PHYSICAL REVIEW B VOLUME 43, NUMBER 10 1 APRIL 1991

Square-lattice Heisenberg antiferromagnet at $T=0$

Zheng Weihong, J. Oitmaa, and C. J. Hamer
School of Physics, University of New South Wales, P.O. Box 1, Kensington, New South Wales 2033, Australia
(Received 8 November 1990; revised manuscript received 11 January 1991)

The spin-$\frac{1}{2}$ and spin-1 Heisenberg antiferromagnets on a square lattice are studied via series expansions around the Ising limit. Series are calculated for the ground-state energy, staggered magnetization, transverse susceptibility, staggered parallel susceptibility, and mass gap. Extrapolating these series to the isotropic limit, we find extremely good agreement with the predictions of spin-wave theory.

I. INTRODUCTION

The discovery of high-T_c superconductivity in materials containing two-dimensional Cu-O planes has generated a surge of interest in two-dimensional models which may be relevant, particularly the Hubbard model, and the Heisenberg antiferromagnet. The square-lattice Heisenberg antiferromagnet, which we consider here, has a long history. A recent review has been given by Barnes.[1] A spin-wave theory was developed for it by Andersen,[2] Kubo,[3] Oguchi,[4] and Stinchcombe,[5] among others. Variational calculations have been presented by Marshall,[6] and Huse and Elser.[7] Series expansions about the Ising limit have been studied by Davis,[8] Parrinello and Arai,[9] Huse,[10] Singh,[11,12] and Singh and Huse.[13] An early finite-cell calculation was performed by Oitmaa and Betts,[14] see also Dagotto and Moreo[15] and Tang and Hirsch.[16] More recently, large-scale Monte Carlo simulations have been carried out by Barnes and Swanson,[17] Manousakis and Salvador,[18] Reger and Young,[19] Barnes, Kotchan, and Swanson,[20] Barnes *et al.*,[21] Gross, Sanchez-Velasco, and Siggia,[22,23] Okabe and Kikuchi,[24,25] Carlson,[26] Trivedi and Ceperley,[27] Liang,[28] and Barnes and Kovarik.[29]

The general conclusion has been that at zero temperature the isotropic Heisenberg antiferromagnet is in an ordered state, with a nonzero staggered magnetization, and is quite well described by spin-wave theory. Liang, Doucot, and Anderson[30] have suggested, however, that a singlet "resonating-valence-bond" state may exist very close to the ground state in energy, so that even a small amount of doping can destroy the Néel order.

In the present paper, we extend the series results for the model using a cluster expansion technique. This is an efficient method of series expansion for quantum Hamiltonian lattice models, which was originally proposed by Nickel,[31] and further elaborated in papers by Marland,[32] Irving and Hamer,[33] and Hamer and Irving.[34] We have recently reviewed the technique in He, Hamer, and Oitmaa.[35] A very similar method seems to have been discovered independently by Singh, Gelfand, and Huse[36] (see also Gelfand, Singh, and Huse[37]), and has been applied by them to the square-lattice Heisenberg antiferromagnet in the works mentioned above. We are able to add several terms to the series for the ground-state energy, staggered magnetization, and perpendicular susceptibility calculated by Singh.[11,12] We have also calculated series for the mass gap and staggered parallel susceptibility which are entirely new, as far as we are aware. Analysis of these series gives estimates for the behavior of isotropic models which are substantially more accurate than any previous treatment.

A careful comparison is made between the series results and the predictions of spin-wave theory. The original spin-wave theory of Anderson[2] was extended to second order by Kubo[3] and Oguchi;[4] and the singular behavior of the anisotropic model was further discussed by Stinchcombe.[5] The results are not comprehensive enough for our purposes, however, and so in Sec. II of the paper we extend the spin-wave calculations for the anisotropic model, following, in the main, the treatment of Oguchi.[4] In Sec. III the series results are analyzed and compared with spin-wave theory. Overall, they agree extremely well—so well, in fact, that an effort to push the spin-wave theory to higher order seems called for.

II. SPIN-WAVE THEORY

The spin-wave (SW) theory has proved to be quite successful in predicting the properties of the ground state (and even low excited states) of spin models such as the Heisenberg antiferromagnet. In this section we present, for comparison with our series expansion results, a spin-wave analysis (to second order in $1/S$) of the anisotropic Heisenberg antiferromagnet, closely following Oguchi.[4] The system of interest is described by the following Hamiltonian:

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

where we have divided the lattice sites into even and odd sublattices, denoted by l and m, respectively, and the sum over $\langle lm\rangle$ denotes a sum over all nearest-neighbor pairs. The limits $x=0$ and $x=1$ correspond to the antiferromagnetic Ising model and isotropic Heisenberg model, respectively.

The application of spin-wave theory to the above Hamiltonian is accomplished by the three following transformations. Firstly, we introduce boson creation and annihilation operators for the "spin deviations" on the two sublattices by means of the Holstein-Primakoff[38] transformation. Let

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

for an "up" spin on the l sublattice, and

$$S_m^+=(2S)^{1/2}b_m^*f_m(S)\ ,\quad S_m^-=(2S)^{1/2}f_m(S)b_m\ ,\quad S_m^z=-S+b_m^*b_m\ , \tag{2.3}$$

for a "down" spin on the m sublattice, where

$$f_l(S)=\left[1-\frac{n_l}{2S}\right]^{1/2} \tag{2.4}$$

and $n_l=a_l^*a_l$ is the "spin deviation operator," and similarly for the m sublattice. The operators a_l^* and a_l (or b_m^*, b_m) satisfy the boson commutation rule

$$[a_l,a_{l'}^*]=\delta_{ll'}\ . \tag{2.5}$$

The Fock space of the new boson operators includes both unphysical states with occupation number $n_l>2S$, and physical states $0\le n_l\le 2S$. They are not mixed by the Hamiltonian if we use Eq. (2.4). In our calculation, however, we employ only the first two terms in an expansion of $f_l(S)$:

$$f_l(S)\simeq 1-n_l/4S\ . \tag{2.6}$$

If the occupation number $\langle n_l\rangle$ is small, the main contribution comes from the physical subspace ($n_l\le 2S$), and it is reasonable to neglect the higher-order terms in the expansion.

