The ground state of two quantum models of magnetism

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The ground state energy and pair correlations have been computed exactly for the spin $\frac{1}{2}$ XY magnet and isotropic Heisenberg antiferromagnet, for a sequence of finite cells on the square and honeycomb lattices. Precise estimates of the ground state energy of the infinite lattices are obtained by extrapolation. It is predicted that the XY magnet has a non-zero transverse magnetization and the Heisenberg antiferromagnet has a non-zero staggered magnetization in the ground state.

L'énergie de l'état fondamental et les corrélations de paires ont été calculées exactement pour le système magnétique XY à spin $\frac{1}{2}$ et le système antiferromagnétique isotrope de Heisenberg, pour une série de mailles finies sur les réseaux carré et en nid d'abeilles. Des estimations précises de l'énergie de l'état fondamental des réseaux infinis sont obtenues par extrapolation. On prédit une aimantation transversale non nulle pour l'état fondamental du système XY et une aimantation non nulle en zigzag pour l'état fondamental de l'antiferromagnétique de Heisenberg.

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Introduction

One of the simplest quantum many-body systems is the spin $\frac{1}{2}$ anisotropic Heisenberg model, characterized by the Hamiltonian

$$[1] \quad \mathscr{H} = 2\sum_{\langle ij\rangle}\{J_{\|}S_i^zS_j^z + J_{\perp}(S_i^xS_j^x + S_i^yS_j^y)\}$$

where the S_i are quantum mechanical spin operators and the sum is over nearest neighbour pairs of sites on a regular lattice. In this paper we consider two special cases of [1], namely the isotropic Heisenberg antiferromagnet

$$[2] \quad \mathscr{H}_{\mathrm{HA}} = 2J\sum_{\langle ij\rangle}\{S_i^zS_j^z + S_i^xS_j^x + S_i^yS_j^y\}$$

and the XY model

$$[3] \quad \mathscr{H}_{\mathrm{XY}} = 2J\sum_{\langle ij\rangle}\{S_i^xS_j^x + S_i^yS_j^y\}$$

(we take $J > 0$ throughout). At finite ($T \sim T_c$ and above) temperatures these models are applicable to a variety of magnetic insulators (1–3) and also as models for a quantum fluid (4, 5). Unfortunately experimental systems which remain well described by the XY or the isotropic Heisenberg model at very low temperature ($T \ll T_c$) have not yet been discovered although a vigorous search is underway.[1,2] The tendency is for small anisotropies in the Hamiltonian of the experimental system to make it behave like an Ising model at very low temperatures. Thus it is not yet possible to compare our calculated ground state energies with experiment.

Despite the apparent simplicity of the Hamiltonians [2] and [3], exact results are scarce. The ground state energy and eigenvector are known exactly for the linear chain for both $\mathscr{H}_{\mathrm{HA}}$ (6, 7) and for $\mathscr{H}_{\mathrm{XY}}$ (8, 9). For two and three dimensional lattices the exact nature of the ground state remains unknown. For the antiferromagnet a number of approximate calculations have been made, using spin wave theory (10, 11), variational methods (12–14), and perturbation theory (15, 16). Partly on the basis of these studies it has been believed that the ground state for loose packed lattices is not too different from the Néel state, in which spins on alternate sublattices point up and down, respectively. Recently Pearson (17) has estimated the ground state energy of the XY model on the square lattice by a perturbational approach in which the ground state of the Ising model is taken as the unperturbed state. Rigorous upper and lower bounds for the ground state energy are also available (10).[3]

The aim of our work is to investigate the nature of the ground state for the models HA and XY by carrying out exact numerical calculations for a sequence of small finite lattices of N spins and then extrapolating to the infinite lattice case. A number of calculations of this type have been reported in the literature. Bonner and Fisher (18) have carried out calculations for linear chains with $N \leq 11$ for the general anisotropic Hamiltonian [1]. They were able to ex-

[1] L. J. de Jongh. Private communication, 1977.
[2] R. L. Carlin. Private communication, 1977.
[3] D. J. Austen. Private communication, 1975.

trapolate successfully from their finite lattice results for the ground state energy to the known result for the infinite chain. Some calculations for 3×3 and 3×4 nets have been carried out by Mubayi *et al.* (19) and by Jain *et al.* (20). However, because for their clusters the number of spins in at least one direction is odd the Néel state will not 'fit' and so they were unable to obtain sensible approximations to the ground state wave function. Accordingly they concentrated their attention on thermodynamic properties of the anisotropic Heisenberg model for a range of temperatures of the order of J/k_B.

