Zero-temperature properties of the quantum *XY* model with anisotropy

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The spin-$\frac{1}{2}$ *XY* model on a square lattice is studied via series expansions around the Ising limit, and spin-wave theory. Series are calculated for the ground-state energy, mass gap, magnetization, and magnetic susceptibilities. Extrapolating these series to the isotropic limit, we find extremely good agreement with the predictions of second-order spin-wave theory.

I. INTRODUCTION

This paper presents the results of a series expansion about the Ising limit for the zero-temperature quantum *XY* model on a square lattice. It forms a companion paper to a similar study of the *XXZ* Heisenberg antiferromagnet which we recently carried out.[1]

The *XY* model has many features in common with the *XXZ* antiferromagnet, but has been less well studied. A recent review has been given by Betts and Miyashita.[2] The spin-wave theory developed by Anderson[3] and others[4–6] was previously thought to be unsatisfactory in the *XY* case,[7] but recently Gomez-Santos and Joannopoulos[8] have shown that by a more judicious choice of the quantized spin axis, one can obtain a good theoretical fit to the model. Numerical studies have included the finite-cell calculations of Betts and co-workers,[9–11] a Monte Carlo (MC) simulation by Okabe and Kikuchi,[12] and a series calculation by Pearson.[13] A renormalization-group analysis has been made by Penson, Jullien, and Pfeuty,[14] and a variational study by Suzuki and Miyashita.[15]

The series results presented here were obtained by an efficient cluster expansion technique proposed originally by Nickel,[16] and further elaborated by Marland[17] and Irving and Hamer.[18,19] A very similar method has been discovered independently by Singh, Gelfand, and Huse.[20,21] We have added several terms to the ground-state energy series of Pearson,[13] and calculated new series for the magnetization, mass gap, and susceptibility in each spin direction.

The results are compared in detail with the predictions of spin-wave theory. In Sec. II we carry out the spin-wave calculations for the anisotropic *XY* model to second order in $1/S$, extending the analysis of Gomez-Santos and Joannopoulos.[8] In Sec. III the series results are confronted with these predictions. Overall, they agree extremely well. The ground state of the isotropic *XY* model is found to exhibit long-range order, as originally predicted by Oitmaa and Betts.[9] The existence of long-range order has been rigorously proven, in fact, in recent papers by Kennedy, Lieb, and Shastry[22] and Kubo and Kishi.[23] Our conclusions are summarized in Sec. IV.

II. SPIN-WAVE THEORY

Spin-wave theory provides a rather accurate picture of the low-lying states of the *XXZ* model, as may be seen from the early works of Anderson and others,[3–5] together with our recent analysis.[1] For the *XY* model, the application of simple first-order spin-wave theory by Gomez-Santos and Joannopoulos[8] has also proved satisfactory in predicting the ground-state energy and magnetization. In this section we extend their treatment to second order for the anisotropic *XY* model.

Gomez-Santos and Joannopoulos[8] showed that it was important to choose the quantized spin axis in the *XY* plane; and in fact such a choice is forced upon us if we are to make contact with the series analysis. Consider then the following Hamiltonian:

$$H=-\sum_{\langle lm\rangle}(S_l^xS_m^x+xS_l^yS_m^y)+h\sum_{\langle i\rangle}S_i^x\ , \tag{2.1}$$

where the indices l,m,i denote lattice sites, $\langle lm\rangle$ a sum over all nearest-neighbor pairs, and $\langle i\rangle$ a sum over all lattice sites. The points $x=0$ and 1 correspond to the ferromagnetic Ising model and isotropic ferromagnetic *XY* model (F), respectively. The isotropic antiferromagnetic *XY* model (A)

$$H^A=\sum_{\langle lm\rangle}(S_l^xS_m^x+S_l^yS_m^y)+h\sum_{\langle i\rangle}S_i^x \tag{2.2}$$

is related to the ferromagnetic one by a simple spin rotation on bipartite lattices. Using a similarity transform with S_m^z on every site m of the odd sublattice, for instance, one can transform: $S_m^z\to S_m^z$, $S_m^x\to -S_m^x$, $S_m^y\to -S_m^y$. Hence there exist relations between the isotropic ferromagnet (F), antiferromagnet (A), and the model described by Eq. (2.1) for the ground-state energy,

