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Heisenberg Antiferromagnet on a Triangular Lattice*

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ABSTRACT

We study two variants of block-spin calculations of the Heisenberg antiferromagnet on a triangular lattice, using a unit block which is a hexagon containing seven spins. The first method allows mixing between the two lowest doublets on each block and leads to vanishing order on the infinite lattice. It gives a strict upper-bound on the energy density of -0.9518. A second analysis, based on a shadow-Hamiltonian approach, gives a slightly higher energy estimate and leads to finite canted magnetization. Comparison with analogous calculations on one and two-dimensional rectangular lattices leads us to prefer the first solution.

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1. Introduction

The Heisenberg Antiferromagnet (HAF) on a triangular lattice is a highly frustrated system. Renewed interest in this model has come from the belief that understanding of the physics of frustrated systems will be important to the study of the new high temperature superconductors. In this paper we discuss several ways of calculating the ground-state of the HAF and compare our results to other approximate methods for treating the same model. Our study is aimed at a comparison of variational treatments and the conclusions that can be drawn from them. In particular we are interested in the question of long range order, and the question of whether or not this theory has a mass gap. The Heisenberg model is defined by the Hamiltonian

$$H = \frac{1}{4} \sum_{\langle ij \rangle} \vec{\sigma}(i) \cdot \vec{\sigma}(j) \tag{1.1}$$

where the sum covers all nearest-neighbor pairs on the triangular lattice (twice). As shown in Fig. 1, a triangular lattice can be divided into three mutually interlaced sub-lattices, which we call the blue (B), green (G), and red (R) sub-lattices. On a triangular lattice each site has six nearest neighbors. Any triangle of the original lattice contains one site from each colored sub-lattice; thus, if we look at a red site, its nearest neighbors are alternating blue and green sites. Just as a staggered mean field state is defined for an anti-ferromagnet on a rectangular lattice, we can similarly define a *canted-mean-field state* in which the spins on each sublattice are all oriented the same way but with a 120° rotation between spins on the different sublattices. For example, choose the red spins to be oriented along the z axis and the blue and green spins to be rotated plus and minus 120° respectively in the x-z plane. This ordered state has an energy per site of -.75. The presence or

absence of *canted magnetization* is then addressed by defining an operator which has an expectation value of unity in the canted mean-field state. Long range antiferromagnetic order is indicated by a non zero value for this canted magnetization operater. The question of whether or not the ground state of the HAF exhibits such order is one of the crucial problems which confronts anyone studying the model.

There is already a considerable literature on this model. Anderson[1] suggested a resonating-valence bond (RVB) ansatz, which predicts the existence of a mass gap and no long range order. He estimated the ground state energy density per site to be $\mathcal{E} = -.98$ but Oguchi et al[2] obtain for this ansatz an estimate of $-.95 \pm .02$. Similar RVB states have recently been used as a basis for models of superconductivity[3] . A trial state suggested by Kalmeyer and Laughlin, based on fractional quantum Hall states,[4] leads to $\mathcal{E} = -.94 \pm .02$.

Huse and Else[5] have recently obtained an energy estimate of -1.0789 by using parametrized variations of the *canted mean-field* wave function to estimate the ground-state energy of systems with finite volume and extrapolated to the infinite volume limit. They concluded that there exists a remnant canted magnetization of 0.68. Other calculations which produce even lower estimates of the energy density contradict this conclusion. Among these are the results of Oguchi,Nishimori and Taguchi[2], who find $\mathcal{E} = -1.098 \pm .018$. They exactly diagonalize the Hamiltonian for small parallelogram (or railroad trestle) lattices and extrapolate in both length and width to obtain an estimate of the infinite volume answer. These authors conclude that the ground state on the infinite lattice has no order.