In principle it is straightforward to compute the energy eigenvalues for a finite spin system, the problem reducing to that of diagonalizing a 2^N dimensional matrix. This becomes intractable at about $N = 8$ unless symmetry considerations can be used to block diagonalize the matrix. Fortunately this is possible. For both models the longitudinal magnetization operator

$$[4] \qquad M_z = \sum_i S_i^z$$

commutes with the Hamiltonian and thus provides a good quantum number for labelling the eigenstates of $\mathscr{H}$. The Hamiltonian thus decomposes into blocks, each block corresponding to an eigenvalue of M_z. For the isotropic Heisenberg antiferromagnet the total magnetization $\boldsymbol{M}$ commutes with $\mathscr{H}$ and it can be shown that the ground state is a singlet, $\boldsymbol{M} = 0$ (12, 8), and thus has $M_z = 0$. For the XY model we also have strong evidence that the ground state has $M_z = 0$, although a rigorous proof has so far eluded us. This conjecture is certainly valid in one dimension and has been confirmed by numerical calculations on clusters of up to 8 spins. Thus we need to consider not the full set of 2^N states but rather the set of $N!/[(\frac{1}{2}N)!]^2$ states with $M_z = 0$. A further important simplification arises through the space group symmetry of the particular cell, since the ground state eigenvector must transform according to one of the irreducible representations of the space group. For the XY model the matrix elements of $\mathscr{H}_{XY}$ are all non-negative and thus by the Frobenius theorem the ground state eigenvector has all coefficients positive and transforms according to the identity representation A_1. For the Heisenberg antiferromagnet it can be shown (12) that for cells of $N = 4n$ spins (n integral) the ground state eigenvector transforms according to A_1, whereas for $N = 4n + 2$ the eigenvector transforms according to the alternating representation A_2, i.e., it changes sign under symmetry operations which interchange the two sublattices. It is the space group symmetry that really leads to a significant reduction in the size of the matrices. To obtain the maximum possible spatial symmetry we use periodic boundary conditions for our cells. Details of the calculations are presented in the following section.

Calculation and Results

As indicated in the Introduction we wish to compute the ground state properties of the Hamiltonians $\mathscr{H}_{HA}$ and $\mathscr{H}_{XY}$ for a number of finite cells on the square and honeycomb lattices. The choice of cells is dictated by the requirement that they contain an even number of spins, so that antiferromagnetic ordering is possible and that they can be repeated periodically to fill the entire lattice. For the square lattice we choose cells of 4, 8, 10, 16, 18 spins and for the hexagonal lattice cells of 6, 8, 14, 18 spins. These are shown in Figs. 1 and 2. The computations become too lengthy for $N > 18$.

The next step is to generate, for each cell, a complete set of basis states which transform according to the irreducible representations A_1 or A_2 of the symmetry group. We start from the Néel state, $\psi_0 = \alpha\beta\alpha\beta\ldots$, with all spins 'up' on one sublattice and 'down' on the other. By overturning a pair of nearest neighbour spins from the Néel state, in all possible ways, we generate a number of states which are all related by symmetry. We choose any one of these and label it ψ_1, a state of 'first order'. By overturning a pair of spins in ψ_1, in all possible ways, and discarding states which are related by symmetry, we generate a number of states of second order, $\psi_{2\nu}$, where the index ν distinguishes between inequivalent states of the same order. An example for the $N = 16$ cell on the square lattice is shown in Fig. 3. This procedure of overturning a pair of spins is continued until no new states are produced and yields a set of states $\{\psi_{\mu\nu}\}$ where μ is the order, and ranges from