$$E_0(x=1)=E_0(x=-1)=E_0^A=E_0^F\ , \tag{2.3a}$$

for the magnetization,

$$M_x(x=1)=M_x(x=-1)=M_x^F=M_x^{A,S} \tag{2.3b}$$

(where S denotes the staggered magnetization), and for the susceptibilities,

$$\chi_{xx}(x=1)=\chi_{xx}(x=-1)=\chi_{xx}^F=\chi_{xx}^{A,S}\ , \tag{2.3c}$$

$$\chi_{yy}(x=1)=\chi_{yy}^{A,S}=\chi_{yy}^F\ , \tag{2.3d}$$

$$\chi_{yy}(x=-1)=\chi_{yy}^A=\chi_{yy}^{F,S}\ , \tag{2.3e}$$

$$\chi_{zz}(x=1)=\chi_{zz}^A=\chi_{zz}^F\ , \tag{2.3f}$$

$$\chi_{zz}(x=-1)=\chi_{zz}^{A,S}=\chi_{zz}^{F,S}\ . \tag{2.3g}$$

Choosing a representation in which S_l^x is diagonal (rather than S_l^z), the Hamiltonian can be rewritten as

$$H=-\sum_{\langle lm\rangle}\left[S_l^x S_m^x+\frac{x}{4}(S_l^+ +S_l^-)(S_m^+ +S_m^-)\right] +h\sum_{\langle i\rangle} S_i^x \ , \tag{2.4}$$

where $S_l^{\pm}$ are raising and lowering operators for S_l^x.

The application of spin-wave theory to the above Hamiltonian is carried out in standard fashion (e.g., Oguchi[5]). First, we introduce "spin deviation" operators by means of the Holstein-Primakoff[24] transformation:

$$\begin{aligned} S_i^x&=S-a_i^*a_i \ ,\\ S_i^+&=(2S)^{1/2}f_i(S)a_i \ ,\\ S_i^-&=(2S)^{1/2}a_i^*f_i(S) \ , \end{aligned} \tag{2.5}$$

where

$$f_i(S)=(1-a_i^*a_i/2S)^{1/2} \ . \tag{2.6}$$

The operators a_i, a_i^* satisfy boson commutation relations:

$$[a_i,a_j^*]=\delta_{ij} \ . \tag{2.7}$$

If the occupation number $\langle a_i^* a_i\rangle$ is small, it is reasonable to keep only the first terms in an expansion in $1/S$ of $f_i(S)$, and so here we take

$$f_i(S)\simeq 1-a_i^*a_i/4S \ . \tag{2.8}$$

Next, we introduce Bloch-type operators a_k, a_k^* by the Fourier transformation:

$$a_k=\left[\frac{1}{N}\right]^{1/2}\sum_l e^{ik\cdot l}a_l \ , \tag{2.9a}$$

$$a_k^*=\left[\frac{1}{N}\right]^{1/2}\sum_l e^{-ik\cdot l}a_l^* \ , \tag{2.9b}$$

where N is the total number of lattice sites, and a_k, a_k^* again satisfy boson commutation relations.

Finally, the terms in the Hamiltonian up to second order in a_k, a_k^* can be diagonalized by a Bogoliubov transformation:

$$a_k=\alpha_k\cosh\theta_k+\alpha_{-k}^*\sinh\theta_k \ , \tag{2.10a}$$

$$a_k^*=\alpha_k^*\cosh\theta_k+\alpha_{-k}\sinh\theta_k \ , \tag{2.10b}$$

where the parameter $\theta_k=\theta_{-k}=\theta_k^*$ is fixed by

$$\tanh(2\theta_k)=\frac{x\gamma_k}{2D-x\gamma_k} \ , \tag{2.11}$$

where

$$D=1-\frac{h}{zS} \ , \tag{2.12}$$

and γ_k is the structure factor of the lattice

$$\gamma_k=\frac{1}{z}\sum_\rho e^{ik\cdot\rho} \ . \tag{2.13}$$

The result is (keeping only terms which contribute up to second order in $1/S$)

$$H=E_h+\sum_k(A_1S+A_2)n_k+\sum_{k_1,k_2}B(k_1,k_2) \ , \tag{2.14}$$

where

$$E_h=-\frac{zS^2}{2}+NSh+zDSNC_1-\frac{zN}{32}\left[\left[\frac{2D^2}{x^2}-1-D\right](C_1-C_{-1})^2+2(1+D)C_1^2+2(1-D)C_{-1}^2+\frac{2D}{x^2}(C_1-C_3)^2\right] \ , \tag{2.15}$$

