1}{2})} (\beta_1 \alpha_2 \alpha_3 + \alpha_1^\dagger \beta_2^\dagger \beta_3^\dagger)], \end{aligned} \quad (2.55)$$

where the two-particle vertex factor $V_0^{(0)}$ and four-particle vertex factors $V_i^{(0)}$ ($i = 1, 2, \dots, 5$) are defined by Eq. (2.13), while the one-particle vertex factors $V_0^{(\frac{1}{2})}$ and $V_0^{(-\frac{1}{2})}$, three-particle vertex factors $V_i^{(\frac{1}{2})}$ ($i = 1, 2, 3$), and $A_k, B^{(i)}$ are defined by

$$\begin{aligned}
 A_k &= z(S - C_1/2)(1 - x^2\gamma_k^2)^{1/2} - \frac{z}{2}(C_{-1} - C_1)(1 - x^2)\gamma_k^2(1 - x^2\gamma_k^2)^{-1/2}, \\
 B^{(i)} &= \mathcal{B}^{(i)}(h_1 = h_2 = 0) \quad (i = 1, 2), \\
 V_0^{(\frac{1}{2})} &= \frac{p}{2}\sqrt{NS}(c_0 - s_0), \\
 V_0^{(-\frac{1}{2})} &= -\frac{p}{4}\sqrt{\frac{N}{S}}C_{-1}(c_0 - s_0), \\
 V_1^{(-\frac{1}{2})} &= c_1c_2c_3 - s_1s_2s_3, \\
 V_2^{(-\frac{1}{2})} &= s_1c_2s_3 - c_1s_2c_3, \\
 V_3^{(-\frac{1}{2})} &= c_1s_2s_3 - s_1c_2c_3.
 \end{aligned}
 \tag{2.56}$$

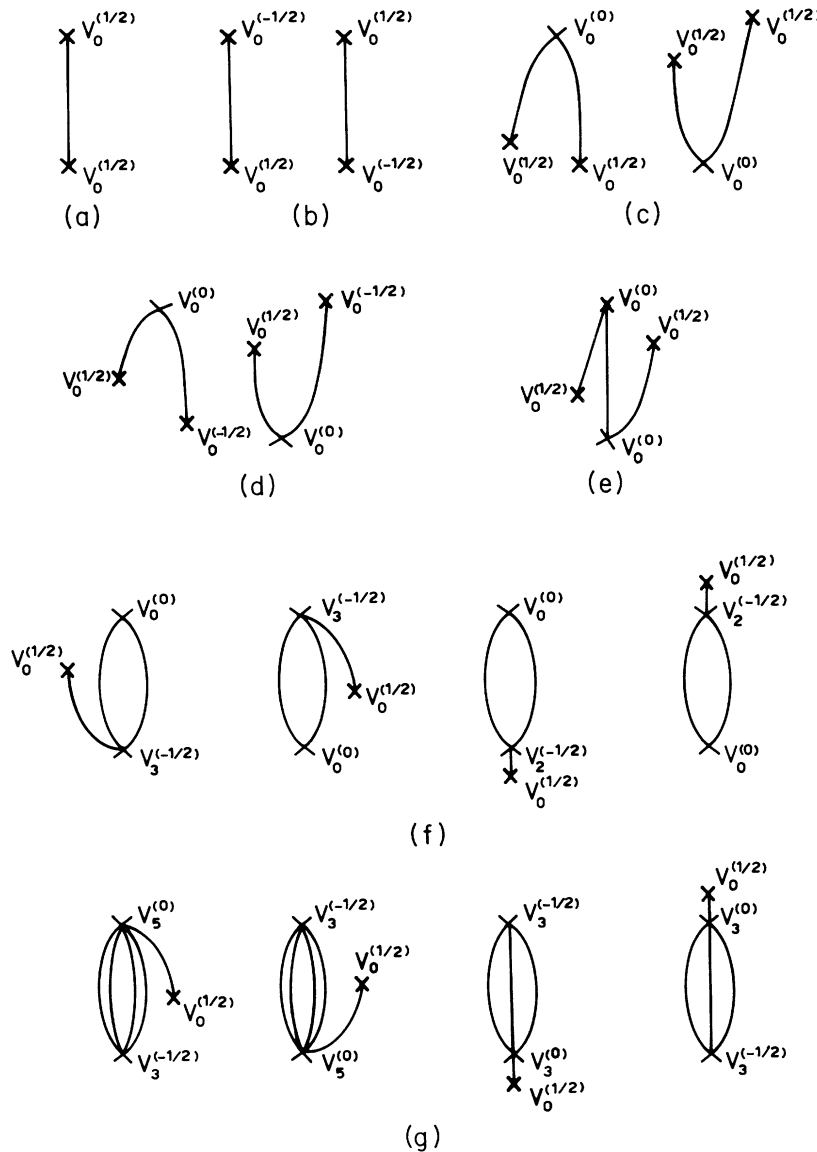


FIG. 3. The perturbation diagrams that contribute to the perpendicular susceptibility χ_{\perp} . To save space, we have not distinguished different possible time orderings of the vertices in the diagrams.

Again, we treat the terms containing V in Eq. (2.55) as perturbation terms. Up to $O(S^{-2})$, there are nine groups of diagrams in Fig. 3 contributing to the p^2 term of the ground-state energy. Denoting the contribution from Fig. 3(a) as E_a^p etc, after some calculations, we get the contribution of each group of diagrams as

