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
(Received 3 May 1996)

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 $J_2/J_1=0.4$ and collinear order sets in around $J_2/J_1=0.6$, 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

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\{ ij \}} \vec{S}_i \cdot \vec{S}_j.$$  \hspace{1cm} (1)

It is known, from a variety of studies,\textsuperscript{1} that the pure $J_1$ model has Néel order in the ground state, reduced by quantum fluctuations. Increasing $J_2$ will act to destabilize the Néel order and at some critical value of $J_2/J_1 (= y)$, 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\textsuperscript{2} to which we refer the reader. The most detailed recent calculations are based on exact diagonalizations of a $6 \times 6$ lattice \textsuperscript{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.\textsuperscript{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

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

$$+ y \sum_{\{ ij \}} \left[ S_i^z S_j^z + y (S_i^x S_j^x + S_i^y S_j^y) \right],$$  \hspace{1cm} (2)

where we have chosen $J_1 = 1$. Our approach follows previous work\textsuperscript{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.\textsuperscript{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

$$H = H_0 + x V_1 + x V_2,$$  \hspace{1cm} (3)

where the unperturbed Hamiltonian is

$$H_0 = - \sum_{\langle ij \rangle} S_i^z S_j^z + y \sum_{\{ ij \}} S_i^z S_j^z,$$  \hspace{1cm} (4)

and the two perturbing terms are

$$V_1 = \frac{1}{2} \sum_{\langle ij \rangle} (S_i^+ S_j^+ + S_i^- S_j^-), \hspace{1cm} V_2 = \frac{y}{2} \sum_{\{ ij \}} (S_i^+ S_j^+ + S_i^- S_j^-).$$  \hspace{1cm} (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 $M^\parallel$, the triplet energy gap $\Delta_t$, and the singlet energy gap $\Delta_s$ in powers of $x$ to order 10 (order 9 for $\chi_{\perp}$ and $\Delta_t$, and order 8 for $\Delta_s$). 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

$$H = H_0 + x V_1 + x V_2 + x V_3,$$  \hspace{1cm} (6)

where the unperturbed Hamiltonian is

$$H_0 = \sum_{\langle ij \rangle} S_i^z S_j^z - \sum_{\langle ij \rangle} S_i^z S_j^z - y \sum_{\{ ij \}} S_i^z S_j^z,$$  \hspace{1cm} (7)

and the three perturbing terms are
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 and connected and disconnected cluster up to 8 sites and have computed series for the same quantities as in the Neél 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. Naïve Dlog Pade 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 $x^-_c$ 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 Neél region spin wave theory gives

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

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

$$x' = (1-x^-_c) x/(x-x^-_c).$$

(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 an extra staggered/collinear field to the Hamiltonian. In the small $y$ region, we add the following staggered field

$$\Delta H = t \sum_i (-1)^i S_i^z$$

(11)

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

$$\Delta H = t (1-x) \sum_i (-1)^i S_i^z$$

(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

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

(13)

to remove the singularity at $x=1$ predicted by spin wave theory. This was first proposed by Huse and was also used in our earlier work on the nearest neighbor case. The pre-
cise form of the singularity in the case without the extra field is in fact \([1 - y/(1 - (1 - x)y)]^{1/2}\), 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 \(0.4 \leq y \leq 0.6\). This indicates that the Néel phase becomes unstable at a value \(y \approx 0.4\) and the collinear phase becomes unstable at a value \(y \approx 0.6\). These critical end points are consistent with previous recent estimates\(^{3–5}\) and thus provide independent confirmation of those results. The perpendicular susceptibility \(\chi_L\) show similar behavior to the magnetization.

The decrease of \(M^+\) and \(\chi_L\) to zero near \(y \approx 0.6\) is much more rapid than that at \(y \approx 0.4\). 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 \(y \leq 0.4\) and \(y \geq 0.6\). In the intermediate region \(\chi_1\) 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 (\(\Delta_t\) and \(\Delta_s\)). 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 \(x = 1\). In the intermediate region \(0.4 \leq y \leq 0.6\) 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 \(\Delta_s/\Delta_t\), 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 \(y \approx 0.4\) and \(y \approx 0.6\) (Fig. 5). This is suggestive of a spin-liquid phase with only short range (nearest neighbor) correlations for \(0.4 \leq y \leq 0.6\).

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. 3.** The ground state energy per site at \(x = 1\) as a function of \(y\).

**FIG. 4.** The ratio of energy gap \(\Delta_s/\Delta_t\) at \(x = 1\) as a function of \(y\).

**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 \(y\).
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

\[
E_k(x=0) = \left[-1 + (2-k)y\right]/(2k)
\]

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

\[
x = \sqrt{6} \eta + 3 \eta + O(\eta^{3/2})
\]

with \( \eta = y - 1/2 \), all states remain degenerate with

\[
E = -1/4 - 5 \eta/2 + O(\eta^2).
\]

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

This work forms part of a research project supported by a grant from the Australian Research Council. We thank Dr. R.R.P. Singh for a number of valuable discussions and suggestions.

---

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

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