Secondly, we introduce Bloch-type operators a_k, b_k by the Fourier transformation

$$a_k=\left[\frac{2}{N}\right]^{1/2}\sum_l e^{ikl}a_l\ ,\quad b_k=\left[\frac{2}{N}\right]^{1/2}\sum_m e^{-ikm}b_m\ , \tag{2.7}$$

where N is the total number of lattice sites, and a_k, b_k satisfy again the boson commutation rules:

$$[a_k,a_{k'}^*]=\delta_{kk'}\ . \tag{2.8}$$

Finally, the terms in the Hamiltonian up to second order in boson operators can be diagonalized by a Bogoliubov transformation:

$$a_k=\alpha_k\cosh\theta_k-\beta_k^*\sinh\theta_k\ ,\quad b_k=-\alpha_k^*\sinh\theta_k+\beta_k\cosh\theta_k\ , \tag{2.9}$$

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

$$\gamma_k=\frac{1}{z}\sum_\rho e^{ik\rho}\ . \tag{2.10}$$

The Hamiltonian now becomes (to second order in an expansion in $1/S$, and keeping only diagonal terms in this bais)

$$H=E_h+\sum_k (A_k^-n_k+A_k^+n_k')+\sum_{k_1,k_2}[B^{(1)}(n_1n_2+n_1'n_2')+B^{(2)}n_1n_2']+\cdots\ , \tag{2.11}$$

where $n_k=\alpha_k^*\alpha_k$, $n_k'=\beta_k^*\beta_k$,

$$E_h=-S^2zN(1-h_1'+h_2')/2+zS\sum_k[(D^2-x^2\gamma_k^2)^{1/2}-D]-\frac{z}{2N}\left\{\left[\sum_k\left[\frac{D-x^2\gamma_k^2}{(D^2-x^2\gamma_k^2)^{1/2}}-1\right]\right]^2+x^2(1-x^2)\left[\sum_k\frac{\gamma_k^2}{(D^2-x^2\gamma_k^2)^{1/2}}\right]^2\right\}, \tag{2.12}$$

$$A_k^{\pm}=zS[(D^2-x^2\gamma_k^2)^{1/2}\pm\tfrac{1}{2}(h_1'+h_2')]-\frac{z}{N}\left[\frac{D-x^2\gamma_k^2}{(D^2-x^2\gamma_k^2)^{1/2}}\sum_{k_2}\left[\frac{D-x^2\gamma_2^2}{(D^2-x^2\gamma_2^2)^{1/2}}-1\right]+\frac{x^2(1-x^2)\gamma_k^2}{(D^2-x^2\gamma_k^2)^{1/2}}\sum_{k_2}\frac{\gamma_2^2}{(D^2-x^2\gamma_2^2)^{1/2}}\right], \tag{2.13}$$

$$B^{(1)}=-\frac{z}{2N}\left[\frac{D^2-2x^2D\gamma_2^2+x^2\gamma_1\gamma_2\gamma_{1-2}}{(D^2-x^2\gamma_1^2)^{1/2}(D^2-x^2\gamma_2^2)^{1/2}}-1\right],\quad B^{(2)}=-\frac{z}{N}\left[\frac{D^2-2x^2D\gamma_2^2+x^2\gamma_1\gamma_2\gamma_{1-2}}{(D^2-x^2\gamma_1^2)^{1/2}(D^2-x^2\gamma_2^2)^{1/2}}+1\right], \tag{2.14}$$

where $\gamma_{1-2}\equiv\gamma_{k_1-k_2}$, etc. These expressions reduce to those of Oguchi[4] in the isotropic limit $x=1$, if one were to make his assumption $\gamma_{1-2}=\gamma_1\gamma_2$ (which seems to be unjustified).

Setting the external magnetic field to zero (i.e., $h_1=h_2=0$), one can derive from Eq. (2.11) the ground-state energy E_0 and mass gap m:

$$E_0/N=-\frac{zS}{2}\left[S-C_1+\frac{1}{4S}\left[C_1^2+\frac{1-x^2}{x^2}(C_{-1}-C_1)^2\right]\right], \tag{2.15}$$

$$m=z(1-x^2)^{1/2}(S-C_{-1}/2), \tag{2.16}$$

where

$$C_n=\frac{2}{N}\sum_k[(1-x^2\gamma_k^2)^{n/2}-1]. \tag{2.17}$$

Let $h_1=-h_2=h$, and differentiate Eq. (2.12) with respect to h, then one finds the staggered magnetization M^+ and parallel staggered susceptibility $\chi_\parallel^S$:

$$M^+=\frac{1}{N}\frac{\partial E_h}{\partial h}\bigg|_{h=0}=S-\frac{C_{-1}}{2}-\frac{1-x^2}{4Sx^2}(C_{-1}-C_1)(C_{-3}-C_{-1}), \tag{2.18}$$

$$\chi_\parallel^S=-\frac{1}{N}\frac{\partial^2 E_h}{\partial h^2}\bigg|_{h=0}=\frac{1}{2zS}(C_{-3}-C_{-1})+\frac{1}{4zS^2}\left[C_1(C_{-3}-C_{-1})+\frac{1-x^2}{x^2}[(C_{-3}-C_{-1})^2+(C_{-1}-C_1)(C_{-1}+3C_{-5}-4C_{-3})]\right]. \tag{2.19}$$