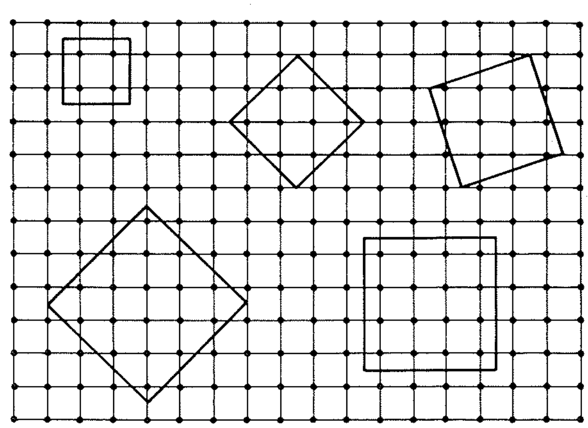

FIG. 1. Finite cells of 4, 8, 10, 16, 18 spins on the square lattice. In each case the infinite lattice is filled by periodic repetition of the cells.

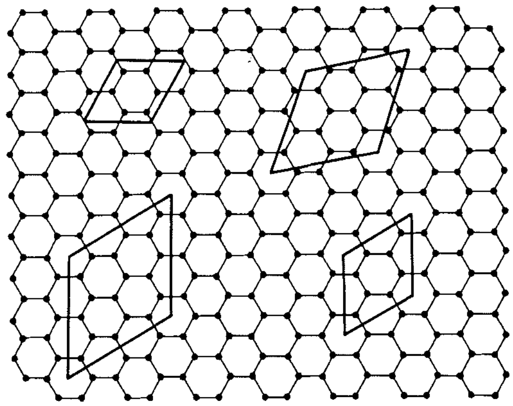

FIG. 2. Finite cells of 6, 8, 14, 18 spins on the honeycomb lattice.

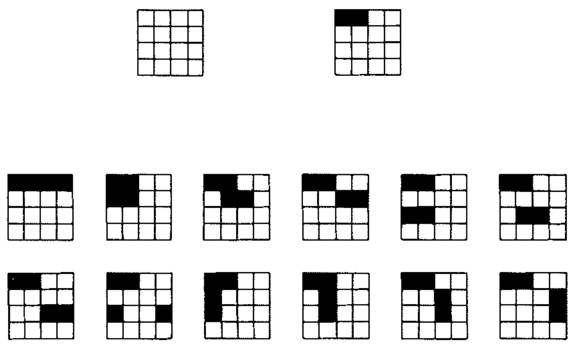

FIG. 3. Generation of basis states. Illustrated are the zeroth order (Néel) state, the singlet first order state, and the twelve second order states for the 16 spin cell on the square lattice. A black square represents a spin which has been overturned from the Néel state.

0 to some value μ_{max}. For example for the $N = 16$ cell on the square lattice we find $\mu_{max} = 6$, and the number of states of each order from 0 to 6, respectively, is 1, 1, 12, 36, 73, 23, and 7, giving a total of 153 states. The normalized symmetric and antisymmetric basis states can be written formally as

$$[5a] \qquad \Psi_{\mu\nu}^{(S)} = \frac{1}{\sqrt{n_{\mu\nu}h}} \sum_{R=1}^{h} P_R \psi_{\mu\nu}$$

and

$$[5b] \qquad \Psi_{\mu\nu}^{(A)} = \frac{1}{\sqrt{n_{\mu\nu}h}} \sum_{R=1}^{h} (-1)^{\varepsilon_R} P_R \psi_{\mu\nu}$$

where P_R is one of the operations of the symmetry group of the cell, the sum is over all h elements of the group, $\varepsilon_R = \pm 1$ depending on whether or not the operation P_R interchanges sublattices, and $n_{\mu\nu}$ is the 'symmetry number' of the state $\psi_{\mu\nu}$, namely the number of operations P_R which leave the state $\psi_{\mu\nu}$ invariant (for example for the Néel state ψ_0 the symmetry number is $\frac{1}{2}h$). For the square lattice the number of basis states for cells with $N = 4$, 8, 10, 16, 18 is, respectively, 2, 6, 9, 153, 398. For the honeycomb lattice the number of basis states for cells with $N =$ 6, 8, 16, 18 is, respectively, 2, 6, 86, 504. These are then the dimensions of the matrices of which the largest eigenvalue and corresponding eigenvector must be determined.