$$\begin{aligned}
 E_a^p &= -\frac{p^2 NS}{2z} (1+x)^{-1} \left[S - \frac{C_{-1}}{2} + \frac{m^{(-1)}}{z(1-x^2)^{1/2}} \right]^{-1}, \\
 E_b^p &= \frac{p^2 N}{4z} \frac{C_{-1}}{(1+x)(S - C_{-1}/2)}, \\
 E_c^p &= \frac{p^2 NS}{4xz} \frac{C_{-1} - C_1}{(1+x)(S - C_{-1}/2)^2}, \\
 E_d^p &= -\frac{p^2 N}{8xzS^2} \frac{C_{-1}(C_{-1} - C_1)}{1+x}, \\
 E_e^p &= -\frac{p^2 N}{8zS^2x^2} \frac{(C_{-1} - C_1)^2}{1+x}, \\
 E_f^p &= \frac{p^2 N}{8x^2zS^2} (1-x)(C_{-1} - C_1)(C_{-3} - C_{-1}), \\
 E_g^p &= \frac{p^2 N}{4zS^2} \frac{(c_0 - s_0)}{(1-x^2)^{1/2}} \left(\frac{2}{N} \right)^2 \sum_{k_i} \delta_{1+2,3} \frac{V_3^{(-\frac{1}{2})}(\mathbf{3}, \mathbf{2}, \mathbf{1}) [V_5^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{2}, \mathbf{1}) - V_3^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{2}, \mathbf{1})]}{\sum_i (1 - x^2 \gamma_i^2)^{1/2}}, \\
 E_h^p &= \frac{p^2 N}{8x^3zS^2} (1-x)^2 (C_{-1} - C_1)(C_{-3} - C_{-1}), \\
 E_i^p &= -\frac{p^2 N}{4zS^2} \frac{(1-x^2)^{-1/2}}{1+x} \left(\frac{2}{N} \right)^2 \\
 &\quad \times \sum_{k_i} \delta_{1+2,3} \left[V_3^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{1}, \mathbf{2}) V_2^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{0}, \mathbf{3}) - V_3^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{1}, \mathbf{2}) V_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{0}, \mathbf{3}) - V_2^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{0}, \mathbf{3}) V_5^{(0)}(\mathbf{0}, \mathbf{3}, \mathbf{1}, \mathbf{2}) \right. \\
 &\quad \left. + V_5^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{1}, \mathbf{2}) V_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{0}) \right] \left[\sum_{i=1}^3 (1 - x^2 \gamma_i^2) \right]^{-1}.
 \end{aligned}
 \tag{2.57}$$

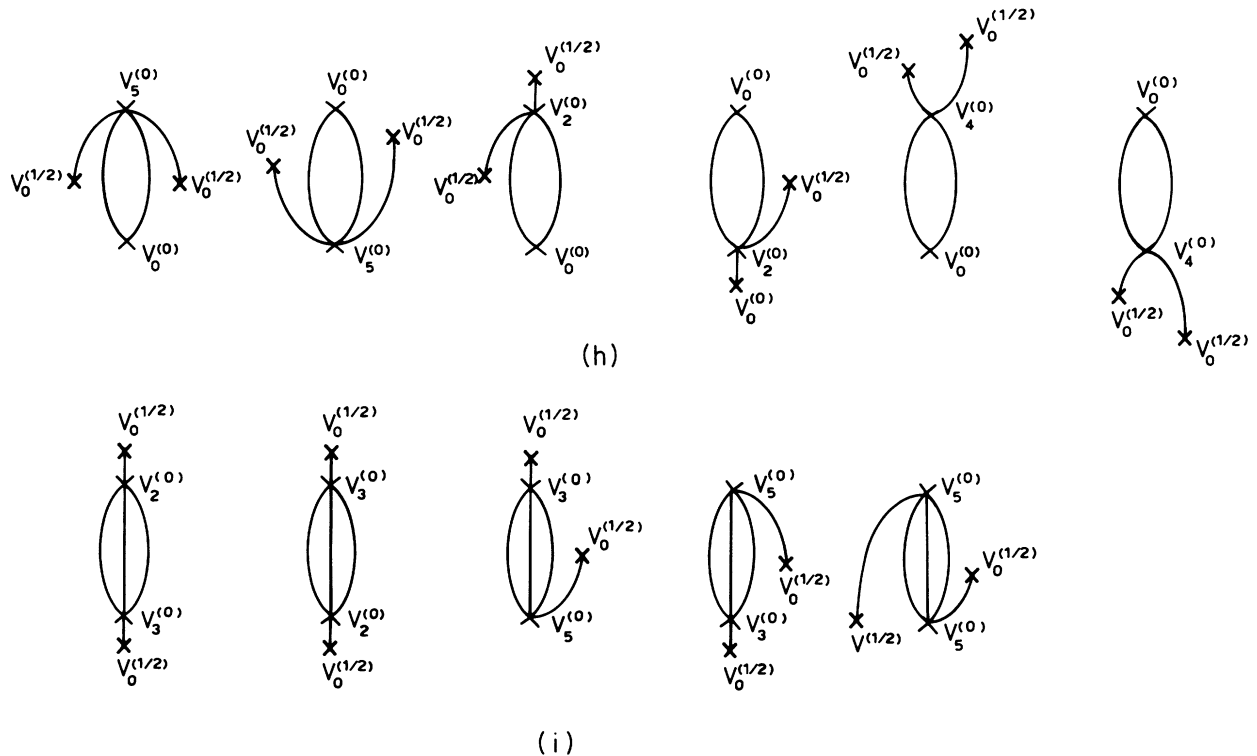


FIG. 3. (Continued).

Therefore, the p^2 term of the ground-state energy is

$$E^p = E_a^p + E_b^p + E_c^p + E_d^p + E_e^p + E_f^p + E_g^p + E_h^p + E_i^p, \quad (2.58)$$

and the uniform perpendicular susceptibility χ_{\perp}^S can be found by

$$\chi_{\perp} = -\frac{1}{N} \frac{\partial^2 E^p}{\partial p^2} \Big|_{p=0} = \chi_{\perp}^{(0)} + \chi_{\perp}^{(-1)} + \chi_{\perp}^{(-2)} + O(S^{-3}), \quad (2.59)$$

where

$$\chi_{\perp}^{(0)} = \frac{1}{z(1+x)}, \quad \chi_{\perp}^{(-1)} = \frac{C_1 - C_{-1}}{2zSx(1+x)}, \quad (2.60)$$

$$\chi_{\perp}^{(-2)} = [(1-x)(1+2x)C_{-1}^2 - (1-x^2)(C_{-1} - C_1)C_{-3} - (1+2x-2x^2)C_{-1}C_1 + C_1^2x - 4x^3Sm^{(-1)}(1-x^2)^{-1/2}/z][4S^2zx^3(1+x)]^{-1} + \chi_g^{(-2)} + \chi_i^{(-2)},$$