In order to derive the perpendicular susceptibility, we set $h_1=h_2=0$ in Eq. (2.1), and add an external magnetic field directed along the x axis:

$$p_1\sum_l S_l^x+p_2\sum_m S_m^x. \tag{2.20}$$

Perform the Holstein-Primakoff and Fourier transformations as before, and then shift the origin of the Bloch operators a_0 and b_0 by

$$t_1=\frac{1}{2z}\left[\frac{N}{S}\right]^{1/2}\frac{xp_2-p_1}{1-x^2}, \tag{2.21}$$

and

$$t_2=\frac{1}{2z}\left[\frac{N}{S}\right]^{1/2}\frac{xp_1-p_2}{1-x^2}, \tag{2.22}$$

respectively, so as to cancel linear terms in $(a_0+a_0^*)$, $(b_0+b_0^*)$. The terms up to second order in the Hamiltonian can be diagonalized by the Bogoliubov transformation as before, and one finds the shift in the ground-state energy caused by the external transverse magnetic field is

$$\Delta E(p_1,p_2)=\frac{N}{4z(1-x^2)}\times\left[(2xp_1p_2-p_1^2-p_2^2)-\frac{x(p_1^2+p_2^2)-2p_1p_2}{2xS}(C_{-1}-C_1)\right]. \tag{2.23}$$

Hence the uniform perpendicular susceptibility can be obtained by setting $p_1=p_2=p$ and differentiating:

$$\chi_\perp=-\frac{1}{N}\frac{\partial^2\Delta E}{\partial p^2}\bigg|_{p=0}=\frac{1}{z(1+x)}\left[1-\frac{(C_{-1}-C_1)}{2Sx}\right]. \tag{2.24}$$

The staggered perpendicular susceptibility $\chi_\perp^S$ can be obtained similarly, and one finds

$$\chi_\perp^S(x)=\chi_\perp(-x). \tag{2.25}$$

This result also reduces to that of Oguchi[4] if $x=1$.

Hitherto, the results have been applicable to any bipartite lattice. We now restrict ourselves to the two-dimensional square lattice (the application of our second-order spin-wave analysis to other lattices will be given elsewhere[39]). Following Kubo[3] and Stinchcombe,[5] we find the following asymptotic expansions for the quantities C_n defined by Eq. (2.17) near $x=1$:

$$\begin{aligned} C_1 &= -0.157\,947\,4+0.275\,575\,6(1-x^2) \\ &\quad -\frac{2}{3\pi}(1-x^2)^{3/2}-0.1741(1-x^2)^2 \\ &\quad -\frac{7}{15\pi}(1-x^2)^{5/2}+\cdots\,, \\ C_{-1} &= 0.393\,203\,9-\frac{2}{\pi}(1-x^2)^{1/2} \\ &\quad +0.4210(1-x^2)-\frac{1}{\pi}(1-x^2)^{3/2} \\ &\quad +0.2577(1-x^2)^2+\cdots\,, \\ C_{-3} &= \frac{2}{\pi}(1-x^2)^{-1/2}-0.4488 \\ &\quad -\frac{1}{\pi}(1-x^2)^{1/2}+0.2323(1-x^2)+\cdots\,, \\ C_{-5} &= \frac{2}{3\pi}(1-x^2)^{-3/2}+\frac{5}{3\pi}(1-x^2)^{-1/2} \\ &\quad -0.603\,64+\frac{3}{4\pi}(1-x^2)^{1/2}+\cdots\,. \end{aligned} \tag{2.26}$$

The coefficients of the analytic terms were found by performing numerical summations of series Eq. (2.17), or its derivatives, while the coefficients of the singular terms can be obtained by the following method. Consider C_1 as an example.

The functions C_1 and $a(1-x^2)^{3/2}+b(1-x^2)^{5/2}$ can be expanded as series in x^2:

$$C_1=\sum_{k=1}^{\infty} d_k x^{2k}\,, \tag{2.27}$$

$$a(1-x^2)^{3/2}+b(1-x^2)^{5/2}=\sum_{k=0}^{\infty} f_k x^{2k}\,, \tag{2.28}$$

where

$$d_k=-[(2k)!/(2^k k!)^2]^3\frac{1}{2k-1}\,, \tag{2.29}$$

$$f_k=\left[3a-\frac{15b}{2k-5}\right]\frac{(2k)!}{(2^k k!)^2(2k-1)(2k-3)}\,. \tag{2.30}$$

If $k\to\infty$, using Stirling's approximation:

$$k!=\sqrt{2\pi k}\,k^k e^{-k}\left[1+\frac{1}{12k}+\cdots\right], \tag{2.31}$$

we find

$$d_k=-\frac{\sqrt{2}}{(2\pi k)^{3/2}k}\left[1+\frac{1}{8k}+\cdots\right], \tag{2.32}$$

$$f_k=\frac{3}{4k^2(\pi k)^{1/2}}\left[a+\frac{15a-20b}{8k}+\cdots\right], \tag{2.33}$$

and so by comparing coefficients of $k^{-5/2}$ and $k^{-7/2}$ in Eqs. (2.32) and (2.33) one may deduce the values of a and b in the asymptotic expansion of C_1 (higher-order singular terms do not contribute to these coefficients).