Using the complete set of basis states for each cell we have generated the Hamiltonian matrices for the antiferromagnet and for the XY model. For $N \leq 16$ all the eigenvalues were obtained using standard diagonalization routines. For the $N = 18$ matrices we used the iterative power method (21) to find only the largest eigenvalue and corresponding eigenvector. In Fig. 4 we plot the ground state energy per spin $-E_0/NJ$ vs. $1/N$ for the square and hexagonal lattices. The plots are strikingly linear with a very slight oscillation and extrapolation to the infinite lattice case can be made with some degree of confidence. It is interesting that Suzuki and Miyashita (22) using their variational approach predict just such a linear $1/N$ dependence of the ground state energy we find empirically. Our estimates are shown in Table 1.

Examination of the coefficients of the symmetrized basis vectors in the ground state eigenvector shows clearly that the true ground state is extremely complicated. For the XY magnet the probability of the Néel state is less than the average probability (e.g. $< 1/153$ for the 16 spin cell on the square lattice). No symmetrized basis state is dominant in the ground state in either model.

From the ground state eigenvector we have computed for each cell all of the pair correlations $\langle S_0^z S_r^z \rangle$ and $\langle S_0^x S_r^x \rangle$. The results shown in Table 2 for the 16 spin cell on the square lattice are

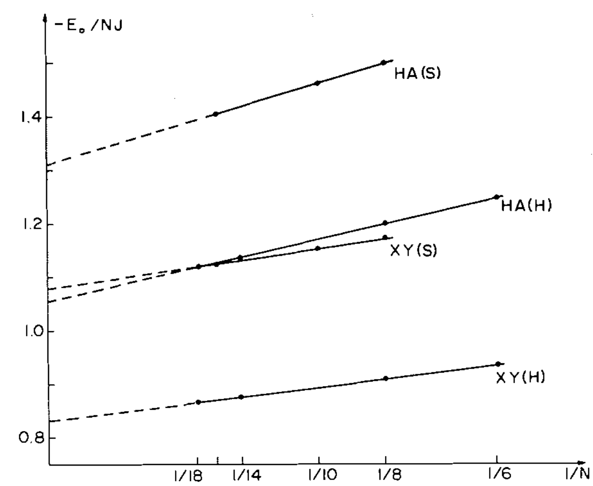

FIG. 4. Ground state energy per spin $(-E_0/NJ)$ for the XY magnet (XY) and the Heisenberg antiferromagnet (HA) for finite cells on the square (S) and honeycomb (H) lattices.

TABLE 1. Estimates of the ground state energy per spin $(-E_0/NJ)$ for the XY magnet and Heisenberg antiferromagnet on the infinite square and honeycomb lattices, obtained by extrapolation from the finite cell data shown in Fig. 4

Model	Square lattice	Honeycomb lattice
XY magnet	1.08 ± 0.01	0.83 ± 0.01
Antiferromagnet	1.31 ± 0.01	1.055 ± 0.01

TABLE 2. Ground state pair correlations for the 16 spin cell on the square lattice

	XY magnet		Heisenberg antiferromagnet
r/δ	$4\langle S_0{}^z S_r{}^z\rangle$	$4\langle S_0{}^x S_r{}^x\rangle$	$4\langle S_0{}^\alpha S_r{}^\alpha\rangle$
1	−0.182	0.562	−0.468
$\sqrt{2}$	−0.027	0.487	0.285
2	−0.027	0.487	0.285
$\sqrt{5}$	−0.023	0.468	−0.270
$2\sqrt{2}$	−0.018	0.458	0.240

typical of the trend seen in all cells. From the pair correlations we have computed the ground state expectation values of the squares of the magnetization M_α and staggered magnetization N_α