with

$$\chi_g^{(-2)} = -\frac{c_0 - s_0}{2zS^2} (1-x^2)^{-1/2} \left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{1+2,3} \frac{[V_3^{(-\frac{1}{2})}(\mathbf{3}, \mathbf{2}, \mathbf{1})][V_5^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{2}, \mathbf{1}) - V_3^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{2}, \mathbf{1})]}{\sum_i (1-x^2\gamma_i^2)^{1/2}}, \quad (2.61)$$

$$\begin{aligned} \chi_i^{(-2)} = \frac{1}{2zS^2} \frac{(1-x^2)^{-1/2}}{1+x} \left(\frac{2}{N}\right)^2 \sum_{k_i} \delta_{1+2,3} & \left[V_3^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{1}, \mathbf{2})V_2^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{0}, \mathbf{3}) \right. \\ & - V_3^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{1}, \mathbf{2})V_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{0}, \mathbf{3}) - V_2^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{0}, \mathbf{3})V_5^{(0)}(\mathbf{0}, \mathbf{3}, \mathbf{1}, \mathbf{2}) \\ & \left. + V_5^{(0)}(\mathbf{3}, \mathbf{0}, \mathbf{1}, \mathbf{2})V_5^{(0)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{0}) \right] \left[\sum_{i=1}^3 (1-x^2\gamma_i^2) \right]^{-1}. \end{aligned}$$

The staggered perpendicular susceptibility χ_{\perp}^S is related to the uniform perpendicular susceptibility χ_{\perp} by⁸

$$\chi_{\perp}^S(x) = \chi_{\perp}(-x). \quad (2.62)$$

The series results for $\chi_g^{(-2)} + \chi_i^{(-2)}$ are

$$\begin{aligned} \chi_g^{(-2)} + \chi_i^{(-2)} = \frac{1}{2S^2z(1+x)} & [-0.010416666666667x^2 + 0.009114583333333x^3 \\ & - 0.0077989366319445x^4 + 0.0070902506510417x^5 - 0.0061216001157407x^6 \\ & + 0.0052963186193396x^7 - 0.0048764370105885x^8 + 0.0040847857793172x^9 \\ & - 0.0039540104981926x^{10} + 0.0032576712484590x^{11} - 0.0032657754357341x^{12} \\ & + 0.0026704605377805x^{13} - 0.0027439034689870x^{14} + 0.002237725639533x^{15} \\ & - 0.0023405818719119x^{16} + 0.0019086610188879x^{17} - 0.0020229705103912x^{18} \\ & + 0.0016518529458875x^{19} - 0.0017684750196474x^{20} + 0.0014470612121930x^{21} \\ & - 0.0015613429143152x^{22} + 0.0012807533130780x^{23} - 0.0013903981283547x^{24} \\ & + 0.0011435872886147x^{25} - 0.0012475640806019x^{26} + 0.0010289340180435x^{27} \\ & - 0.0011268985903297x^{28} + 0.00093197606974512x^{29} - 0.0010239556525932x^{30} \\ & + 0.00084913916280841x^{31} - 0.00093535661273403x^{32} + 0.00077772256732402x^{33} \\ & - 0.00085849706759527x^{34} + 0.00071565239973556x^{35} - 0.00079134309218339x^{36} \\ & + 0.00066131304941856x^{37} - 0.00073228722854356x^{38} + O(x^{39})]. \quad (2.63) \end{aligned}$$

For the spin- $\frac{1}{2}$ model, the series for χ_{\perp} in x from second-order and third-order spin-wave theory, and the exact series⁸ for χ_{\perp} are, respectively,

$$\begin{aligned}
\chi_{\perp}^{2\text{nd}} &= \frac{1}{4} - \frac{5x}{16} + \frac{5x^2}{16} - \frac{169x^3}{512} + \frac{169x^4}{512} - 0.33923340x^5 + 0.33923340x^6 \\
&\quad - 0.34507465x^7 + 0.34507465x^8 - 0.34921464x^9 + 0.34921464x^{10} + O(x^{11}), \\
\chi_{\perp}^{3\text{rd}} &= \frac{1}{4} - \frac{21x}{64} + \frac{139x^2}{384} - 0.384765625x^3 + 0.391928779x^4 - 0.40289476x^5 + 0.40481929x^6 \\
&\quad - 0.41138267x^7 + 0.41171885x^8 - 0.41614476x^9 + 0.41592491x^{10} + O(x^{11}), \\
\chi_{\perp}^{\text{exact}} &= \frac{1}{4} - \frac{x}{3} + \frac{17x^2}{48} - 0.37962963x^3 + 0.38352225x^4 - 0.39315892x^5 + 0.39586801x^6 \\
&\quad - 0.40295421x^7 + 0.40531565x^8 - 0.40921498x^9 + 0.41102770x^{10} + O(x^{11}).
\end{aligned} \tag{2.64}$$

Again, the series for the third-order spin-wave theory is closer to the exact series than that for second-order spin-wave theory.

The results of numerical integration for $\chi_g^{(-2)} + \chi_i^{(-2)}$ at $x = 1$ and $x = -1$ are

$$x = 1: \quad \chi_g^{(-2)} + \chi_i^{(-2)} = -\frac{0.021771(2)}{32S^2}, \tag{2.65}$$

$$x = -1: \quad \chi_g^{(-2)} + \chi_i^{(-2)} = -\frac{0.6075(3)}{32S^2(1+x)},$$

which are consistent with the series estimates

$$x = 1: \quad \chi_g^{(-2)} + \chi_i^{(-2)} = -\frac{0.0219(2)}{32S^2}, \tag{2.66}$$

$$x = -1: \quad \chi_g^{(-2)} + \chi_i^{(-2)} = -\frac{0.6082(5)}{32S^2(1+x)}.$$

Therefore, the conclusions for the uniform perpendicular susceptibility χ_{\perp} and staggered perpendicular susceptibility χ_{\perp}^S at the limit $x \rightarrow 1$ are

$$\chi_{\perp} = 0.125 - 0.034447S^{-1} + 0.001701(3)S^{-2} + O(S^{-3}), \tag{2.67}$$

$$(1-x)\chi_{\perp}^S = 0.25 + 0.0688939S^{-1} + 0.01280(5)S^{-2} + O(S^{-3}).$$

Given in Table I and Figures 4–7 is a detailed comparison for the ground-state energy E_0/N , staggered magnetization