III. SERIES RESULTS AND ANALYSIS

Series expansions have been obtained for the thermodynamic functions in this model using Nickel's cluster expansion method. By a simple similarity transformation with S_m^x on every site of the odd sublattice, one can transform

$$S_m^z\to -S_m^z\,,\quad S_m^x\to S_m^x\,,\quad S_m^y\to -S_m^y\,, \tag{3.1}$$

and obtain a ferromagnetic Hamiltonian equivalent to Eq. (2.1):

$$\begin{aligned} H' &= -\sum_{\langle lm\rangle}[S_l^zS_m^z-x(S_l^xS_m^x-S_l^yS_m^y)] \\ &\quad +h_1\sum_l S_l^z-h_2\sum_m S_m^z \\ &= -\sum_{\langle lm\rangle}\left[S_l^zS_m^z-\frac{x}{2}(S_l^+S_m^++S_l^-S_m^-)\right] \\ &\quad +h_1\sum_l S_l^z-h_2\sum_m S_m^z \end{aligned} \tag{3.2}$$

in terms of the spin raising and lowering operators of Eqs. (2.2) and (2.3). The unperturbed ground state at $x=0$ has all spins "up"; the operator proportional to x is treated as a perturbation term, 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,[35] and will not repeat the details here. The major difference in this case is that a "low temperature" expansion is involved, requiring the calculation of "strong" embedding constants for the clusters (Domb[40]). The calculations involved a list of 11 131 linked clusters of up to 14 sites together with their lattice constants and embedding constants; the mass gap required a further list of 2525 clusters, both linked and unlinked, up to 11 sites. Generating the cluster data occupied some 20 h of CPU time on an IBM3090; Calculating the contribution of each cluster to various series took up a further 40 h of CPU time for the spin-$\frac{1}{2}$ model, and 10 h for the spin-1 model.

The resulting series are listed in Table I and Table II. They agree with the results of Singh,[11,12] and extend the series he obtained for the spin-$\frac{1}{2}$ model by two terms for E_0 and M^+, and six terms for $\chi_\perp$. The series for mass gap and staggered parallel susceptibility are new, as far as we know.

As a first step in the treatment of these series, we have endeavored to test whether the singularities of these functions at $x=1$ are of the form predicted by spin-wave theory, as outlined in Sec. II. The results are shown in Table III. For the most part, a standard Dlog Padé analysis in the variable x^2 was performed, after first differentiating the function where necessary in order to promote the singular term to leading order in $(1-x^2)$. In the case of the transverse susceptibility $\chi_\perp$, the series is dominated by a simple pole at $x=-1$, corresponding to the staggered transverse susceptibility, and so we re-

TABLE I. Series coefficients for the ground-state energy per site E_0/N, the staggered magnetization M^+, staggered parallel susceptibility $\chi_\parallel^S$, and the mass gap m. Coefficients of x^n are listed for both the spin-$\frac{1}{2}$ and spin-1 models.

n	E_0/N	M^+	$\chi_\parallel^S$	m
		Spin-$\frac{1}{2}$ model		
0	$-\frac{1}{2}$	$\frac{1}{2}$	0	2
2	$-\frac{1}{6}$	$-\frac{1}{9}$	$\frac{4}{27}$	$-\frac{5}{3}$
4	0.925 925 925 926[−3]	−0.177 777 777 778[−1]	0.108 691 358 025	0.317 129 629 630
6	−0.158 156 966 490[−2]	−0.947 129 349 682[−2]	0.798 717 918 565[−1]	−0.419 233 764 146
8	−0.825 212 846 235[−3]	−0.744 291 529 381[−2]	0.774 790 791 855[−1]	0.270 996 990 417
10	−0.311 850 649 269[−3]	−0.437 691 024 484[−2]	0.636 977 861 687[−1]	−0.389 433 514 875
12	−0.241 942 079 720[−3]	−0.360 570 635 434[−2]	0.602 759 642 393[−1]	
14	−0.151 122 678 477[−3]	−0.280 100 515 146[−2]	0.558 300 121 347[−1]	
		Spin-1 model		
0	−2	1	0	4
2	$-\frac{2}{7}$	$-\frac{4}{49}$	$\frac{160}{343}$	$-\frac{50}{21}$
4	−0.252 298 721 686[−1]	−0.269 590 990 605[−1]	0.373 146 890 919[−1]	−0.401 853 664 099
6	−0.723 812 205 411[−2]	−0.136 997 515 033[−1]	0.305 409 765 642[−1]	−0.199 264 281 768
8	−0.328 119 045 071[−2]	−0.880 047 084 950[−2]	0.267 818 058 353[−1]	−0.129 925 423 262
10	−0.179 344 795 467[−2]	−0.625 519 624 340[−2]	0.241 638 397 155[−1]	−0.892 317 430 503[−1]
12	−0.110 240 947 222[−2]	−0.473 924 235 610[−2]	0.222 072 275 512[−1]	

moved this pole by performing an Euler transformation

$$z=\frac{2x}{1+x}\ , \tag{3.3}$$

before looking for the behavior near $x=1$.

The estimates of the singularity parameters in Table III are not very accurate, because our series are neither very long nor very smooth. The results are particularly poor for the ground-state energy, where the singularity is weakest. There is little room for doubt, however, that the singular point lies at $x=1$; and the index estimates are by and large consistent with the spin-wave predictions, within errors of order 10%. Henceforward we assume that the indices predicted by spin-wave theory are correct.