$$A_1=zD(1-x\gamma_k/D)^{1/2} \ , \tag{2.16}$$

$$\begin{aligned} A_2=&-\frac{z}{16}\left\{4(1+D)C_1+4(1-D)C_{-1}+\left[\left[\frac{4D}{x}-3x\right]C_{-1}-xC_1-\frac{4DC_3}{x}\right]\gamma_k\right\}\cosh(2\theta_k)\\ &-\frac{z}{16}\left\{\left[\frac{4DC_3}{x}+\left[\frac{4D}{x}-3x\right]C_{-1}-\left[\frac{8D}{x}+x\right]C_1\right]\gamma_k-2D(C_{-1}-C_1)\right\}\sinh(2\theta_k) \ , \end{aligned} \tag{2.17}$$

$$\begin{aligned} B(k_1,k_2)=&-\frac{z}{2N}(n_1n_2\cosh(2\theta_1)\cosh(2\theta_2)\\ &+\gamma_{1-2}\{(n_1\cosh^2\theta_1+n_1'\sinh^2\theta_1)(n_2\cosh^2\theta_2+n_2'\sinh^2\theta_2)+\tfrac{1}{4}\sinh(2\theta_1)\sinh(2\theta_2)(n_1+n_1')(n_2+n_2')\}\\ &-x\gamma_2[\cosh(2\theta_1)+\tfrac{1}{2}\sinh(2\theta_1)][\cosh(2\theta_2)+\sinh(2\theta_2)]n_1n_2\}) \ , \end{aligned} \tag{2.18}$$

and

$$C_n=\frac{1}{N}\sum_k\left[\left[1-\frac{x\gamma_k}{D}\right]^{n/2}-1\right] \ , \tag{2.19}$$

$$n_1=\alpha^*_{k_1}\alpha_{k_1},\quad n'_1=\alpha^*_{-k_1}\alpha_{-k_1},\quad \gamma_{1-2}\equiv\gamma_{k_1-k_2}\ . \tag{2.20}$$

The first-order results above reduce to those of Gomez-Santos and Joannopoulos[8] in the isotropic limit $x=1$.

Setting the external magnetic field to zero (i.e., $h=0$, $D=1$), one can derive from Eq. (2.14) the ground-state energy E_0 and mass gap m:

$$\frac{E_0}{N}=-\frac{zS^2}{2}+\frac{zSC_1}{2}-\frac{Z}{16}\left[\frac{1-x^2}{x^2}(C_1-C_{-1})^2+2C_1^2+\frac{1}{x^2}(C_1-C_3)^2\right], \tag{2.21}$$

$$m=\left[zS-\frac{z}{4}\left[C_1-\frac{C_3}{x}+\frac{1+x}{x}C_{-1}\right]\right](1-x)^{1/2}\ . \tag{2.22}$$

Differentiating with respect to h, one can obtain the magnetization and susceptibility in the **x** direction:

$$M_x=\frac{1}{N}\frac{\partial E_h}{\partial h}\bigg|_{h=0}=S-\frac{1}{4}(C_1+C_{-1})$$
$$+\frac{1}{32S}\left[\frac{4-3x^2}{x^2}(C_1-C_{-1})^2+\frac{2}{x^2}(C_1-C_3)(C_3-2C_1+C_{-1})+2\frac{1-x^2}{x^2}(C_1-C_{-1})(C_{-3}-C_1)\right], \tag{2.23}$$

$$\chi_{xx}=-\frac{1}{N}\frac{\partial^2 E_h}{\partial h^2}\bigg|_{h=0}=\frac{1}{8zS}(C_1+C_{-3}-2C_{-1})$$
$$+\frac{1}{32zS^2}\left[\frac{1-x^2}{x^2}(C_1-C_{-1})(3C_1-C_{-1}+C_{-3}-3C_{-5})\right.$$
$$+\frac{4}{x^2}(C_1-C_{-1})^2+2\frac{4-x^2}{x^2}(C_1-C_{-1})(C_{-3}-C_1)$$
$$+\frac{1-x^2}{x^2}(C_{-3}-C_1)^2+2(C_{-1}-C_1)(C_{-1}-2C_1)+\frac{1}{x^2}(C_{-1}-4C_1+3C_3)^2$$
$$\left.+2(C_{-1}-C_{-3})(C_1-2C_{-1})+\frac{1}{x^2}(C_1-C_3)(-C_{-3}+3C_{-1}-7C_1+5C_3)\right]. \tag{2.24}$$