TABLE I. A comparison of the first-order, second-order, and third-order spin-wave results with the recent estimates from exact series expansions (Ref. 8) for the ground-state energy E_0/N , staggered magnetization M^+ , parallel staggered susceptibility $\chi_{//}^S$, energy gap m , uniform perpendicular susceptibility χ_{\perp} , and staggered perpendicular susceptibility χ_{\perp}^S at the isotropic limit $x \rightarrow 1$.

Function	Spin-wave predictions			Series estimate
	First-order	Second-order	Third-order	
Spin-$\frac{1}{2}$ model				
E_0/N	-0.65795	-0.67042	-0.66999	-0.6693(1)
M^+	0.30340	0.30340	0.3069	0.307(1)
χ_{\perp}	0.125	0.056106	0.06291	0.0659(10)
$(1-x^2)^{-1/2}m$	2	1.2136	1.235	1.27(2)
$(1-x^2)^{1/2}\chi_{//}^S$	0.15916	0.22174	0.243	0.264(10)
$(1-x)\chi_{\perp}^S$	0.25	0.38779	0.439	0.47(1)
Spin-1 model				
E_0/N	-2.31590	-2.32837	-2.32815	-2.3279(2)
M^+	0.80340	0.80340	0.80427	0.8039(4)
χ_{\perp}	0.125	0.090553	0.09225	0.0925(10)
$(1-x^2)^{-1/2}m$	4	3.21359	3.2245	3.26(4)
$(1-x^2)^{1/2}\chi_{//}^S$	0.079577	0.09522	0.0978	0.098(3)
$(1-x)\chi_{\perp}^S$	0.25	0.31889	0.3317	0.333(2)

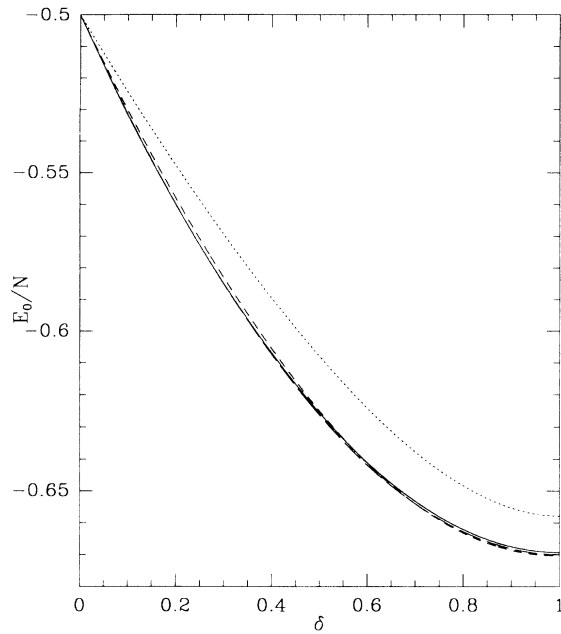


FIG. 4. Graph of the ground-state energy per site E_0/N against $\delta = 1 - (1 - x^2)^{1/2}$ for the spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice. The four curves shown are the series estimate (Ref. 8), and the first, second and third-order spin-wave predictions, corresponding to solid, dot, short-dashed, and long-dashed lines, respectively.

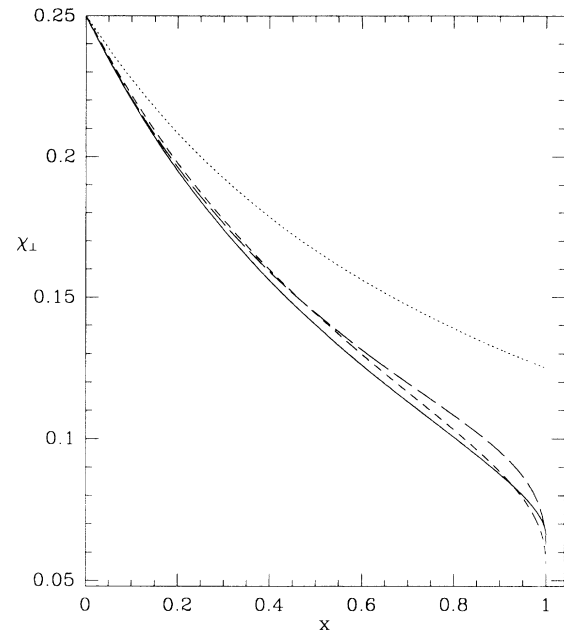


FIG. 6. Graph of the perpendicular susceptibility χ_{\perp} against x for spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice. Notation as Fig. 4.

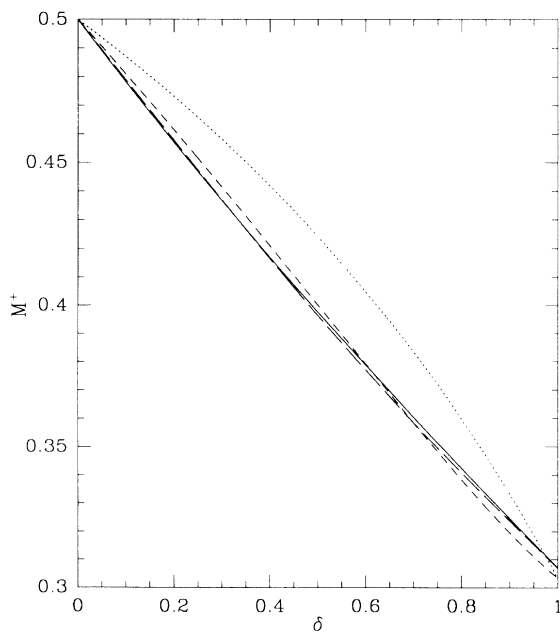


FIG. 5. Graph of the staggered magnetization M^+ against δ for the spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice. Notation as Fig. 4.