At the next stage of the analysis, we have tried to estimate the coefficients of the leading order terms in the asymptotic expansion near $x=1$, by extrapolation of the series. For this purpose, we first transform to a new variable proposed by Huse:[10]

$$1-\delta=(1-x^2)^{1/2}\ , \tag{3.4}$$

so that according to spin-wave theory each function should be analytic in δ. Next, we have extrapolated each series to the point $\delta=1$ (or $x=1$) using three different methods. In the first method, simple Padé approximants in δ were calculated for each series, from which the value of the function and its derivatives at $\delta=1$ can be calculated directly. Secondly, differential approximants[41] were

TABLE II. Series coefficients for the perpendicular susceptibility $\chi_\perp$. Coefficients of x^n are listed for both the spin-$\frac{1}{2}$ and spin-1 models.

n	Spin-$\frac{1}{2}$	Spin-1
0	$\frac{1}{4}$	$\frac{1}{4}$
1	$-\frac{1}{3}$	$-\frac{2}{7}$
2	0.354 166 666 667	0.289 285 714 286
3	−0.379 629 629 630	−0.299 831 800 852
4	0.383 522 247 942	0.301 344 414 137
5	−0.393 158 923 672	−0.306 189 718 951
6	0.395 868 009 007	0.306 873 914 417
7	−0.402 954 211 929	−0.309 864 843 278
8	0.405 315 646 692	0.310 323 237 180
9	−0.409 214 981 572	−0.312 399 393 569
10	0.411 027 697 321	0.312 738 010 344
11	−0.414 448 978 063	
12	0.415 617 280 171	
13	−0.418 179 085 518	

TABLE III. Estimates of singularity parameters for the series given in Tables I and II. Both unbiased estimates (UB), 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 UB	Singularity index B	Spin-wave prediction
		Spin-$\frac{1}{2}$ model		
m	1.0(1)	0.6(2)	0.57(6)	0.5
$\chi_\parallel^S$	1.05(10)	$-0.7(2)$	$-0.60(10)$	-0.5
$\frac{dM^+}{dx^2}$	1.0(1)	$-0.5(2)$	$-0.49(2)$	-0.5
$\frac{d^2E_0}{d(x^2)^2}$	0.8(5)			-0.5
$\frac{d\chi_\perp}{dx}$	$x_c=1.03(4)$	$-0.6(2)$	$-0.41(2)$[a]	-0.5
$\chi_\perp^S$	$x_c=1.00(1)$	$-1.1(1)$	$-1.07(10)$	-1.0
		Spin-1 model		
m	1.00(4)	0.55(8)	0.53(4)	0.5
$\chi_\parallel^S$	1.03(2)	$-0.70(10)$	$-0.65(10)$	-0.5
$\frac{dM^+}{dx^2}$	1.01(6)	$-0.6(1)$	$-0.58(8)$	-0.5
$\frac{d^2E_0}{d(x^2)^2}$	1.07(8)	$-0.95(6)$	$-0.7(2)$	-0.5
$\frac{d\chi_\perp}{dx}$	$x_c=0.98(10)$	$-0.24(20)$	$-0.37(15)$	-0.5
$\chi_\perp^S$	$x_c=1.00(1)$	$-1.05(8)$	$-1.04(4)$	-1.0

[a]All estimates defective.

calculated for each series, from which the value of the function and its derivatives at $\delta=1$ can be found by numerical integration. Lastly, we used the technique of Singh,[11] whereby partial sums S_N are computed at $x=1$ for the original series in the variable x^2. If the leading singularity is of the form $(1-x^2)^\lambda$, then asymptotically one expects

$$S_N \sim S_\infty + \frac{C}{(N+\alpha)^\lambda}, \tag{3.5}$$

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. The error is gauged by extrapolating with $\alpha=0$. Comparing the results of all three methods of extrapolation, one can form good estimates of the extrapolated values S_∞ and its associated error. In cases where the function is singular at leading order, it was first multiplied by the appropriate power of $(1-\delta)$ in order to estimate the amplitude of the singularity.

The perpendicular susceptibility again requires special treatment. The effects of the simple pole at $x=-1$ were first removed by the Euler transformation [Eq. (3.3)], or else by multiplying by a factor $(1+x)$; and then we changed to a new variable $\delta'=1-(1-z)^{1/2}$, or $\delta''=1-(1-x)^{1/2}$, respectively, before performing the extrapolations. These two methods give consistent results.

The results of these procedures are listed in Table IV. For each given function $f(x)$, we defined asymptotic amplitudes A_n via

$$f(x)=\sum_{n=n_0}^{\infty} A_n(1-x^2)^{n/2}. \tag{3.6}$$

Table IV lists our estimates of the leading amplitudes A_n, as obtained by the procedures outlined above, together with the predictions of spin-wave theory at first and second orders in $1/S$. For those quantities with a finite limit at $x=1$, the agreement is remarkably good. Second-order spin-wave theory predicts the leading amplitude for the ground-state energy in the spin-$\frac{1}{2}$ model to within 0.2%, the magnetization to 1%, and $\chi_\perp$ to about 14% (Takahashi[42] has developed a modified spin-wave theory using the Dyson-Maleev transformation instead of the Holstein-Primakoff transformation: it predicted $\chi_\perp=0.065\,50$ for $S=\frac{1}{2}$, which is in excellent agreement with our series expansion result). For those quantities whose leading terms are singular at $x=1$, and for the nonleading amplitudes, the agreement is not so nearly exact, as one might expect, but it is still reasonable.

The agreement is further illustrated in Figs. 1–3, which graph the series estimates and spin-wave predictions as

TABLE IV. Series estimates for the leading order amplitudes A_n at $x=1$ [as defined by Eq. (3.6)]. Also listed are the spin-wave predictions at first and second order.

