Series expansion for the J_1-J_2 Heisenberg antiferromagnet on a square lattice

J. Oitmaa* and Zheng Weihong†
School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
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We have developed series expansions about the Ising limit for the ground state energy, magnetization, susceptibility, and energy gap of the frustrated J_1-J_2 antiferromagnet. We find that the Néel order vanishes at $J_2/J_1 \simeq 0.4$ and collinear order sets in around $J_2/J_1 \simeq 0.6$, in broad agreement with other recent work. We also explore the nature of the phase diagram for the spin-anisotropic case. [S0163-1829(96)07730-2]

There is considerable current interest in the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet with frustrating interactions. We consider specifically the square lattice with both nearest neighbor and second neighbor antiferromagnetic interactions, often referred to as J_1-J_2 model. The Hamiltonian is

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{[ij]} \vec{S}_i \cdot \vec{S}_j . \tag{1}$$

It is known, from a variety of studies,[1] that the pure J_1 model has Néel order in the ground state, reduced by quantum fluctuations. Increasing J_2 will act to destabilitize the Néel order and at some critical value of $J_2/J_1(\equiv y)$, a phase transition to a different kind of state will occur, perhaps to a ''spin liquid.'' For large J_2/J_1, on the other hand, the system will order in the collinear phase, with alternating rows (or columns) of spins up and down, again with reduction of complete order by quantum fluctuations. As J_2/J_1 is reduced this phase will become unstable at some critical ratio.

Previous studies have given conflicting estimates of the two phase transition points. References to much of the early work are given in a recent paper by Dotsenko and Sushkov,[2] to which we refer the reader. The most detailed recent calculations are based on exact diagonalizations of a 6×6 lattice,[3–5] and suggest that the intermediate phase is stable for $0.4 < J_2/J_1 < 0.6$. The nature of this intermediate phase remains unclear, despite many suggestions and calculations.[6–9]

In this paper we use series expansion techniques to study this system, to estimate the limit of stability of the Néel and collinear phases and also to investigate the effects of spin anisotropy. For this purpose we write the Hamiltonian in the form

$$H = \sum_{\langle ij \rangle} [S_i^z S_j^z + x(S_i^x S_j^x + S_i^y S_j^y)] + y \sum_{[ij]} [S_i^z S_j^z + x(S_i^x S_j^x + S_i^y S_j^y)], \tag{2}$$

where we have chosen $J_1 = 1$. Our approach follows previous work[10–12] in expanding about the Ising limit $x = 0$, and we refer to these papers for a discussion of technical details. In the present problem there is of course a second possible expansion variable, y, and one could expand quantities of interest in two variables.[13] However we find it more convenient to choose fixed values of y and expand in powers of x only. Apart from technical advantages this means that y is included to all orders in the final results.

We first consider the Néel region (small y). Carrying out a spin rotation on sublattice B allows the Hamiltonian to be written as

$$H = H_0 + xV_1 + xV_2 , \tag{3}$$

where the unperturbed Hamiltonian is

$$H_0 = -\sum_{\langle ij \rangle} S_i^z S_j^z + y \sum_{[ij]} S_i^z S_j^z \tag{4}$$

and the two perturbing terms are

$$V_1 = \frac{1}{2} \sum_{\langle ij \rangle} (S_i^+ S_j^+ + S_i^- S_j^-), \quad V_2 = \frac{y}{2} \sum_{[ij]} (S_i^+ S_j^- + S_i^- S_j^+). \tag{5}$$

The ground state of H_0 is ferromagnetic and stable for $y < \frac{1}{2}$. We compute the ground state energy E_0, the parallel and perpendicular susceptibility, the staggered magnetization M^+, the triplet energy gap Δ_t and the singlet energy gap Δ_s in powers of x to order 10 (order 9 for $\chi_\perp$ and Δ_t, and order 8 for Δ_s). This requires consideration of 99357 distinct connected clusters of up to 10 sites for the ground state properties, and 30336 connected and disconnected clusters of up to 9 sites for the energy gap. We do not display the series here but can provide them on request.