In order to derive the susceptibility in the **y** direction, set $h=0$ in Eq. (2.1) and add an external magnetic field directed along the y axis, $p\sum_i S_i^y$. Perform the Holstein-Primakoff and Fourier transformations as before, and then shift the origin of the Bloch operators a_0 by $-(1/z)\sqrt{N/2S}\,p/(1-x)$, so as to cancel linear terms in $(a_0+a_0^*)$. The Hamiltonian can then be diagonalized by the Bogoliubov transformation as before, and one finds that the shift in ground-state energy caused by the external magnetic field is

$$\Delta E_y(p)=-\left[\frac{S}{1-x}+\frac{C_{-1}-C_1}{2x(1-x)}\right]\frac{N}{2zS}p^2\ . \tag{2.25}$$

Hence one can find the required susceptibility:

$$\chi_{yy}=-\frac{1}{N}\frac{\partial^2\Delta E_y}{\partial p^2}\bigg|_{p=0}=\frac{1}{z(1-x)}\left[1+\frac{C_{-1}-C_1}{2Sx}\right]. \tag{2.26}$$

The susceptibility in the **z** direction can be obtained in a similar fashion:

$$\chi_{zz}=\frac{1}{z}\left[1-\frac{C_3-C_1}{2Sx}\right]. \tag{2.27}$$

Note that the C_n appearing in Eqs. (2.21)–(2.27) are evaluated from Eq. (2.19) after setting $h=0$, i.e., $D=1$.

Up to this point, the results have been applicable to the ferromagnetic XY model on any lattice or to the antiferromagnetic XY model on any bipartite lattice following a simple spin rotation. We now restrict our attention to the two-dimensional square lattice (the application of our second-order spin-wave analysis to other lattices will be given elsewhere[25]).

Using the same techniques applied in our calculation of XXZ model,[1] we can find the asymptotic expansion near $x=\pm1$ of the C_n for the two-dimensional square lattice:

$$C_3 = 0.098\,184\,35 - 0.105\,069\,7(1-x^2) + 0.017\,585\,6(1-x^2)^2 - \frac{1}{10\sqrt{2}\pi}(1-x^2)^{5/2} + 0.023\,772(1-x^2)^3 - \frac{59}{560\sqrt{2}\pi}(1-x^2)^{7/2} + \cdots , \tag{2.28a}$$

$$C_1 = -0.041\,908\,60 + 0.081\,918\,3(1-x^2) - \frac{1}{3\sqrt{2}\pi}(1-x^2)^{3/2} + 0.065\,780(1-x^2)^2 - \frac{31}{120\sqrt{2}\pi}(1-x^2)^{5/2} + \cdots , \tag{2.28b}$$

$$C_{-1} = 0.285\,764\,5 - \frac{\sqrt{2}}{\pi}(1-x^2)^{1/2} + 0.280\,482(1-x^2) - \frac{11}{12\sqrt{2}\pi}(1-x^2)^{3/2} + 0.1643(1-x^2)^2 + \cdots , \tag{2.28c}$$

$$C_{-3} = \frac{2\sqrt{2}}{\pi}(1-x^2)^{-1/2} - 0.836\,163\,5 - \frac{1}{2\sqrt{2}\pi}(1-x^2)^{1/2} + 0.087\,706\,2(1-x^2) + \cdots , \tag{2.28d}$$

$$C_{-5} = \frac{4\sqrt{2}}{3\pi}(1-x^2)^{-3/2} + \frac{5}{3\sqrt{2}\pi}(1-x^2)^{-1/2} - 0.953\,105 + \cdots . \tag{2.28e}$$

Hence one can deduce the asymptotic behavior near $x=\pm1$ of the physical quantities above:

$$E_0/N = -2S^2 - 0.083\,817\,2S - 0.005\,784\,67 + (0.163\,836\,6S - 0.025\,031)(1-x^2) + (-0.150\,05S + 0.006\,535\,3)(1-x^2)^{3/2} + \cdots \quad (x\sim\pm1) , \tag{2.29a}$$

$$m = [4S - 0.431\,436 + 1.2732(1-x)^{1/2}](1-x)^{1/2} + \cdots \quad (x\sim1) , \tag{2.29b}$$

$$m = [4S - 0.056\,276 + 0.233\,88(1+x)](1-x)^{1/2} + \cdots \quad (x\sim-1) , \tag{2.29c}$$

$$M_x = S - 0.060\,964 - 7.4036\times10^{-4}/S + (0.112\,539 - 0.023\,715\,6/S)(1-x^2)^{1/2} + \cdots \quad (x\sim\pm1) , \tag{2.29d}$$