Function	n	Amplitudes A_n Spin-wave predictions First order	Second order	Series estimate
		Spin-$\frac{1}{2}$ model		
E_0/N	0	-0.6579	-0.6704	$-0.6693(1)$
	2	0.2756	0.1672	0.188(3)
	3	-0.2122	0.1052	$-0.037(2)$
M^+	0	0.3034	0.3034	0.307(1)
	1	0.3183	0.1429	0.17(1)
$\chi_\perp$	0	0.125	0.0561	0.0659(10)
	1		0.0796	0.037(3)
m	1	2	1.214	1.27(2)
	2		1.273	0.46(8)
$\chi_\parallel^S$	-1	0.1592	0.2217	0.264(10)
	0	-0.2105	-0.1773	$-0.230(8)$
$(1-x)\chi_\perp^S$	0	0.25	0.388	0.47(1)
	1		-0.159	$-0.24(3)$
		Spin-1 model		
E_0/N	0	-2.3159	-2.3284	$-2.3279(3)$
	2	0.5512	0.4428	0.455(2)
	3	-0.4244	-0.1071	$-0.195(3)$
M^+	0	0.8034	0.8034	0.8039(4)
	1	0.3183	0.2306	0.241(4)
$\chi_\perp$	0	0.125	0.09055	0.0925(10)
	1		0.0398	0.031(6)
m	1	4	3.2136	3.26(4)
	2		1.2732	0.7(1)
$\chi_\parallel^S$	-1	0.0796	0.0952	0.098(3)
	0	-0.1053	-0.0970	$-0.101(5)$
$(1-x)\chi_\perp^S$	0	0.25	0.319	0.333(2)
	1		-0.0796	$-0.083(10)$

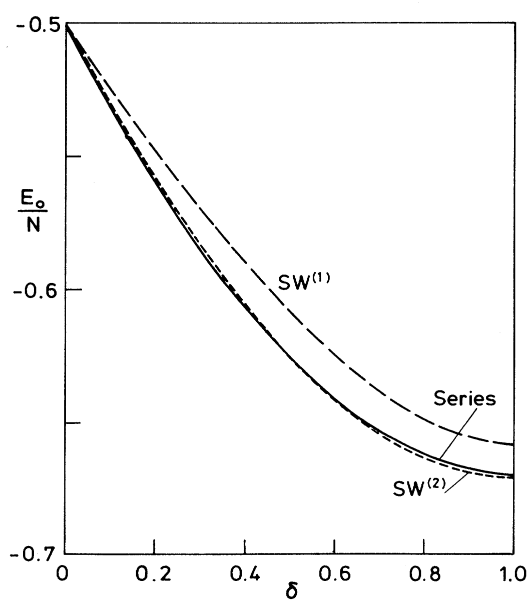

FIG. 1. Graph of the ground state energy per site E_0/N against δ for spin-$\frac{1}{2}$. The three curves shown are the series estimate, and the first- and second-order spin-wave predictions, marked $SW^{(1)}$ and $SW^{(2)}$, respectively.

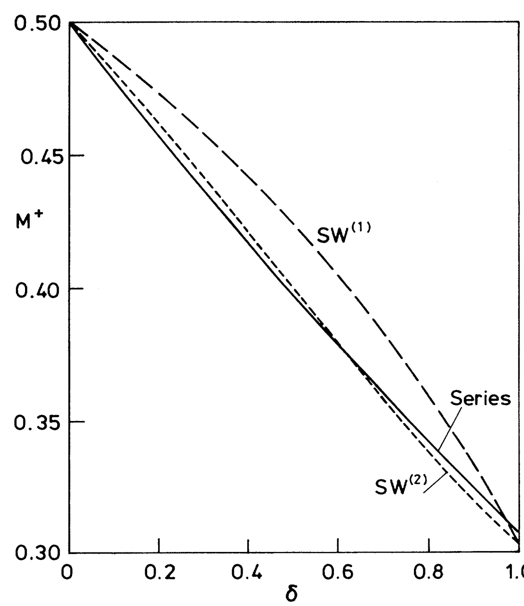

FIG. 2. Graph of the staggered magnetization M^+ against δ for the spin-$\frac{1}{2}$ model. Notation as in Fig. 1.

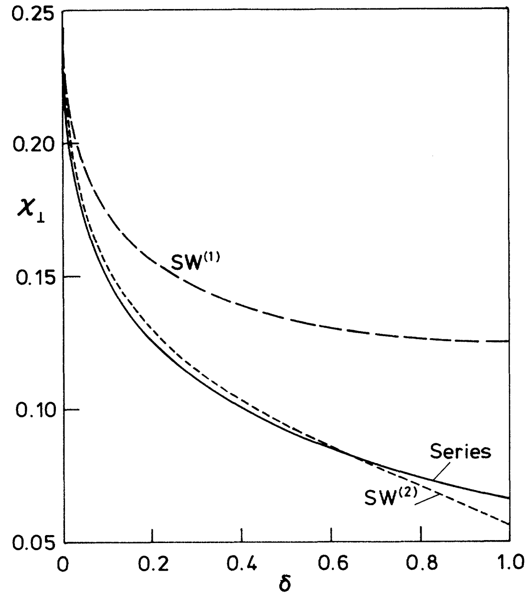

FIG. 3. Graph of the perpendicular susceptibility $\chi_\perp$ against δ for the spin-$\frac{1}{2}$ model. Notation as in Fig. 1.