Turning now to the collinear phase (large y), we carry out a spin rotation on every second row of spins, to transform the Hamiltonian into

$$H = H_0 + xV_1 + xV_2 + xV_3 , \tag{6}$$

where the unperturbed Hamiltonian is

$$H_0 = \sum_{\langle ij \rangle}^{(\mathrm{row})} S_i^z S_j^z - \sum_{\langle ij \rangle}^{(\mathrm{col})} S_i^z S_j^z - y \sum_{[ij]} S_i^z S_j^z \tag{7}$$

and the three perturbing terms are

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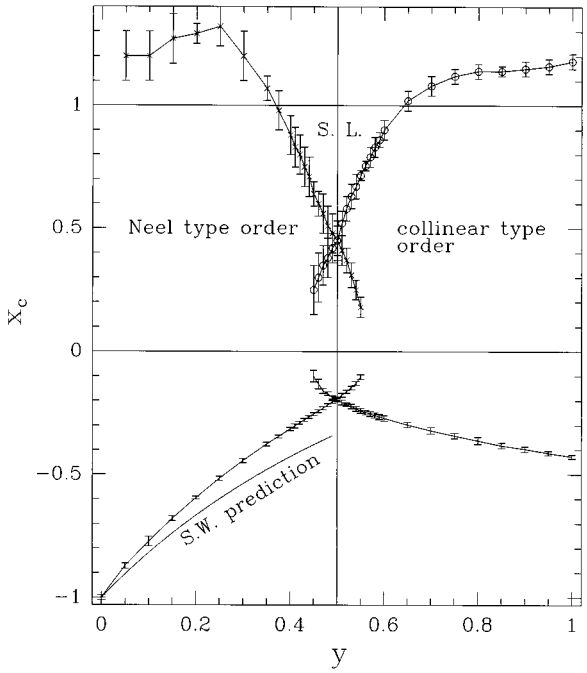

FIG. 1. Singularities obtained from analysis of the series for magnetization M^+ (for both positive and negative x_c), and the series for perpendicular and parallel susceptibilities (for negative x_c only). The prediction of x_c^- by the spin wave theory is also shown.

$$V_1=\frac{1}{2}\sum_{\langle ij\rangle}^{(\mathrm{row})}(S_i^+S_j^-+S_i^-S_j^+),$$

$$V_2=\frac{1}{2}\sum_{\langle ij\rangle}^{(\mathrm{col})}(S_i^+S_j^++S_i^-S_j^-),$$

$$V_3=\frac{y}{2}\sum_{[ij]}(S_i^+S_j^++S_i^-S_j^-). \tag{8}$$

In this case we need to distinguish between vertical and horizontal nearest neighbor bonds, and the resulting clusters have 3 bond types. We have obtained connected clusters up to 9 sites (61654 clusters) and connected and disconnected cluster up to 8 sites (18137 clusters) and have computed series for the same quantities as in the Néel phase, but to one order less).

Having obtained the series we attempt to identify critical points and to determine the nature of the phase diagram in the $(x-y)$ plane. Naive Dlog Padé analysis reveals lines of singularities, as shown in Fig. 1. These are obtained consistently for the magnetization, perpendicular and parallel susceptibilities, and the energy gap. We note, in particular, that for any y there is a singularity $x_c^-<0$ which lies closer to the origin than the positive singularity. This is reflected directly in the alternating sign of series coefficients. The singularity x_c^- appears to correspond to the leading spin-wave prediction. For the perpendicular susceptibility in the Néel region spin wave theory gives

$$\chi_\perp\sim[1-y+x(1+y)]^{-1}, \tag{9}$$

which gives $x_c^-=-(1-y)/(1+y)$. This is shown as the solid line in Fig. 1. The increasing deviation between x_c^- from the series and the spin wave result suggests that, unlike the case $y=0$, leading order spin wave theory does not give x_c exactly. To attempt a more precise analysis we have used an Euler transformation

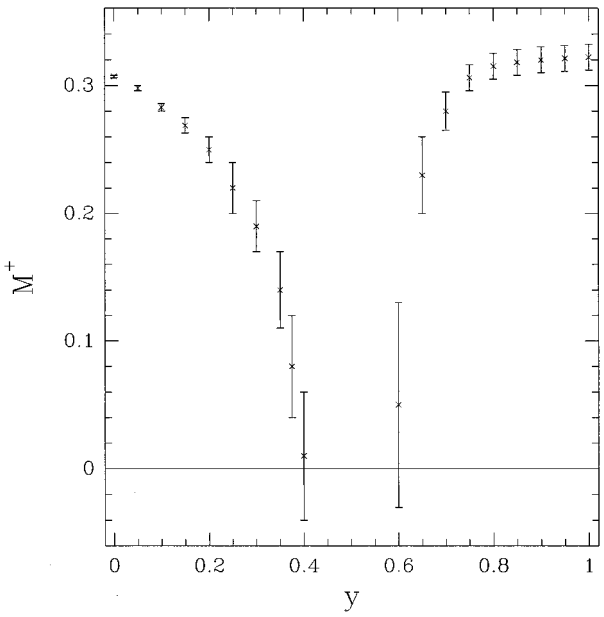

FIG. 2. The staggered/collinear magnetization M^+ at $x=1$ against y.

$$x'=(1-x_c^-)x/(x-x_c^-). \tag{10}$$

The transformed series yield more accurate estimates of the positive singularity x_c^+ and the curves shown in Fig. 1 are based on this analysis.