The methods we describe in this paper are variants of the the Hamiltonian block-spin or real-space renormalization group technique .[6] The virtue of this method is that it allows one to explicitly construct infinite-volume trial wave-

functions specifically tailored to the problem at hand. Furthermore, it allows one to explore the space of non-trivial symmetry-breaking trial states as well as those constructed to preserve the symmetries of the problem. In what follows our fundamental blocking unit is chosen to be the seven-site hexagons shown in Fig. 1. This is a particularly suitable tiling for a triangular lattice . At each stage this blocking reproduces the triangular lattice with no loss of symmetry. In addition, the pattern of three interlaced sub-lattices is also preserved if one identifies the block color as the color of the central site. Such a seven-site, two state block-spin calculation was performed by van de Braak, Caspers and Willemse [7]. Truncating the Hilbert space of every block onto the lowest doublet they obtained the result $\mathcal{E} = -0.91012$ for the average energy per site of the triangular lattice.

We will present two different generalizations of this approach. Each of these calculations introduces some admixture of other states within the Hilbert-space of each block. The calculation explained in section 2 uses an admixture between the lowest lying doublet and the first excited doublet within each block. This leads to $\mathcal{E} = -0.9518$, and implies a vanishing mass-gap. The second method, explained in section 3, selects the states to retain on the basis of a shadow-Hamiltonian that includes a background term, which induces canted magnetization. Section 4 presents the conclusions which we draw from a comparison of these results with similar calculations for one and two dimensional rectangular lattices.

2. Triangular HAF and 7-Site Blocks

In the naive block-spin method, at each stage one retains the lowest eigenstates of a block Hamiltonian,H_B, obtained from the true Hamiltonian H by simply dropping all terms that link the individual blocks to one another. When one diagonalizes the seven-site Hamiltonian, one finds that the lowest two eigenstates lie in a degenerate spin 1/2 doublet. The naive block-spin calculation obtained by retaining just this multiplet was described in Ref.7. The block-Hamiltonian can be written as

$$H_7 = H_6 + 2\vec{s}_7 \cdot \vec{S}_6 \tag{2.1}$$

where H_6 is the Heisenberg-model on the chain of six spins on the periphery whose total spin is S_6, and s_7 is the spin at the center of the hexagon. The two lowest lying spin multiplets are both doublets, that is the total spin $S_7 = 1/2$. The lowest doublet has $S_6 = 1$ and $E_7 = -6.236$ and the first excited multiplet has $S_6 = 0$ and $E_7 = -5.6056$. The next excitation lies at $E_7 = -4.56$. Our variational ansatz is to keep a linear combination of the lowest two doublets at each iteration and vary over the mixing angle, at the conclusion of the recursion. Clearly the choice $\theta = 0$ reproduces the result of Ref. 7. Since the Hamiltonian reproduces itself up to an overall scale factor which is less than unity, this calculation predicts that this system is at its critical point.

After the first truncation one obtains a Hamiltonian which is a function of the mixing angle, θ, given by the formula

$$H_{tr} = -6.236\cos^2\theta - 5.6056\sin^2\theta + K\sum_{\langle ij\rangle}\vec{\sigma}(i)\cdot\vec{\sigma}(j) \tag{2.2}$$

where

$$K = \frac{12}{81} \cos^4\theta + 0.67857 \sin^2 2\theta \ .$$

Applying the same transformation n times one finds that the recoupling term scales as K^n. Successive iterations of the truncation yield a vanishing mass-gap and a geometrical series for the energy density. We find the minimum energy for the infinite volume system occurs when the mixing angle between the two doublets is $\theta = \theta_{min} = 35.8.°$. The energy per site is then - 0.9518.

We can calculate the expectation value of any operater in this trial state. Of particular interest here is the canted magnetization, defined by

$$M = \sum_{i\in R} \sigma_z(i) + \sum_{i\in B} \left(-\frac{\sigma_z(i)}{2} + \frac{\sqrt{3}}{2}\, \sigma_x(i) \right) + \sum_{i\in G} \left(-\frac{\sigma_z(i)}{2} - \frac{\sqrt{3}}{2}\, \sigma_x(i) \right) . \quad (2.3)$$