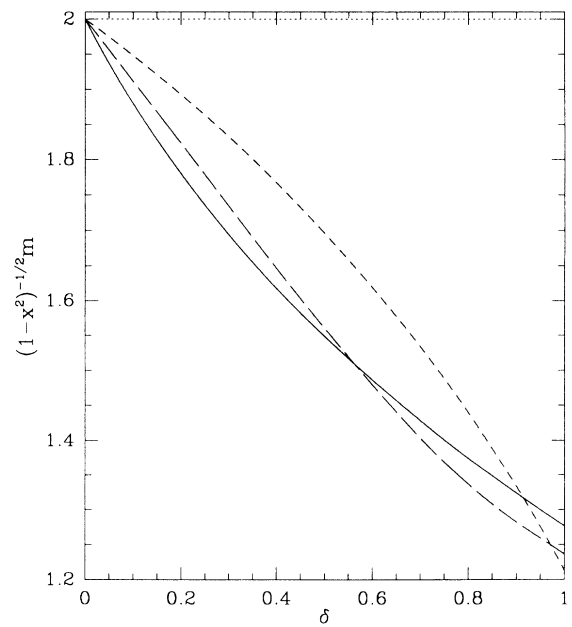


FIG. 7. Graph of $(1 - x^2)^{-1/2}m$ against δ for spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice (m is the energy gap). Notation as Fig. 4.

M^+ , parallel staggered susceptibility $\chi_{//}^S$, energy gap m , uniform perpendicular susceptibility χ_{\perp} , and staggered perpendicular susceptibility χ_{\perp}^S between the results of the first, second, and third-order spin-wave theory, and the recent estimates from exact series expansions.⁸ One finds in general that the third-order corrections are small, but in the right direction to give improved convergence. For the spin- $\frac{1}{2}$ model, the third-order corrections reduce the discrepancy between spin-wave theory and exact series results by around 50%. For the spin-1 model, the third-order theory agrees completely with the series results, within errors.

III. HOLSTEIN-PRIMAKOFF FORMALISM

The Holstein-Primakoff transformation is

$$l \text{ sublattice : } S_l^z = S - a_l^\dagger a_l, \quad S_l^+ = (2S)^{1/2} f_l(S) a_l, \quad S_l^- = (2S)^{1/2} a_l^\dagger f_l(S), \quad (3.1)$$

$$m \text{ sublattice : } S_m^z = b_m^\dagger b_m - S, \quad S_m^+ = (2S)^{1/2} b_m^\dagger f_m(S), \quad S_m^- = (2S)^{1/2} f_m(S) b_m,$$

where f is

$$f_l(S) = \left(1 - \frac{a_l^\dagger a_l}{2S}\right)^{1/2} = 1 - \frac{a_l^\dagger a_l}{4S} - \frac{a_l^\dagger a_l a_l^\dagger a_l}{32S^2} + O(S^{-3}). \quad (3.2)$$

In terms of these boson operators a_l and b_m , the Hamiltonian in Eq. (2.1) can be expressed as

$$\begin{aligned} H = & -SN(Sz - h_1 + h_2)/2 \\ & + (zS - h_1) \sum_l a_l^\dagger a_l + (zS + h_2) \sum_m b_m^\dagger b_m + xS \sum_{\langle lm \rangle} (a_l b_m + a_l^\dagger b_m^\dagger) \\ & - \sum_{\langle lm \rangle} a_l^\dagger a_l b_m^\dagger b_m - \frac{x}{4} \sum_{\langle lm \rangle} (a_l^\dagger a_l a_l b_m + a_l^\dagger b_m^\dagger b_m^\dagger b_m + a_l^\dagger a_l^\dagger a_l b_m^\dagger + a_l b_m^\dagger b_m b_m) \\ & - \frac{x}{32S} \sum_{\langle lm \rangle} (a_l b_m^\dagger b_m b_m^\dagger b_m b_m - 2a_l^\dagger a_l a_l b_m^\dagger b_m b_m + a_l^\dagger a_l a_l^\dagger a_l a_l b_m \\ & \quad + a_l^\dagger b_m^\dagger b_m^\dagger b_m b_m^\dagger b_m - 2a_l^\dagger a_l^\dagger a_l b_m^\dagger b_m^\dagger b_m + a_l^\dagger a_l^\dagger a_l a_l^\dagger a_l b_m^\dagger) + O(S^{-2}). \end{aligned} \quad (3.3)$$

Note that in this case the Hamiltonian is manifestly Hermitian; but it is more complicated than the Dyson-Maleev Hamiltonian, because of the final, third-order correction term. As before, we can introduce Bloch-type operators a_k , b_k by a Fourier transformation, diagonalize the quadratic part of H by a Bogoliubov transformation, and express the Hamiltonian as (here we only need to consider the diagonal part of the third order term):

$$\begin{aligned} H = & \mathcal{E}_h + \Delta\mathcal{E}_0^{(-1)} + \sum_k [(\mathcal{A}_k^- + \Delta\mathcal{A}_k) n_k + (\mathcal{A}_k^+ + \Delta\mathcal{A}_k) n'_k] + \sum_{k_1, k_2} [\mathcal{B}^{(1)}(n_1 n_2 + n'_1 n'_2) + \mathcal{B}^{(2)} n_1 n'_2] \\ & + \sum_k \mathcal{V}_0^{(0)} (\alpha_k \beta_k + \alpha_k^\dagger \beta_k^\dagger) - \frac{z}{2N} \sum_{k_i} \delta_{1+2,3+4} [\mathcal{V}_1^{(0)} (\beta_1^\dagger \beta_2^\dagger \beta_3 \beta_4 + \alpha_3^\dagger \alpha_4^\dagger \alpha_1 \alpha_2) \\ & \quad - 2\mathcal{V}_2^{(0)} (\alpha_3^\dagger \beta_4 \alpha_1 \alpha_2 + \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger \beta_3) - 2\mathcal{V}_3^{(0)} (\alpha_3^\dagger \alpha_4^\dagger \alpha_2 \beta_1^\dagger + \alpha_1 \beta_2^\dagger \beta_3 \beta_4) \\ & \quad + 2\mathcal{V}_4^{(0)} (\alpha_3^\dagger \alpha_1 \beta_2^\dagger \beta_4 + \alpha_4^\dagger \alpha_2 \beta_1^\dagger \beta_3) + \mathcal{V}_5^{(0)} (\alpha_3^\dagger \alpha_4^\dagger \beta_1^\dagger \beta_2^\dagger + \alpha_1 \alpha_2 \beta_3 \beta_4)], \end{aligned} \quad (3.4)$$