$$\chi_{xx} = (0.028\,134\,8/S + 3.958\,26\times10^{-4}/S^2)(1-x^2)^{-1/2} - 0.045\,30/S + 0.008\,352\,1/S^2 + \cdots \quad (x\sim\pm1) , \tag{2.29e}$$

$$\chi_{yy} = (1-x)^{-1}[0.25 + 0.004\,095\,9/S - 0.079\,577(1-x)^{1/2}/S + \cdots] \quad (x\sim1) , \tag{2.29f}$$

$$\chi_{yy} = 0.125 - 0.020\,479\,5/S + 0.039\,788\,6(1+x)^{1/2}/S + \cdots \quad (x\sim-1) , \tag{2.29g}$$

$$\chi_{zz} = 0.25 - 0.017\,511\,6/S + 0.046\,747(1-x)/S + \cdots \quad (x\sim1) , \tag{2.29h}$$

$$\chi_{zz} = 0.25 + 0.017\,511\,6/S - 0.046\,747(1+x)/S + \cdots \quad (x\sim-1) . \tag{2.29i}$$

III. SERIES RESULTS AND ANALYSIS

Series expansions for the model have been obtained using Nickel's cluster expansion method.[16–19] The Hamiltonian (2.1) in zero magnetic field can be rewritten

$$H = -\sum_{\langle lm\rangle} [S_l^x S_m^x + \tfrac{1}{4}x(S_l^+ + S_l^-)(S_m^+ + S_m^-)] , \tag{3.1}$$

in a representation where S_i^x is diagonal and S_i^+, S_i^- are spin raising and lowering operators. The unperturbed ground state at $x=0$ has all spins "up," and the operator proportional to x is treated as a perturbation operator, which "flips" spins on neighboring pairs of sites $\langle lm \rangle$. We have reviewed the techniques necessary for performing such a perturbation expansion in He, Hamer and Oitmaa.[26] Technically, the present case is a "low-temperature" expansion, requiring the calculation of "strong" embedding constants for the clusters involved.[27]

TABLE I. Series coefficients for the ground-state energy per site E_0/N, the magnetization M_x, and the parallel susceptibility χ_{xx}. Coefficients of x^n are listed.

n	E_0/N	M_x	χ_{xx}
0	$-\frac{1}{2}$	$\frac{1}{2}$	0
2	$-\frac{1}{24}$	$-\frac{1}{36}$	$\frac{1}{2}$
4	$-0.428\,240\,740\,741\times10^{-2}$	$-0.906\,828\,703\,704\times10^{-2}$	$0.263\,244\,598\,765\times10^{-1}$
6	$-0.125\,118\,955\,761\times10^{-2}$	$-0.456\,675\,158\,859\times10^{-2}$	$0.205\,169\,648\,395\times10^{-1}$
8	$-0.553\,856\,724\,242\times10^{-3}$	$-0.287\,374\,997\,710\times10^{-2}$	$0.174\,432\,424\,029\times10^{-1}$
10	$-0.299\,040\,060\,244\times10^{-3}$	$-0.201\,587\,464\,747\times10^{-2}$	$0.154\,267\,331\,542\times10^{-1}$
12	$-0.182\,300\,413\,146\times10^{-3}$	$-0.151\,362\,706\,889\times10^{-2}$	$0.139\,861\,198\,156\times10^{-1}$
14	$-0.120\,533\,943\,936\times10^{-3}$	$-0.118\,982\,714\,152\times10^{-2}$	$0.128\,870\,990\,841\times10^{-1}$

TABLE II. Series coefficients for the transverse susceptibilities χ_{yy}, χ_{zz}, and the energy gap m. Coefficients of x^n are listed.

n	χ_{yy}	χ_{zz}	m
0	$\frac{1}{4}$	$\frac{1}{4}$	2
1	$\frac{7}{24}$	$-\frac{1}{24}$	-1
2	0.296 875 000 000	$0.520\,833\,333\,333\times10^{-2}$	$-0.416\,666\,666\,667$
3	0.308 738 425 926	$-0.318\,287\,037\,037\times10^{-2}$	$-0.416\,666\,666\,667\times10^{-1}$
4	0.310 543 491 191	$0.395\,921\,746\,399\times10^{-2}$	$-0.104\,745\,370\,370$
5	0.316 136 021 397	$-0.665\,530\,922\,374\times10^{-3}$	$-0.252\,674\,093\,364\times10^{-1}$
6	0.317 170 886 064	$0.323\,355\,318\,811\times10^{-4}$	$-0.471\,861\,677\,758\times10^{-1}$
7	0.320 603 704 686	$-0.228\,148\,917\,862\times10^{-3}$	$-0.201\,121\,534\,927\times10^{-1}$
8	0.321 338 412 658	$-0.134\,630\,116\,992\times10^{-4}$	$-0.260\,801\,516\,831\times10^{-1}$
9	0.323 692 938 356	$-0.100\,425\,218\,103\times10^{-3}$	$-0.151\,060\,413\,907\times10^{-1}$
10	0.324 245 837 203	$-0.191\,327\,790\,202\times10^{-4}$	$-0.180\,459\,338\,722\times10^{-1}$
11	0.325 992 915 511	$-0.519\,134\,609\,996\times10^{-4}$	
12	0.326 426 520 258	$-0.173\,983\,050\,553\times10^{-4}$	
13	0.327 789 189 125	$-0.298\,654\,517\,495\times10^{-4}$	