We will evaluate the average canted magnetization on a block of size $V = 7^n$, obtained after n recursive applications of the RG truncation procedure. On such a block one can represent this operator as

$$M_n = \frac{M}{V} = V^{-k}(\cos n\alpha\ \sigma_z + \sin n\alpha\ \sigma_x) \quad (2.4)$$

where k and α depend on the variational angle θ. For $\theta = 0$, i.e. truncating onto the lowest state of H_7, one finds $k = 1$. This is the largest possible value, it gives the most rapid decrease of the expectation value with the volume of the system. This behavior coincides with that found for regular magnetization, which decays linearly with volume because the system has to have all the spins but one canceling each other to produce a final state of spin one half. For $\theta = \theta_{min}$ we obtain $k = .278$. Hence the mean canted magnetization drops more slowly than the

regular one and the wave-function has some alignment in the canted directions for small blocks. Nonetheless it does decrease as a power of the volume. Therefore over large scales no remnant of the canted magnetization is left. This is unavoidable when the truncated state is chosen as a linear superposition of two spin $\frac{1}{2}$ doublets. For finite volumes we find some canted magnetization. Thus for $V = 49$ the result is $V^{-k} = .34$. We note that this is already significantly smaller than the estimate derived from the wave-function of ref.5. Hence the two wave-functions are very different. Neither does our wave-function correspond to an RVB state. We do have couplings of the various spins to the lowest possible total spin, but not just via spin 0 nearest neighbor pairings.

For comparison let us apply the same method to the two-dimensional square lattice, choosing a similar form for the blocks, namely a central site plus all its nearest neighbours (a cross). We get a very different result. In this five-site block spin the lowest state is not a doublet, but a multiplet of spin 3/2 after the first iteration and $3^n/2$ after n iterations. This block-spin transformation does not lead to a self-similar system at each scale, because of the increasing spin of the retained multiplet. Nonetheless, it does yield a variational ansatz which converges to a stable result for the ground state energy density and a large expectation value (.75) for the staggered magnetization. The finite value of the magenetization operator is possible because the single-site states belong to larger and larger irreducible spin representations. This contrasts with the previous case where the lowest multiplets were always spin 1/2 and the canted magnetization was forced to fall to zero asymptotically. Since the Hamiltonian in this problem eventually scales to zero faster than its block expectation-value grows with the spin, this calculation does give a vanishing mass gap. On a one dimensional lattice the equivalent calculation

uses three site blocks and the result looks more like the triangular lattice case. The lowest two multiplets are both spin one half. A truncation which keeps a linear combination of these multiplets at each step gives a description of the system as one with zero mass gap and no order, which is correct for this model. Numerical results for these calculations are given in the table in the following section.

3. Block Spin Method with a Shadow Hamiltonian

We now consider a generalization of the block-spin method in which the choice of retained states is made by picking the eigenstates of some effective block Hamiltonian, which we call a *shadow Hamiltonian*, H_S . For example, let

$$H_S(j) = H_B + jM \tag{3.1}$$

where M can be chosen to be any operater, preferably the order-parameter of interest, and j is a parameter to be determined variationally. Let $|\psi(j)\rangle$ be the infinite volume wavefunction generated by retaining the n lowest eigenstates of $H_S(j)$ on each block at each stage of the iteration. At every stage of the calculation we carry along enough information to reconstruct both H_S and H in the truncated basis of states. The truncation procedure is repeated until the energy per site converges to the desired accuracy. One computes, for each value of j, the expectation value of the original Hamiltonian in the state constructed from the thinning algorithm based upon $H_S(j)$. The best trial state is that which minimizes the resulting function of j. Note that the quantity

$$E(j) = \langle\psi(j)|\, H\, |\psi(j)\rangle \tag{3.2}$$

is a bound on the infinite volume energy of the system for any value of j. Having

chosen j_{min}, that value of j which minimizes $E(j)$, we can then obtain a best estimate for the expectation value of M,

$$\mathcal{M} = \langle \psi(j_{min}) | \, M \, | \psi(j_{min}) \rangle \, . \tag{3.3}$$

We have carried out calculations of this kind for the case of the one-dimensional HAF, the two-dimensional HAF on a square lattice, and the two-dimensional HAF on a triangular lattice. In all calculations we retain the lowest two eigenstates of the shadow Hamiltonian on the block at each step. In the one-dimensional problem the blocks are constructed by using three points in each block, on the square lattice we used same kind of blocks alternating between the two orthogonal directions on consecutive steps, and in the triangular problem we used the hexagonal units of Fig. 1. The best energies and corresponding magnetizations are given in in Table 1.