[6] $$M_\alpha = \sum_i S_i{}^\alpha; \quad N_\alpha = \sum_i \varepsilon_i S_i{}^\alpha$$

where $\varepsilon_i = \pm 1$, depending on whether i is on the A or B sublattice. The expectation values are given by

[7] $$\langle M_\alpha{}^2\rangle = N \sum_r \langle S_0{}^\alpha S_r{}^\alpha\rangle$$
$$\langle N_\alpha{}^2\rangle = N \sum_r \varepsilon_r \langle S_0{}^\alpha S_r{}^\alpha\rangle$$

In Figs. 5 and 6 we plot these quantities vs. $1/N$ for the square and hexagonal lattices, respectively. For the XY model the result $\langle M_z{}^2\rangle = 0$ and for the antiferromagnet the result $\langle M_z{}^2\rangle = \langle M_x{}^2\rangle = 0$ are of course identically satisfied. We predict that for the XY model on the infinite lattice $\langle N_x{}^2\rangle = \langle N_z{}^2\rangle = 0$ whereas $\langle M_x{}^2\rangle \neq 0$. In particular we estimate

$$\langle M_x{}^2\rangle/N^2 = 0.116 \pm 0.002 \text{ (square)}$$
$$\langle M_x{}^2\rangle/N^2 = 0.104 \pm 0.002 \text{ (honeycomb)}$$

In other words there is partial long range order in the xy plane. For the antiferromagnet we find that $\langle N_x{}^2\rangle = \langle N_z{}^2\rangle \neq 0$ and our estimates are

$$\langle N_\alpha{}^2\rangle/N^2 = 0.059 \pm 0.003 \text{ (square)}$$
$$\langle N_\alpha{}^2\rangle/N^2 = 0.054 \pm 0.003 \text{ (honeycomb)}$$

For the XY model there are two independent nearest neighbour correlations, $\langle S_0{}^x S_\delta{}^x\rangle \propto E_0$ and $\langle S_0{}^z S_\delta{}^z\rangle$. The finite lattice values for the latter correlation in the ground state are as linear on a $1/N$ plot as the

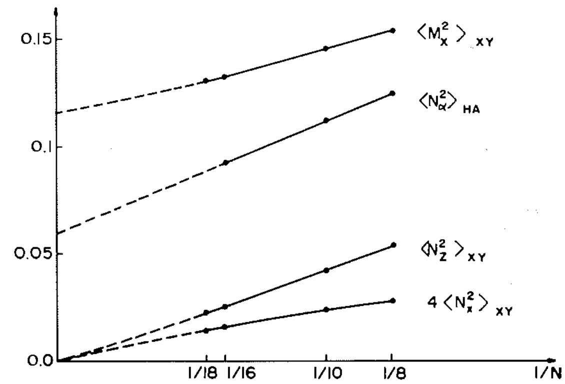

FIG. 5. Plot of ground state magnetizations vs. $1/N$ for finite cells on the square lattice.

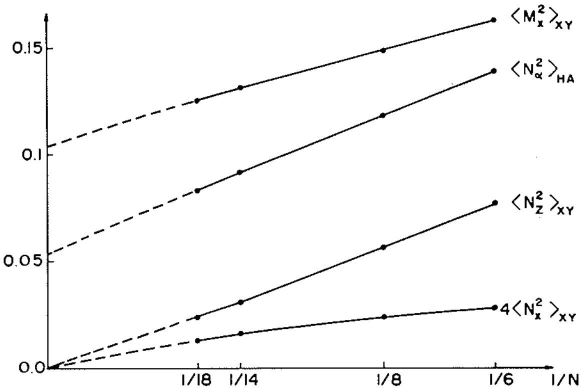

FIG. 6. Plot of ground state magnetizations vs. $1/N$ for finite cells on the honeycomb lattice.