We used the same list of clusters as in our previous paper.[1] Calculating the contribution of each cluster to the various series took up some 150 h CPU time on an IBM3090 computer.

The resulting series are listed in Tables I and II. The only previous series analysis that we know of is that of Pearson,[13] who calculated terms up to $O(x^8)$ in the series for the ground-state energy. Our results agree with his to that order.

The analysis of these series was carried out along the same line as Zheng, Oitmaa, and Hamer.[1] First, the form of any singularities at $x=\pm1$ was investigated. For the most part, a standard *D*log Padé analysis was performed,[28] after first differentiating each function where necessary in order to promote the singular term into the dominant term. The estimated singularity parameters are shown in Table III. They show that the singularities do indeed lie at the expected positions $x=\pm1$; and although the index estimates are not very accurate, they are by and large quite consistent with the predictions of spin-wave theory.

Next, we assume the singularity indices are those predicted by spin-wave theory and attempt to estimate the amplitudes of leading-order terms in the asymptotic expansions near $x=\pm1$. First, we transform to a new variable, as proposed by Huse:[29]

$$\delta=1-(1-x^2)^{1/2}\ , \tag{3.2a}$$

TABLE III. Estimates of singularity parameters for the series given in Tables I and II. Both unbiased estimates (u.b.) and estimates biased by setting $x_c^2=1$ (b.) are listed. The index values predicted by spin-wave theory are also given for comparison.

Function		Singular point x_c^2	Singularity index	Spin-wave prediction
$\frac{d^2E_0}{d(x^2)^2}$	u.b.	1.0(1)	$-0.7(2)$	-0.5
	b.	1	$-0.6(1)$	
m $(x>0)$	u.b.	1.005(5)	0.56(8)	0.5
	b.	1	0.54(3)	
$\frac{dM_x}{dx^2}$	u.b.	1.01(1)	$-0.55(6)$	-0.5
	b.	1	$-0.52(4)$	
χ_{xx}	u.b.	1.000(1)	$-0.6(1)$	-0.5
	b.	1	$-0.51(1)$	
χ_{yy} $(x>0)$	u.b.	$x_c=1.002(2)$	$-1.06(5)$	-1
	b.	1	$-1.03(4)$	
$\frac{d\chi_{yy}}{dx}$ $(x<0)$	u.b.	$x_c=-0.95(10)$	$-0.3(2)$	-0.5
	b.	-1	$-0.35(10)$	
$\frac{d^2\chi_{zz}}{dx^2}$ $(x>0)$	u.b.	$x_c=1.04(4)$	$-0.9(2)$	-0.5
	b.	1	$-0.55(8)$	
$\frac{d^2\chi_{zz}}{dx^2}$ $(x<0)$	u.b.	$x_c=-1.3(1)$[a]	$-0.9(2)$[a]	-0.5
	b.	-1	$-0.55(10)$	

[a]All estimates defective.

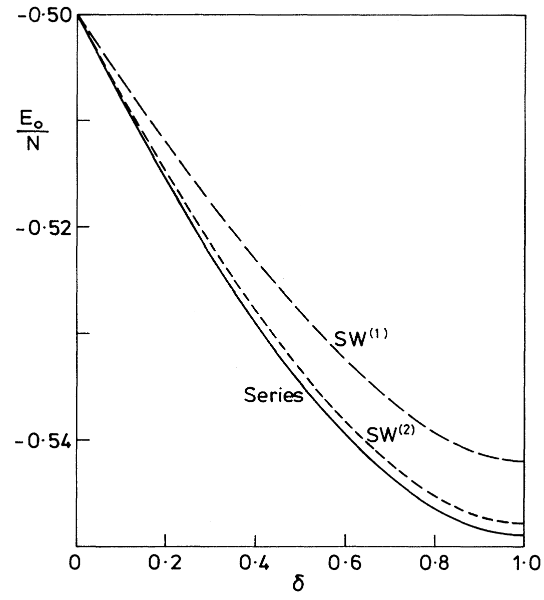

FIG. 1. Graph of the ground-state energy per site, E_0/N, against δ. The three curves shown are the series estimate and the first- and second-order spin-wave predictions, marked $SW^{(1)}$ and $SW^{(2)}$, respectively.