The energies and magnetizations converge quite rapidly as a function of the iteration. This fact, and the simplicity of interpretation, make this sort of calculation very appealing. Unfortunately, one has to remember that the ground-state of the one-dimensional anti-ferromagnet cannot exhibit long range order while by this method one would conclude that it does. The shadow Hamiltonian technique is useful for studying symmetry breaking quantities such as the magnetization of a system, but, as this result indicates, it does introduce a bias in favor of such breaking. In the neighborhood of a critical point, where long-range structures play an important role, it may lead to erroneous conclusions. This same criticism applies to the procedure of Huse and Else[5] . Their method also chooses trial states in a way which is biased toward the symmetry breaking mean-field state. As in the method described here applying their method to a one-dimensional Heisenberg antiferro-

magnet, it yields a result known to be incorrect. In the square-lattice problem both studies lead to higher and more stable values of staggered-magnetization.

On the basis of the calculation described in this section one would conclude that the triangular lattice behaves like the square lattice, and that its ground state has a non-zero canted magnetization. The lesson of the one dimensional calculation, however, is that one should also explore options which do not bias the calculation towards order before drawing any conclusion. The calculation described in the previous section is an example of such a method.

4. Conclusions

We have discussed two variational calculations which provide upper bounds on the vacuum energy density. While the resulting energies were quite similar the wave-functions are very different. In particular, one exhibits non-vanishing *canted anti-ferromagnetic order* whereas the other does not. As discussed in the introduction, this reflects the situation in the literature. For every approximation which predicts *canted anti-ferromagnetic order* one can find a calculation which produces a comparable estimate of the ground-state energy density but which predicts no long range order.

In our first calculation we allowed for the mixture of the two doublets which belong to the low-lying structure of the Hamiltonian inside the hexagonal block. The state so obtained indeed has some non-vanishing expectation value for the canted magnetization for small lattices but it shows no order in the infinite volume limit. The value of the energy-density obtained in this way provides an upper bound on the infinite volume energy that is, as far as we know, the lowest obtained to date.

We consider the long-range-order found in the second calculation, based on the shadow Hamiltonian, to be unreliable. When one biases the calculation towards such order by the choice of shadow Hamiltonian, one indeed obtains an ordered state. We saw this happening in the one-dimensional chain. The calculation for the frustrated system may suffer from the same problems that invalidate the calculation for the one-dimensional chain, namely the appearance of large-scale structures which destroy the magnetization and which are missed by this method.

The bounds on the energy-density obtained in these two calculations differ only slightly. Although the state which has no order lies a little lower, this by itself is not sufficient evidence to decide that it correctly reflects the properties of the true ground state. What we find much more convincing is the comparison with the one- and two-dimensional rectangular lattice results. Table 1 summarizes our results, as well as those of Ref. 5, for the three cases. It appears to us on examining this table that the triangular lattice results look much more like those of the one dimensional case than the two dimensional. This leads us to conclude that it is most likely that the ground state of this system is indeed disordered. Note, because of the slow fall-off of the magnetization the distinction between order and disorder cannot readily be made upon the basis of small lattice calculations.

Both of our block-spin calculations lead to a vanishing mass-gap. In our θ-dependent calculation we keep an exact spin doublet at each recursion step. Hence the Hamiltonian is unchanged except by an overall scale factor at each recursion. This indicates a massless spectrum since the Hamiltonian scales to zero as the block size increases. In the other calculation we obtain spontaneous symmetry-breaking. This should be accompanied by a Goldstone-boson leading again to a vanishing mass-gap.

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Lattice / Method	1 dimension		square lattice		triangular lattice	
	$\mathcal{E}$	$\mathcal{M}$	$\mathcal{E}$	$\mathcal{M}$	$\mathcal{E}$	$\mathcal{M}$
Spin Multiplets	− 0.7826	0	− 1.10	0.75	− 0.9518	0
Shadow Hamiltonian	− 0.7861	0.478	− 1.12	0.944	− 0.939	0.59
Huse & Elser	− 0.88	< 0.2	− 1.32	0.71	− 1.07	0.68

Table 1: Comparison of calculations for the energy-density $\mathcal{E}$ and the staggered or canted magnetization $\mathcal{M}$. First line refers to the block-spin calculation using a string of 3 sites in 1-dimension, a cluster of 5 sites forming a cross on a square lattice, and a 7-site hexagon on the triagonal lattice. Second line gives the resuls of Shadow Hamiltonian calculations described in section 3. The third line contains the results of Ref. 5.