where the definitions of \mathcal{E}_h , D , γ_k , n_i , n'_i , \mathcal{A}_k^\pm , and $\mathcal{B}^{(i)}$ are the same as before, and $\Delta\mathcal{E}_0^{(-1)}$ and $\Delta\mathcal{A}_k$ are the corrections from third-order terms to \mathcal{E}_h and \mathcal{A}_k^\pm :

$$\Delta\mathcal{E}_0^{(-1)} = -\frac{zN}{64S} \left\{ \frac{D^3}{x^2} (C_{-1} - C_1)^2 - D[(C_{-1} + 1)^2 - 1] \right\} (C_{-1} - C_1), \quad (3.5)$$

$$\Delta\mathcal{A}_k = \frac{zD}{32S} \left\{ 2(C_{-1} - C_1)(C_{-1} + 1) + \frac{x^2 \gamma_k^2}{D^2} \left(C_{-1}(C_{-1} + 2) - \frac{3D^2}{x^2} (C_{-1} - C_1)^2 \right) \right\} (1 - x^2 \gamma_k^2 D^{-2})^{-1/2},$$

and we have neglected the correction to $\mathcal{B}^{(i)}$ from third-order terms. The vertices $\mathcal{V}_0^{(0)}(k)$ and $\mathcal{V}_i^{(0)}(1, 2, 3, 4)$ ($i = 1, \dots, 5$) are the Holstein-Primakoff vertices; they are related to the Dyson-Maleev vertices by

$$\begin{aligned}
\mathcal{V}_0^{(0) \text{ H-P}} &= \mathcal{V}_0^{(0) \text{ D-M}} , \\
\mathcal{V}_i^{(0) \text{ H-P}}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}) &= \frac{1}{2}[\mathcal{V}_i^{(0) \text{ D-M}}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}) + \mathcal{V}_i^{(0) \text{ D-M}}(\mathbf{4}, \mathbf{3}, \mathbf{2}, \mathbf{1})] \quad (i = 1, 4, 5) , \\
\mathcal{V}_2^{(0) \text{ H-P}}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}) &= \mathcal{V}_3^{(0) \text{ H-P}}(\mathbf{4}, \mathbf{3}, \mathbf{2}, \mathbf{1}) = \frac{1}{2}[\mathcal{V}_2^{(0) \text{ D-M}}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}) + \mathcal{V}_3^{(0) \text{ D-M}}(\mathbf{4}, \mathbf{3}, \mathbf{2}, \mathbf{1})] .
\end{aligned} \tag{3.6}$$

A. Ground-state energy

Up to order $O(S^{-1})$, the ground-state energy \mathcal{E}_0 is

$$\begin{aligned}
\frac{\mathcal{E}_0}{N} &= -S^2 z(D - \frac{1}{2}) + \frac{z}{2} D S C_1 - \frac{z}{8} \left\{ [(1-D)C_{-1} + D C_1]^2 \right. \\
&\quad \left. + \frac{D^2}{x^2} (C_{-1} - C_1)^2 (1-x^2) \right\} + (\Delta \mathcal{E}_0^{(-1)} + \Delta \mathcal{E}_a^{(-1)} + \Delta \mathcal{E}_b^{(-1)})/N,
\end{aligned} \tag{3.7}$$

where $\Delta \mathcal{E}_a^{(-1)}$ and $\Delta \mathcal{E}_b^{(-1)}$ are the contributions from diagram Fig. 1(a) and Fig. 1(b). They have the same form as Eqs. (2.14) and (2.15), except that the vertices $\mathcal{V}_i^{(0)}$ are the Holstein-Primakoff vertices. For zero external magnetic field (i.e. $h_1 = h_2 = 0$), the ground-state energy E_0 is

$$\begin{aligned}
E_0/N &= -\frac{zS}{2} \left(S - C_1 + \frac{1}{4S} \left[C_1^2 + \frac{1-x^2}{x^2} (C_{-1} - C_1)^2 \right] \right) \\
&\quad - \frac{z}{16x^4 S} (1-x^2)^2 (C_{-1} - C_1)^2 (C_{-3} - C_{-1}) + \frac{\Delta E_0^{(-1)}}{N} + \frac{\Delta E_b^{(-1)}}{N},
\end{aligned} \tag{3.8}$$

where

$$\Delta E_0^{(-1)} = \Delta \mathcal{E}_0^{(-1)}(h_1 = h_2 = 0) = -\frac{zN}{64S} [x^{-2} (C_{-1} - C_1)^2 - C_{-1}^2 - 2C_{-1}] (C_{-1} - C_1). \tag{3.9}$$

For the square lattice, one finds that the singularity of $\Delta E_0^{(-1)}/N$ at $x \rightarrow 1$ is $(1-x^2)^{1/2}$ instead of $(1-x^2)^{3/2}$. The series result for $\Delta E_b^{(-1)}$ is

$$\begin{aligned}
\Delta E_b^{(-1)} &= -\frac{N}{2S} [0.00457763671875x^4 + 0.00400924682617x^6 + 0.00319408625x^8 \\
&\quad + 0.00254846725147x^{10} + 0.00206869514204x^{12} + 0.0017111998614x^{14} \\
&\quad + 0.00144019926x^{16} + 0.0012306616159x^{18} + 0.001065532227x^{20} \\
&\quad + 0.000933118259x^{22} + 0.00082527290x^{24} + O(x^{26})].
\end{aligned} \tag{3.10}$$

The singular behavior of $\Delta E_b^{(-1)}$ at $x \rightarrow 1$ seems also to be $(1-x^2)^{1/2}$, but the series for $\Delta E_0^{(-1)} + \Delta E_b^{(-1)}$ is the same as $\Delta E_b^{(-1)}$ in the Dyson-Maleev formalism. Therefore, the Holstein-Primakoff formalism finally produces the same results for the ground-state energy as the Dyson-Maleev formalism, and the singular behavior of the ground-state energy at the isotropic limit $x = 1$ still remains as $(1-x^2)^{3/2}$ when the spin wave theory is promoted to the third order.