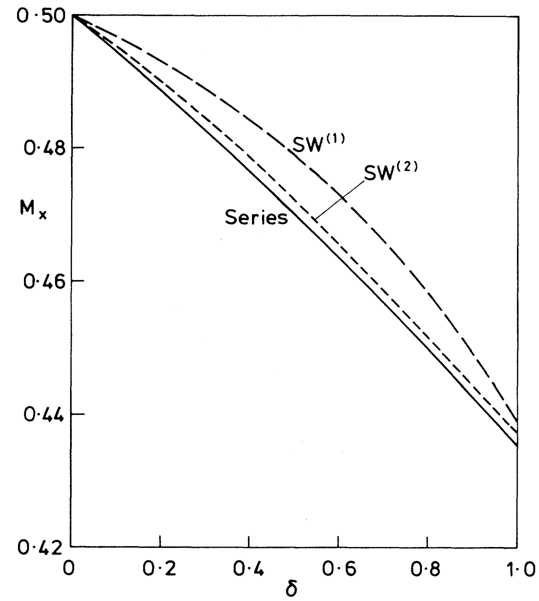

FIG. 2. Graph of the magnetization M_x against δ. Notation as in Fig. 1.

or

$$\delta' = 1-(1\mp x)^{1/2} , \tag{3.2b}$$

depending whether the quantity is a function of x^2 or x, and whether we are expanding about $x=+1$ or -1. The function should then be analytic in the new variable δ (or δ′), according to spin-wave theory. We then extrapolate to $x=\pm1$ using three different methods. In the first method, simple Padé approximants in δ (or δ′) were calculated for each series, from which the value of the function and its derivatives at $\delta=1$ (or $\delta'=1$) can be calculated directly. In the second method, differential approxi-

TABLE IV. Series estimates for the leading-order amplitudes A_n at $x=\pm1$ [as defined by Eq. (3.4)]. Also listed are the spin-wave predictions at first and second order.

Function	x	n	Amplitudes A_n Spin-wave predictions First-order	Second-order	Series estimate
E_0/N	±1	0	−0.541 91	−0.547 69	−0.548 83(3)
		2	0.081 92	0.056 89	0.069 80(2)
		3	−0.075 03	−0.009 67	−0.031 1(1)
M_x	±1	0	0.439 04	0.437 56	0.435 48(3)
		1	0.112 54	0.065 11	0.0740(2)
χ_{xx}	±1	−1	0.056 27	0.057 85	0.0588(6)
		0	−0.0906	−0.0572	−0.034(5)
m	1	1	2	1.569	1.61(1)
		2		1.273	0.68(6)
$(1-x)^{-1/2}m$	−1	0	2	1.9437	1.763(4)
		2		0.2339	0.68(2)
$(1-x)\chi_{yy}$	1	0	0.25	0.3319	0.3505(5)
		1		−0.1592	−0.1515(14)
χ_{yy}	−1	0	0.125	0.084 04	0.0900(5)
		1		0.079 58	0.038(3)
χ_{zz}	1	0	0.25	0.214 98	0.209 54(3)
		2		0.0935	0.0486(6)
χ_{zz}	−1	0	0.25	0.285 02	0.301 515(2)
		2		−0.093 49	−0.069 734(4)

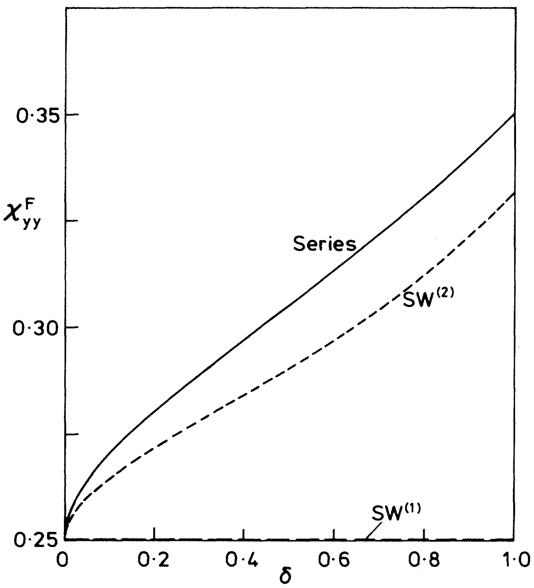

FIG. 3. Graph of the susceptibility χ_{yy} $(x>0)$ against δ. Notation as in Fig. 1.