energies, hence we obtain the infinite lattice estimates

$$\langle S_0{}^z S_\delta{}^z\rangle = -0.052 \pm 0.002 \text{ (honeycomb)}$$
$$\langle S_0{}^z S_0{}^\delta\rangle = -0.038 \pm 0.001 \text{ (square)}$$

Of the four cases which we have considered only the case of the Heisenberg antiferromagnet on the square lattice has received much previous attention. Previous authors have calculated the ground state energy and also in some cases the ground state spin deviation from the Néel state, usually denoted ΔS_z, where

[8] $$\Delta S_z = \tfrac{1}{2} - \sqrt{\langle N_\alpha{}^2\rangle}/N$$

Table 3 gives a comparison of previous estimates of E_0 and ΔS_z with the present estimates. Our result for the ground state energy is close to the mean of other estimates. Excluding Boon's result (16) all energy estimates are 1% to 4% below the mean field value. The variation among the estimates of ΔS_z is much greater.

For the XY model on the square lattice Pearson (17) quotes $E_0/NJ = -1.098 \pm 0.004$. We feel that his confidence limits are somewhat too optimistic.

TABLE 3. Comparison with previous results for the Heisenberg antiferromagnet on the square lattice

Method	Reference	$-E_0/NJ$	ΔS_z
Mean field		1.333	0
Spin wave	Anderson (10)	1.32	0.20
Spin wave	Kubo (11)	1.29	—
Variational	Marshall (12)	1.31	—
Perturbational	Davis (15)	1.33	0.12
Perturbational	Boon (16)	1.43	—
Variational	Oguchi (13)	1.29	0.07
Variational	Bartkowski (14)	1.32	0.10
Finite lattice	Oitmaa and Betts (24)	1.30	0.25

Pearson has not calculated the ground state magnetization.

Conclusions

We have introduced a method for estimating the ground state properties of quantum mechanical spin models for infinite plane lattices by extrapolation from exact numerical calculations on finite cells. Rather precise estimates of the ground state energy per spin have been obtained for the XY model and the isotropic Heisenberg antiferromagnet on the two dimensional square and honeycomb lattices.

The ground state expectation values of the squares of the magnetizations $\langle M_\alpha{}^2\rangle$, and of the staggered magnetizations $\langle N_\alpha{}^2\rangle$, have also been computed. For the infinite lattice XY magnet we predict that the staggered magnetizations are zero, while there is partial ordering in the xy plane (68% for the square lattice, 64% for the honeycomb lattice). For the infinite isotropic antiferromagnet we predict that the ground state has non-zero staggered magnetization. The staggered ordering is 49% complete for the square lattice and 46% complete for the honeycomb lattice whereas for the Néel state the staggered ordering would be 100%. Thus we postulate a state of finite long range order for both models at $T = 0$. For the XY model this is a new prediction but for the Heisenberg antiferromagnet ground state long range order was first predicted by Anderson (10). When expressed in terms of spin deviation Table 3 shows that our prediction for the degree of order in the ground state of the Heisenberg antiferromagnet is considerably less than that of most earlier calculations.

Mermin and Wagner (23) have proved that two dimensional quantum spin models have zero long range order for all $T > 0$. Our results are not in conflict with this theorem but indicate that both models undergo a phase transition of first order at $T = 0$.

Partially motivated by our work, Suzuki and Miyashita (22) have very recently carried out a study of the ground state of the spin $\frac{1}{2}$ XY model. Using a variational wave function which is a linear combination of all states with $M_z = 0$ they obtain results for the ground state energy and long range order which are in excellent agreement with our results.

There are a number of ways in which the present work can be extended. The ground state properties of the anisotropic Hamiltonian [1] could be estimated by the same method, assuming that the ground state has $M_z = 0$. The same techniques can also be applied to three dimensional lattices, and work along these lines is in progress. For the antiferromagnet it would be possible in principle to reduce the number of basis states by including only singlet states. This may make numerical calculations for larger cells practicable. Finally a rigorous proof that the ground state of the infinite XY model has $M_z = 0$ remains an unsolved problem.

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