B. Staggered magnetization and parallel staggered susceptibility

The staggered magnetization M^+ and parallel staggered susceptibility $\chi_{//}^S$ are found to be

$$M^+ = \frac{1}{N} \frac{\partial \mathcal{E}_0}{\partial h} \Big|_{h=0} = S - \frac{C_{-1}}{2} - \frac{1-x^2}{4Sx^2} (C_{-1} - C_1)(C_{-3} - C_{-1}) + \Delta M_0^{(-2)} + \Delta M_a^{(-2)} + \Delta M_b^{(-2)}, \tag{3.11}$$

$$\begin{aligned}
\chi_{//}^S &= -\frac{1}{N} \frac{\partial^2 \mathcal{E}_0}{\partial h^2} \Big|_{h=0} = \frac{1}{2zS} (C_{-3} - C_{-1}) \\
&\quad + \frac{1}{4zS^2} \left\{ \frac{1-x^2}{x^2} \left[(C_{-1} - C_1)(C_{-1} + 3C_{-3} - 4C_{-5}) + (C_{-3} - C_{-1})^2 \right] + C_1(C_{-3} - C_{-1}) \right\} \\
&\quad + \Delta \chi_0^{(-3)} + \Delta \chi_a^{(-3)} + \Delta \chi_b^{(-3)},
\end{aligned}$$

where $\Delta M_a^{(-2)}$ and $\Delta \chi_a^{(-3)}$ are the same as in the Dyson-Maleev formalism, and $\Delta M_b^{(-2)}$ and $\Delta \chi_b^{(-3)}$ have the same expressions as in the Dyson-Maleev formalism except that the vertices $\mathcal{V}_i^{(0)}$ are the Holstein-Primakoff vertices, while

$\Delta M_0^{(-2)}$ and $\Delta \chi_0^{(-3)}$ are

$$\Delta M_0^{(-2)} = -\frac{1}{64S^2x^2}(C_{-1} - C_{-3})(4x^2C_{-1} - 3C_{-1}^2 + 3x^2C_{-1}^2 - 2x^2C_1 + 6C_{-1}C_1 - 2x^2C_{-1}C_1 - 3C_1^2), \quad (3.12)$$

$$\begin{aligned} \Delta \chi_0^{(-3)} = \frac{1}{64S^3zx^2} & (-4x^2C_{-3}^2 - 12x^2C_{-5}C_{-1} + 22x^2C_{-3}C_{-1} + 6C_{-3}^2C_{-1} - 6x^2C_{-3}^2C_{-1} \\ & - 6x^2C_{-1}^2 + 9C_{-5}C_{-1}^2 - 9x^2C_{-5}C_{-1}^2 - 24C_{-3}C_{-1}^2 + 22x^2C_{-3}C_{-1}^2 \\ & + 9C_{-1}^3 - 7x^2C_{-1}^3 + 6x^2C_{-5}C_1 - 6x^2C_{-3}C_1 - 6C_{-3}^2C_1 + 2x^2C_{-3}^2C_1 \\ & - 18C_{-5}C_{-1}C_1 + 6x^2C_{-5}C_{-1}C_1 + 36C_{-3}C_{-1}C_1 - 10x^2C_{-3}C_{-1}C_1 \\ & - 12C_{-1}^2C_1 + 2x^2C_{-1}^2C_1 + 9C_{-5}C_1^2 - 12C_{-3}C_1^2 + 3C_{-1}C_1^2). \end{aligned}$$

Note that for the square lattice and at the isotropic limit $x \rightarrow 1$, $\Delta M_0^{(-2)}$ and $\Delta \chi_0^{(-3)}$ diverge as $(1 - x^2)^{-1/2}$ and $(1 - x^2)^{-3/2}$, respectively, and the series results for $\Delta M_b^{(-2)}$ and $\Delta \chi_b^{(-3)}$ are

$$\begin{aligned} \Delta M_b^{(-2)} = -\frac{1}{8S^2} & [0.01116943359375x^4 + 0.0170173645019531x^6 + 0.0194610878825x^8 \\ & + 0.02031743025873x^{10} + 0.0204286399521x^{12} + 0.020184390093x^{14} \\ & + 0.01977314298840x^{16} + 0.0192896622252x^{18} + 0.018782800461x^{20} \\ & + 0.0182779348960x^{22} + 0.01778803837706x^{24} + O(x^{26})], \end{aligned} \quad (3.13)$$

$$\begin{aligned} \Delta \chi_b^{(-3)} = \frac{1}{16S^3} & [0.01983642578125x^4 + 0.0456085205078125x^6 \\ & + 0.0702325329184532x^8 + 0.092511795228347x^{10} + O(x^{12})]. \end{aligned}$$

At $x \rightarrow 1$, $\Delta M_b^{(-2)}$ and $\Delta \chi_b^{(-3)}$ also diverge as $(1 - x^2)^{-1/2}$ and $(1 - x^2)^{-3/2}$, respectively. But we can easily prove that the series for $\Delta M_0^{(-2)} + \Delta M_b^{(-2)}$ and $\Delta \chi_0^{(-3)} + \Delta \chi_b^{(-3)}$ are equal to those for $\Delta M_b^{(-2)}$ and $\Delta \chi_b^{(-3)}$ in the Dyson-Maleev formalism, respectively. Therefore, the Holstein-Primakoff formalism again gives the same results for the staggered magnetization and the staggered parallel susceptibility as the Dyson-Maleev formalism, and the singular behavior for the staggered magnetization and the staggered parallel susceptibility at $x = 1$ still remains as $(1 - x^2)^{1/2}$ and $(1 - x^2)^{-1/2}$, respectively.