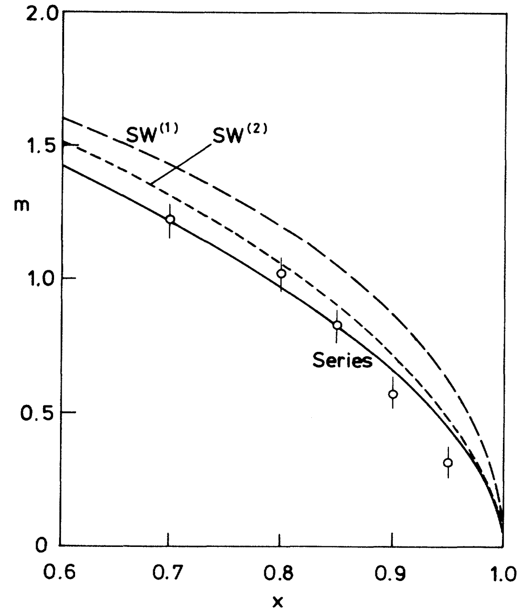

FIG. 4. Graph of the mass gap m against x for the spin-$\frac{1}{2}$ model. Notation as in Fig. 1. The data points are the Monte Carlo estimates of Barnes *et al.* (Ref. 21).

functions of δ for the ground-state energy, the staggered magnetization, and transverse susceptibility of the spin-$\frac{1}{2}$ model. The series estimates here were obtained by integrating the differential approximants in δ. For the spin-1 model the agreement is even better than for the spin-$\frac{1}{2}$ model, as one might expect since the spin-wave theory involves an expansion in $1/S$.

In a recent paper, Barnes *et al.*[21] performed a Monte Carlo calculation of the mass gap near the isotropic point, and found it to lie about a factor of 2 below the first-order spin-wave prediction. This apparent discrepancy with spin-wave theory is largely removed if one goes to second order: a glance at Table IV shows that the leading amplitude A_1 for the mass gap is then reduced by 40%. Figure 4 compares the data of Barnes *et al.*[21] with our series extrapolation, and the spin-wave prediction. The agreement between the series extrapolation and the Monte Carlo estimates is very good. The second-order spin-wave theory still runs a little high, but provides a substantial improvement on first-order theory.

A hypothesis of universality for the singularity ampltiudes has been discussed by Singh,[11] and Singh and Huse.[13] For instance, if we write

$$\begin{aligned} M^+ &\sim M_0(1+At), \quad t\to 0 , \\ \chi_\perp &\sim \chi_\perp^0(1+Bt), \quad t\to 0 \end{aligned} \tag{3.7}$$

where $t=(1-x^2)^{1/2}$, then since the singularities are due to Goldstone modes, i.e., long-distance effects, they argue that the ratio $R=A/B$ should be universal, and independent of short-distance properties such as spin. In the $S\to\infty$ limit the spin-wave theory gives $R=1$. From the series estimates in Table IV, we find values

$$\begin{aligned} R(S=\tfrac{1}{2}) &= 0.98(4) , \\ R(S=1) &= 0.88(13) , \end{aligned} \tag{3.8}$$

which are in quite good agreement with this universality hypothesis. We note, however, that the spin-wave theory does not exhibit this universality, and predicts an S-dependent ratio R. At second order, it predicts

$$\begin{aligned} R(S=\tfrac{1}{2}) &= 0.332 , \\ R(S=1) &= 0.653 . \end{aligned} \tag{3.9}$$

Finally, a comparison of our results with some recent estimates from other sources is presented in Table V. It can be seen that our results agree with the earlier ones within errors, but are substantially more accurate in most cases.

IV. SUMMARY

By extrapolation of our series expansions to the isotropic limit, we have obtained estimates for the behavior of the Heisenberg antiferromagnet which are generally more accurate than 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 convergence appears so extremely rapid, in fact, that one is tempted to ask whether it is feasible to push the spin-wave calculations to third order. This would probably require the use of a symbolic manipulation package on a

TABLE V. Comparison of some recent numerical estimates obtained by different authors for the ground-state energy, the staggered magnetization, and the perpendicular susceptibility at $x=1$.

Reference	Method	$4E_0/N$	$2M^+$	$\chi_\perp$
	Spin-$\frac{1}{2}$ model			
Gross *et al.* (Ref. 22)	Monte Carlo	$-2.669(3)$	0.57(5)	
Reger and Young (Ref. 19)	Monte Carlo	$-2.680(8)$	0.60(4)	
Singh (Ref. 11)	Series	$-2.6785(10)$	0.605(15)	0.065(3)
Auerbach and Arovas (Ref. 43)	Mean field			0.066(1)
Liang *et al.* (Ref. 30)	Variational	$-2.6752(16)$		
Tang and Hirsch (Ref. 16)	Finite cell	$-2.688(4)$	0.50(6)	
Okabe *et al.* (Refs. 24 and 25)	Monte Carlo	$-2.680(4)$		
Barnes *et al.* (Ref. 20)	Monte Carlo	$-2.676(4)$		
Gross *et al.* (Ref. 23)	Monte Carlo	$-2.6692(12)$		
Carlson (Ref. 26)	Monte Carlo	$-2.6767(4)$	0.68(2)	
Trivedi *et al.* (Ref. 27)	Monte Carlo	$-2.6768(8)$	0.62(4)	
Liang (Ref. 28)	Monte Carlo	$-2.6784(32)$	0.608(8)	
Barnes *et al.* (Ref. 29)	Monte Carlo	$-2.6769(5)$		
Present work	Series	$-2.6772(4)$	0.614(2)	0.0659(10)
	Spin-1 model			
		E_0/N	M^+	$\chi_\perp$
Lin and Emery (Ref. 44)	Finite lattice	$-2.3323(6)$	0.767(4)	
Singh (Ref. 12)	Series	$-2.327(1)$	0.81(1)	0.095(2)
Present work	Series	$-2.3279(2)$	0.8039(4)	0.093(1)

computer, however.