The singularity x_c^- can be removed and the series made much more regular by adding a extra staggered/collinear field to the Hamiltonian. In the small y region, we add the following staggered field

$$\Delta H=t(1-x)\sum_i(-1)^iS_i^z \tag{11}$$

and in large y region, we can add the following collinear field:

$$\Delta H=t(1-x)\sum_i(-1)^{i_x}S_i^z \tag{12}$$

both of which vanish at the isotropic limit $x=1$. Leading order spin wave theory has the singularity x_c^- moved to $-\infty$ with $t=4S(1+y)$.

Our first goal is to estimate the appropriate order parameter (magnetization) for the isotropic limit $x=1$ as a function of y using the above series with/without the extra field. In order to do this we follow the Euler transformation if needed by a second transformation

$$\delta=1-(1-x)^{1/2}, \tag{13}$$

to remove the singularity at $x=1$ predicted by spin wave theory. This was first proposed by Huse[14] and was also used in our earlier work on the nearest neighbor case.[12] The pre-

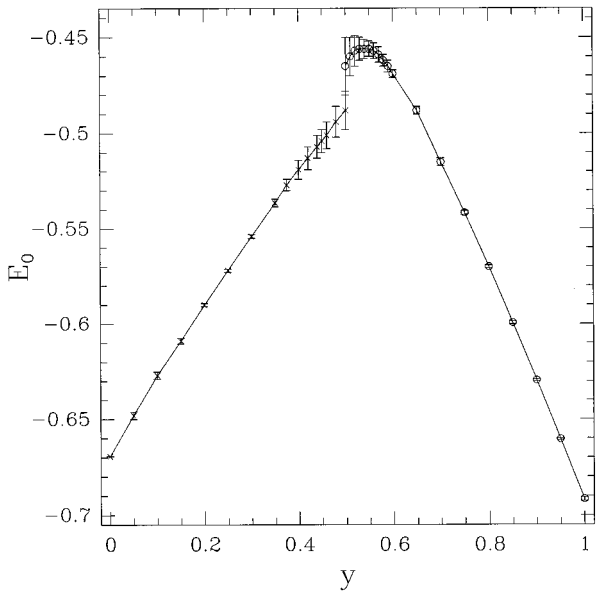

FIG. 3. The ground state energy per site at $x=1$ as a function of y.

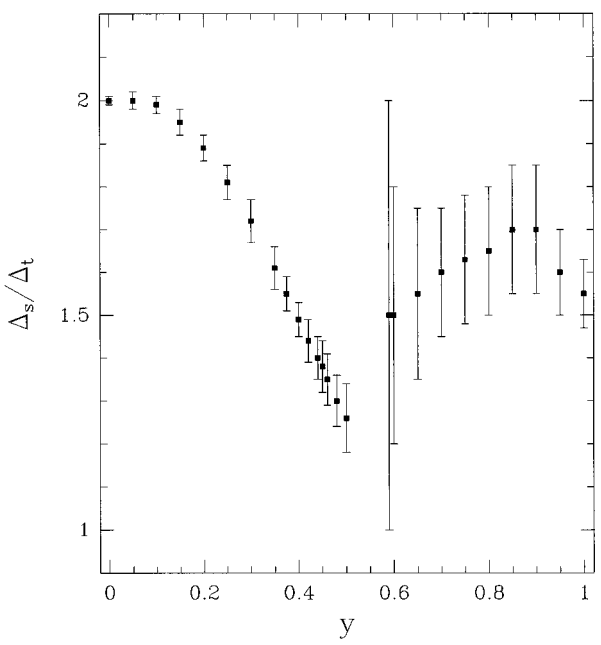

FIG. 4. The ratio of energy gap Δ_s/Δ_t at $x=1$ as a function of y.