C. Energy gap

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

$$m = m^{(1)} + m^{(0)} + m^{(-1)}, \quad (3.14)$$

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

$$m^{(-1)} = \Delta m_0^{(-1)} + \Delta m_a^{(-1)} + \Delta m_b^{(-1)} + \Delta m_c^{(-1)} + \Delta m_d^{(-1)} + \Delta m_e^{(-1)}. \quad (3.15)$$

Here

$$\Delta m_0^{(-1)} = \frac{z}{32S} [(C_{-1} - C_1)(3C_1 + 2 - C_{-1}) + x^2C_{-1}(C_{-1} + 2)](1 - x^2)^{-1/2}, \quad (3.16)$$

while the results for $\Delta m_a^{(-1)}$ and $\Delta m_d^{(-1)} + \Delta m_e^{(-1)}$ are the same as in the Dyson-Maleev formalism for all bipartite lattices. For the square lattice and at the isotropic limit $x \rightarrow 1$, $\Delta m_0^{(-1)}$ is divergent as $(1 - x^2)^{-1/2}$. The terms $\Delta m_b^{(-1)}$ and $\Delta m_c^{(-1)}$ have the same expression as in the Dyson-Maleev formalism except that the vertices $V_i^{(0)}$ are the Holstein-Primakoff vertices, and the series result of $\Delta m_b^{(-1)} + \Delta m_c^{(-1)}$ for the square lattice is

$$\begin{aligned} \Delta m_b^{(-1)} + \Delta m_c^{(-1)} = -\frac{2}{S} & [0.03125x^2 + 0.0240783691406x^4 + 0.0251989364624x^6 \\ & + 0.0240877438337x^8 + 0.0226435948716x^{10} + 0.0212619411675x^{12} \\ & + 0.0200293216798x^{14} + 0.0189491069375x^{16} + 0.0180039755581x^{18} \\ & + 0.0171735719197x^{20} + 0.0164394356085x^{22} + 0.0157860396618x^{24} + O(x^{26})]; \end{aligned} \quad (3.17)$$

$\Delta m_b^{(-1)} + \Delta m_c^{(-1)}$ also diverges at the isotropic limit $x = 1$. But the series result for $\Delta m_0^{(-1)} + \Delta m_b^{(-1)} + \Delta m_c^{(-1)}$ is the same as $\Delta m_b^{(-1)} + \Delta m_c^{(-1)}$ in the Dyson-Maleev formalism. Therefore, the two formalisms give the same final results for the energy gap, which vanishes near the isotropic limit as $(1 - x^2)^{1/2}$.

Since the results for the ground state energy E_0/N , staggered magnetization M^+ , parallel staggered susceptibility $\chi_{//}^S$, energy gap m in the Holstein-Primakoff formalism are the same as those in the Dyson-Maleev formalism, we will not repeat the calculation of the perpendicular susceptibility χ_{\perp} in Holstein-Primakoff formalism.

IV. SUMMARY AND CONCLUSIONS

As noted in the Introduction, the Dyson-Maleev formalism is the easier of two to work with. Within this formalism, we have used Rayleigh-Schrödinger perturbation theory to calculate expressions for the ground-state energy, energy gap, staggered magnetization, parallel staggered susceptibility, and transverse susceptibility, correct to third order in a $1/S$ expansion. These expressions are valid for any bipartite lattice. For the particular case of the square lattice model, these expressions have been converted firstly into series expansions in the coupling x about the (anisotropic) Ising limit; and secondly, into estimated values at the isotropic point $x = 1$, using series extrapolation and Monte Carlo integration.

Comparing these results with the previous second-order spin-wave estimates,⁸ and with “exact” numerical estimates, we find that in most cases the third-order corrections are small, but in the right direction to give improved convergence towards the “exact” results. Roughly speaking, for the $S = \frac{1}{2}$ model the discrepancy between the spin-wave theory and the exact results decreases by about 50% when the third-order spin-wave corrections are added in. Whether this trend will continue to higher orders, or whether the spin-wave expansion will eventually begin to diverge again as expected for an asymptotic expansion, is of course impossible to say. For the $S = 1$

model, the third-order spin-wave theory already agrees with the “exact” results, within errors.

Our results for the staggered magnetization disagree with those of Castilla and Chakravarty²¹ and Igarashi and Watabe,²² so that we found improved convergence towards the “exact” results at third order, whereas they did not. Our results for the transverse susceptibility agree with those of Igarashi and Watabe.²² This only serves to reinforce the conclusion that the spin-wave expansion at $T = 0$ is a useful asymptotic expansion.

Turning to the Holstein-Primakoff formalism, one finds that the Hamiltonian is longer and more complicated than that in the Dyson-Maleev case and some of the individual perturbation diagrams contain extra divergences in the isotropic limit $x \rightarrow 1$. Nevertheless, these extra divergences cancel exactly in the final result for any physical quantity, as we have checked for the ground-state energy, energy gap, staggered magnetization, and parallel staggered susceptibility, so that the two formalisms agree in the final outcome. The asymptotic behavior of all these quantities in the limit $x \rightarrow 1$, which typically involves square-root singular terms in powers of $(1 - x^2)^{1/2}$, also remains the same as in second-order spin-wave theory. It is noteworthy that the apparent lack of hermiticity in the Dyson-Maleev Hamiltonian has caused no ill effects to this order; and indeed the specific perturbation theory diagrams of Figs. 1–3 show the correct time-reversal symmetry. This is true provided one does not distinguish between α and β bosons; and indeed the Hamiltonian is symmetric under interchange of α 's and β 's. The agreement between the two formalisms also helps to give us confidence that our results are correct.

In summary, then, we have found that when carried to third order in the $1/S$ expansion, the spin-wave theory continues to give consistent results, and improved convergence towards the exact values for the square-lattice Heisenberg antiferromagnet at $T = 0$.

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