One might object that these conclusions rest on the assumption that the singularity exponents at $x=1$ are those predicted by spin-wave theory [i.e., powers of $(1-x^2)^{1/2}$]. Our direct numerical evidence for this assumption is not enormously strong; but once the assumption has been made, the quantitative agreement with spin-wave theory provides very strong *a posteriori* evidence that it is correct.

The overall picture that emerges from this work is the same as in previous treatments. The isotropic model at $x=1$ possesses rotational SU(2) symmetry [rather than O(3), if we are dealing with spin-$\frac{1}{2}$ representations], which is broken when $x\neq 1$ into a product of a Z(2) symmetry in the z direction times a U(1) symmetry in the x-y plane. The ground state of the isotropic model exhibits spontaneous symmetry breaking by the Goldstone mechanism, so that if the isotropic limit is approached from the Ising side ($x\rightarrow 1-$) there is long-range antiferromagnetic order in the z direction, i.e., a finite M^+ value, which vanishes discontinuously beyond $x=1$. The mass gap, on the other hand, goes to zero in the isotropic limit, corresponding to the appearance of a massless Goldstone mode. The system thus possesses an intriguing mixture of the characteristics of a first-order transition and a second-order transition. Further discussuion of these points may be found in Barnes *et al.*,[21] for example.

ACKNOWLEDGMENTS

This work forms parts of a research project supported by a grant from the Australian Research Council.

[1]T. Barnes (unpublished).
[2]P. W. Anderson, Phys. Rev. **86**, 694 (1952).
[3]R. Kubo, Phys. Rev. **87**, 568 (1952).
[4]T. Oguchi, Phys. Rev. **117**, 117 (1960).
[5]R. B. Stinchcombe, J. Phys. C **4**, L79 (1971).
[6]W. Marshall, Proc. R. Soc. London, Ser. A **232**, 48 (1955).
[7]D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).
[8]H. L. Davis, Phys. Rev. **120**, 789 (1960).
[9]M. Parrinello and T. Arai, Phys. Rev. B **10**, 265 (1974).
[10]D. Huse, Phys. Rev. B **37**, 2380 (1988).
[11]R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989).
[12]R. R. P. Singh, Phys. Rev. B **41**, 4873 (1990).
[13]R. R. P. Singh and D. A. Huse, Phys. Rev. B **40**, 7247 (1989).
[14]J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978).
[15]E. Dagotto and A. Moreo, Phys. Rev. B **38**, 5087 (1988).
[16]S. Tang and J. E. Hirsch, Phys. Rev. B **39**, 4548 (1989).
[17]T. Barnes and E. S. Swanson, Phys. Rev. B **37**, 9405 (1988).
[18]E. Manousakis and R. Salvador, Phys. Rev. Lett. **60**, 840 (1988).
[19]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).
[20]T. Barnes, D. Kotchan, and E. S. Swanson, Phys. Rev. B **39**, 4357 (1989).
[21]T. Barnes *et al.*, Phys. Rev. B **40**, 8945 (1989).
[22]M. Gross, E. Sanchez-Velasco, and E. Siggia, Phys. Rev. B **39**, 2484 (1989).
[23]M. Gross, E. Sanchez-Velasco, and E. Siggia, Phys. Rev. B **40**, 11 328 (1989).
[24]Y. Okabe and M. Kikuchi, J. Phys. Soc. Jpn. **57**, 4351 (1988).
[25]Y. Okabe and M. Kikuchi, J. Phys. (Paris) Colloq. **49**, C8-1393 (1988).

[26]J. Carlson, Phys. Rev. B **40**, 846 (1989).
[27]N. Trivedi and D. M. Ceperley, Phys. Rev. B **40**, 2737 (1989).
[28]S. Liang, Phys. Rev. B **42**, 6555 (1990).
[29]T. Barnes and M. D. Kovarik, Phys. Rev. B **42**, 6159 (1990).
[30]S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).
[31]B. G. Nickel (unpublished).
[32]L. G. Marland, J. Phys. A **14**, 2047 (1981).
[33]A. C. Irving and C. J. Hamer, Nucl. Phys. **B230**, 361 (1984).
[34]C. J. Hamer and A. C. Irving, J. Phys. A **17**, 1649 (1984).
[35]H. X. He, C. J. Hamer, and J. Oitmaa, J. Phys. A **23**, 1775 (1990).
[36]R. R. P. Singh, M. P. Gelfand, and D. A. Huse, Phys. Rev. Lett. **61**, 2484 (1988).
[37]M. P. Gelfand, R. R. P. Singh, and D. A. Huse, J. Stat. Phys. **59**, 1093 (1990).
[38]J. Holstein and N. Primakoff, Phys. Rev. **58**, 1908 (1940).
[39]Zheng Weihong, J. Oitmaa, and C. J. Hamer (unpublished).
[40]C. Domb, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (New York, Academic, 1974), Vol. 3.
[41]A. J. Guttmann, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. Lebowitz (Academic, New York, 1989), Vol. 13.
[42]M. Takahashi, Phys. Rev. B **40**, 2494 (1989).
[43]A. Auerbach and D. P. Arovas, Phys. Rev. Lett. **61**, 617 (1988).
[44]H. G. Lin and V. J. Emery, Phys. Rev. B **40**, 2730 (1989).