cise form of the singularity in the case without the extra field is in fact $[1-x/(1-(1-x)y)]^{1/2}$, but this reduces to the above for $x=1$. We have then used integrated first-order inhomogeneous differential approximants[15] to extrapolate each series to the point $\delta=1$ (or $x=1$). The results for the magnetization and ground state energy are shown in Figs. 2 and 3. We note that the magnetization vanishes in the region $0.4\lesssim y\lesssim 0.6$. This indicates that the Néel phase becomes unstable at a value $y\simeq 0.4$ and the collinear phase becomes unstable at a value $y\simeq 0.6$. These critical end points are consistent with previous recent estimates[3–5] and thus provide independent confirmation of those results. The perpendicular susceptibility $\chi_\perp$ show similar behavior to the magnetization. The decrease of M^+ and $\chi_\perp$ to zero near $y\simeq 0.6$ is much more rapid than that at $y\simeq 0.4$. This is consistent with the prediction that the transition from the collinear phase is first order.[16] The parallel susceptibility appears to diverge at the isotropic limit $x=1$ for both $y\lesssim 0.4$ and $y\gtrsim 0.6$. In the intermediate region $\chi_\parallel$ appears to diverge at smaller x values, consistent with the singularity structure shown in Fig. 1.

We have also obtained series for both triplet and singlet energy gaps (Δ_t and Δ_s). In both the Néel and collinear regions the triplet energy gap appears to be finite for $x<1$ and to approach zero at the isotropic limit $x\to 1$. In the intermediate region $0.4\lesssim y\lesssim 0.6$ the extrapolation to $x=1$ is inconclusive, consistent with either a gapless state or a small gap of order 0.1. The series for the singlet gap is irregular and we have been unable to make a consistent extrapolation to $x=1$. We have estimated the ratio Δ_s/Δ_t, shown in Fig. 4. At $y=0$, we find $\Delta_s/\Delta_t=2.00(1)$, consistent with the spin wave prediction, reducing with increasing y.

The nature of the intermediate phase remains unclear and our methods, based on expansions about Ising ordered states, are unable to probe this directly. In an effort to address this question we have computed series for the second neighbor (diagonal) and third neighbor (axial) ZZ correlations. These correlations are nonzero in the spin-ordered phases and approach zero at $y\simeq 0.4$ and $y\simeq 0.6$ (Fig. 5). This is suggestive of a spin-liquid phase with only short range (nearest neighbor) correlations for $0.4\lesssim y\lesssim 0.6$.

Finally we have investigated the region $x\ll 1$. In the Ising limit there exists a multiphase point at $y=1/2$, separating the Néel and collinear phases. An infinite number of ground

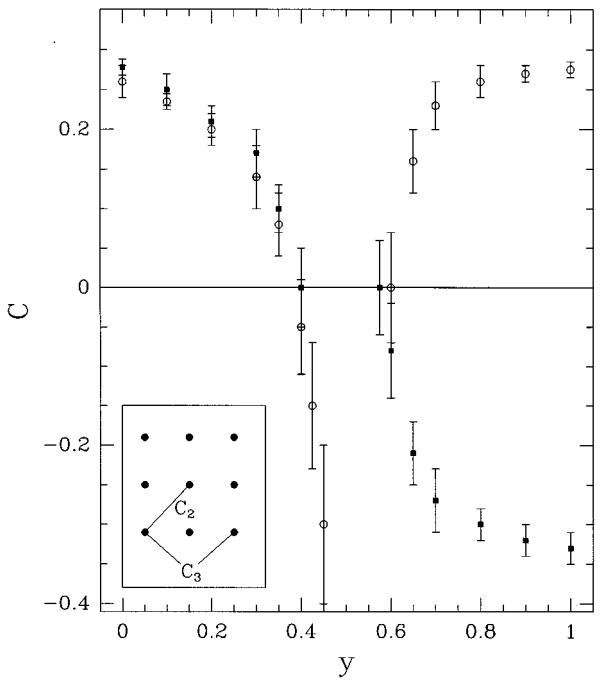

FIG. 5. The second neighbor correlation C_2 (filled symbols) and the third neighbor correlation C_3 (open symbols) at $x=1$ as a function of y.