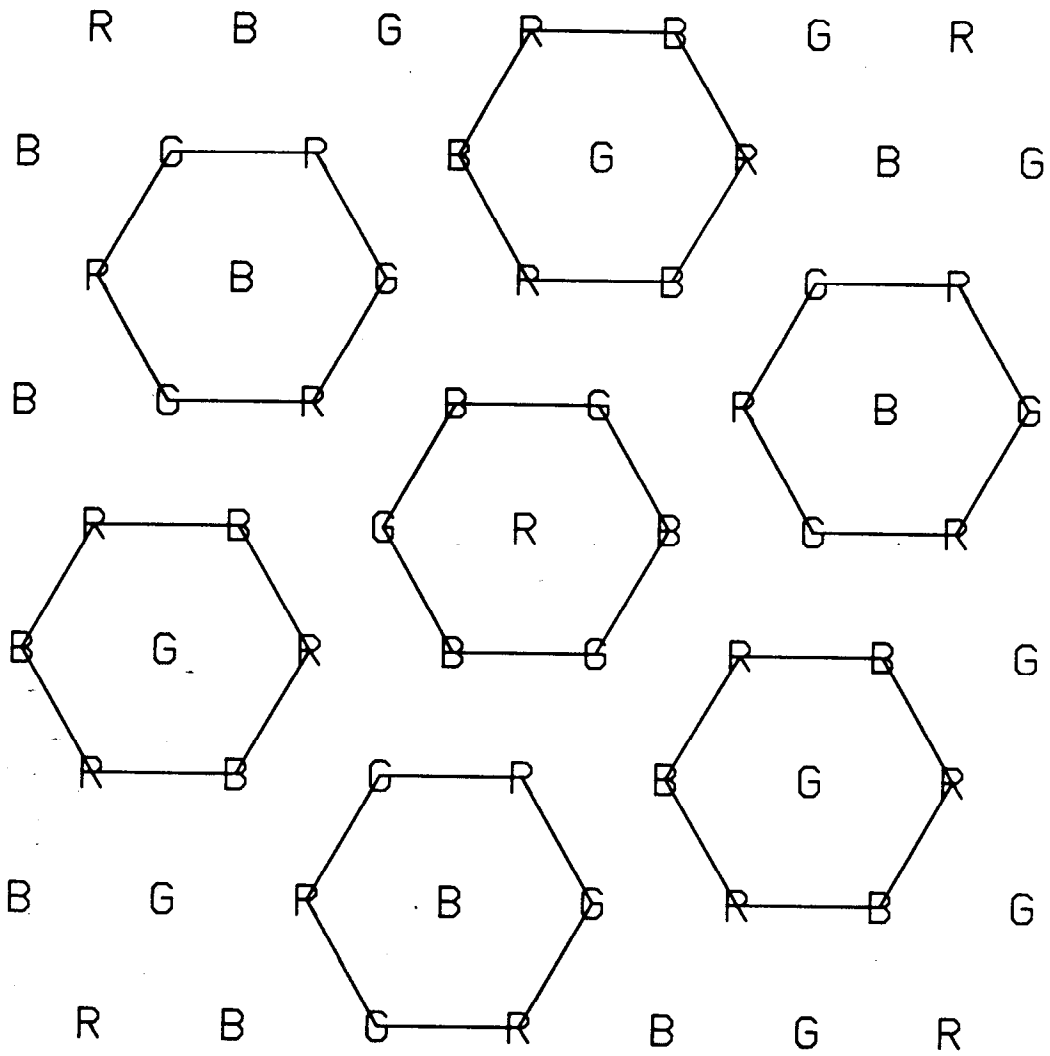

Figure 1: Triangular lattice grouped into seven-site blocks.