mants[28] were calculated for each series, from which the value of the function and its derivatives at $\delta=1$ (or $\delta'=1$) can be found by numerical integration. Last, we used the technique of Singh,[30] whereby partial sums S_N are computed at $x^2=1$ for the original series in the variable x^2 (or x). If the leading singularity is of the form $(1-x^2)^\lambda$, then asymptotically one expects.

$$S_N \sim S_\infty + \frac{c}{(N+\alpha)^\lambda} , \tag{3.3}$$

where S_∞ is the sum of the infinite series and c,α are constants. The sums S_N are plotted against $(N+\alpha)^{-\lambda}$, and α is adjusted so as to get the best fit to a straight line; then S_∞ can be estimated by a simple linear extrapolation. Comparing the results of all these methods, one can form good estimates of the extrapolated value S_∞ and its associated error.

The results of these procedures are listed in Table IV. For each given function f, the asymptotic amplitudes are defined by

$$f(x^2) \sim \sum_{n=n_0}^{\infty} A_n (1-x^2)^{n/2} \quad (x^2 \sim 1) \tag{3.4a}$$

or

$$f(x) \sim \sum_{n=n_0}^{\infty} A_n (1 \mp x)^{n/2} \quad (x \sim \pm 1) , \tag{3.4b}$$

as the case may be. Our series estimates of these amplitudes A_n are listed in Table IV, together with the predictions of spin-wave theory at first and second order in $1/S$.

The agreement between the spin-wave predictions and the series estimates is very good, even better than in the case of the Heisenberg antiferromagnet.[1] The reason presumably is that the average "spin deviation" $\langle n_l \rangle$ is smaller here than in the Heisenberg case, and so the truncated spin-wave analysis is more accurate. Second-order spin-wave theory predicts the leading amplitude for the ground-state energy to within 0.2%, the magnetization M_x to 0.5%, and χ^A_{yy} to about 7%. The agreement is further illustrated in Figs. 1, 2, and 3, which graph the series estimates and spin-wave predictions as functions of δ for E_0, M_x, and χ_{yy} $(x>0)$. The series estimates here were obtained by integrating the differential approximants in δ (or δ′).

Finally, a comparison of our results for the ground-state energy with estimates from other sources is shown in Table V. Our results are clearly consistent with the earlier ones, but much more accurate.

IV. SUMMARY

Our conslusions are much the same as in the Heisenberg case.[1] By extrapolation of our series expansions to the isotropic limit, estimates for the behavior of the XY spin model have been obtained which are substantially more accurate than the few previous treatments. A detailed comparison has shown excellent agreement between the numerical results and spin-wave theory. In every case, the second-order spin-wave theory provides a much more accurate representation than the first-order theory.

The isotropic XY ferromagnet at $x=1$ possesses a rotational O(2) symmetry in the x-y spin plane, which is broken when $x<1$ into a $\mathbb{Z}_2$ symmetry in the **x** direction. The ground state of the isotropic model exhibits spontaneous symmetry breaking by the Goldstone mecha-

TABLE V. Comparison of some numerical estimates obtained by different authors for the ground-state energy of the $S=\frac{1}{2}$ isotropic XY model on a square lattice.

Reference	Method	$4E_0/N$
Oitmaa, Betts, and Marland (Ref. 10)	Finite lattice calculation	−2.16(2)
Pearson (Ref. 13)	Series	−2.198(8)
Okabe and Kikuchi (Ref. 12)	8×8 MC	−2.008(8)
Okabe and Kikuchi (Ref. 12)	12×12 MC	−2.1968(80)
Okabe and Kikuchi (Ref. 12)	16×16 MC	−2.1960(20)
Present work	Series	−2.1953(1)

nism, so that if the isotropic limit is approached from the Ising side ($x < 1$), there is long-range order in the **x** direction, i.e., a nonzero M_x value, in accordance with the rigorous proofs of Kennedy, Lieb, and Shastry[22] and Kubo and Kishi.[23] The mass gap goes to zero in the isotropic limit, corresponding to the appearance of a massless Goldstone mode. All these characteristics are very similar to those of the *XXZ* Heisenberg antiferromagnet.

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