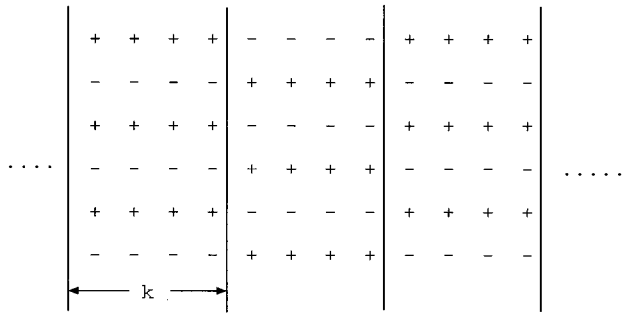

FIG. 6. Band state $\langle k \rangle$ in the Ising limit $x=0$.

states are degenerate at this point. We consider the band states, denoted by $\langle k \rangle$ and shown in Fig. 6. Note that $k=1,\infty$ correspond to the Néel and collinear states, respectively. A simple calculation shows that the ground state energy is

$$E_k(x=0)=[-1+(2-k)y]/(2k) \tag{14}$$

which for $y=\frac{1}{2}$ is independent of k. This does not exhaust the possible degenerate states. We have used perturbation theory through third order to compute the energies of states with $k=1,2,3,4,\infty$. We find that along the line

$$x=\sqrt{6\eta}+3\eta+O(\eta^{3/2}) \tag{15}$$

with $\eta \equiv y-1/2$, all states remain degenerate with

$$E=-1/4-5\eta/2+O(\eta^2). \tag{16}$$

This suggests that the Néel and collinear phases do not separate until some finite x.

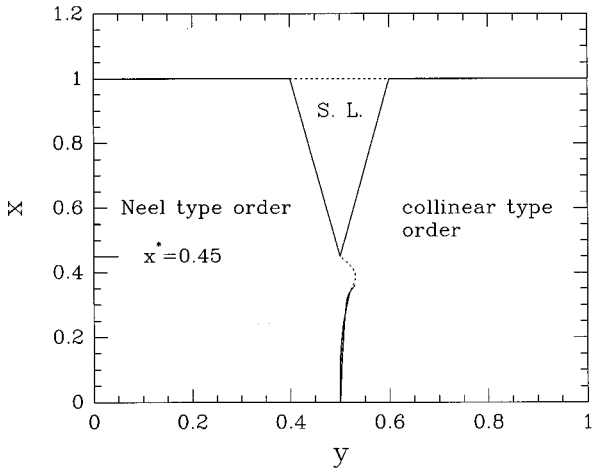

FIG. 7. Schematic phase diagram obtained from series and perturbation theory.

In Fig. 7 we show a schematic phase diagram for this system, based on our results and conjectures. For $x=1$ there is an intermediate phase with short range correlations between Néel and collinear phases, for $0.4 \lesssim y \lesssim 0.6$. The nature of this phase remains uncertain. For decreasing x the width of intermediate phase also decreases until it terminates at an estimated $x^* \simeq 0.45$. This point appears to occur at or close to $y=\frac{1}{2}$. For $x<x^*$ there is no intermediate phase separating Néel and collinear phases.

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*Electronic address: otja@newt.phys.unsw.edu.au
†Electronic address: w.zheng@unsw.edu.au

[1] E. Manousakis, Rev. Mod. Phys. **63**, 1(1991).
[2] A.V. Dotsenko and O.P. Sushkov, Phys. Rev. B **50**, 13 821 (1994).
[3] H.J. Schulz and T.A.L. Ziman, Europhys. Lett. **18**, 355 (1992).
[4] H.J. Schulz, T.A.L. Ziman, and D. Poiblanc (unpublished).
[5] T. Einarsson and H.J. Schulz, Phys. Rev. B **51**, 6151 (1995).
[6] E. Dagotto and A. Moreo, Phys. Rev. Lett. **63**, 2148 (1989).
[7] R.R.P. Singh and R. Narayanan, Phys. Rev. Lett. **65**, 1072 (1990).
[8] H.A. Ceccatto, C.J. Gazza, and A.E. Trumper, Phys. Rev. B **45**, 7832 (1992).
[9] J. Richter, Phys. Rev. B **47**, 5794 (1993).
[10] M.P. Gelfand, R.R.P. Singh, and P.A. Huse, J. Stat. Phys. **59**, 1093 (1990).
[11] H.X. He, C.J. Hamer, and J. Oitmaa, J. Phys. A **23**, 1775 (1990).
[12] W.H. Zheng, J. Oitmaa, and C.J. Hamer, Phys. Rev. B **43**, 8321 (1991).
[13] J. Oitmaa and W.H. Zheng, J. Phys. A **25**, 5849 (1992).
[14] D.A. Huse, Phys. Rev. B **37**, 2380 (1988).
[15] A.J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic, New York, 1974), Vol. 13.
[16] M.J de Oliveira, Phys. Rev. B **43**, 6181 (1991).