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EXACT GROUND STATE OF A QUANTUM MECHANICAL ANTIFERROMAGNET

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We present some exact results for the ground state of a quantum mechanical antiferromagnetic model in the two dimensions with next-nearest neighbor interactions.

We have found some exact results for the ground state(s) of an anisotropic quantum spin Heisenberg-Hamiltonian with next neighbor interactions in two and three dimensions. For clarity we present the two dimensional case in detail and postpone the three dimensional results to a forthcoming paper. We consider a two dimensional lattice (Fig. 1) where each dashed line represents a bond with strength 2α and each nearest neighbor bond has strength unity. The Hamiltonian is

$$H = \sum_{\langle ij\rangle} h_{ij} + 2\alpha \sum_{\langle \ell m\rangle} h_{\ell m} - h \sum_i S_i^z \qquad (1)$$

where $\langle ij\rangle$ represents a sum over all nearest neighbors and $\langle \ell m\rangle$ represents a sum over the diagonal bonds. Also

$$h_{ab} = J_z S_a^z S_b^z + J_x S_a^x S_b^x + J_y S_a^y S_b^y \qquad (2)$$

We restrict our attention to the non-trivial case $J_x, J_y, J_z > 0$. This model resembles the triangular lattice Heisenberg antiferromagnet, which has been studied extensively in recent literature, [1,2,3] in that the Ising limit exhibits frustration [4]. It is our hope that the exact solution sheds light on the interplay between quantum effects and spinglass ordering [5].

A. QUANTUM CASE Our solution is inspired by the surprising solution of Majumdar's, [6] for a linear chain Heisenberg antiferromagnet with a nearest and next nearest neighbor coupling which is half as strong as the first. We first observe that the state

$$|\psi\rangle = \prod_{\langle \ell m\rangle} [\ell, m] \qquad (3)$$

is an eigenstate of the Hamiltonian Eq. (1) with eigenvalue

$$E_0/N = W \equiv -\alpha \frac{1}{3} S(S+1)[J_x + J_y + J_z] \qquad (4)$$

(We use the notation $[\ell,m]$ for a singlet combination of the spins ℓ and m.) This is seen most readily by using the identity $s_i^\alpha(s_j^\alpha + s_k^\alpha) \times [j,k] = 0$ and hence the first term in Eq. (3) annihilates $|\psi\rangle$. We further show that E_0 saturates a lower bound to the ground state energy for suitable values of the parameters and hence $|\psi\rangle$ is the rigorous ground state. We write $H = \Sigma_t h_t$, where the sum is over the N triagles (each diagonal bond supports two triangles). Each triangular Hamiltonian has the form

$$h_t = h_{i\ell} + h_{i\ell} + \alpha h_{\ell m} - \frac{h}{2}(S_\ell^z + S_m^z) \qquad (5)$$

Hence a use of the variational principle implies $E_0 > N e_t$ where e_t is the ground state energy of Eq. (5). We have shown that e_t equals W and hence $|\psi\rangle$ is the ground state of H, provided $\alpha > \alpha_b$, where α_b is: (a) $1 + h/J_z$ for $s = 1/2$ and for arbitrary J_x, J_y and J_z. (For the isotropic case we have a better bound $\alpha_b = 1 + h/2J$.) (b) $1 + s + h/2J$ for $s > 1$ in the isotropic limit ($J_x = J_y = J_z = J$).

The nature of ground state correlations in $|\psi\rangle$ is seen to be liquid like, with only short ranged order and hence we have termed it the "quantum spin liquid" phase (Q.S.L.). This wave function is of the type suggested by Anderson [1] and is familiar from valence bond theory in chemistry. For α smaller than the bounding value α_b, we have not succeeded in solving the model exactly. However, we can show that the character of the ground state must change at some value of α between α_b and $2s/(2s+1)$ since at the latter value, the Néel (Ising) state provides a better upper bound to the ground state energy.

B. ISING LIMIT We have studied the ground state degeneracy of the Hamiltonian in the Ising limit $J_x = J_y = 0$ and $h = 0$ for $s = 1/2$. It is readily established that for $\alpha < 1$, the ground state entropy is O(1) whereas for $\alpha > 1$, it is of O(N). The case $\alpha > 1$ is quite simple since in this case the only constraint is that spins at the ends of a diagonal bond must be antiparallel. The entropy then is $S = k_B N(0.3466)$. The case $\alpha = 1$ is much more complex, since in this case, more configurations are allowed than for $\alpha > 1$. We have established that the case $\alpha = 1$ can be mapped on to a 10 vertex model containing N/2 sites with two sublattices, which is a generalization of the ice problem solved by Lieb [7]. We have obtained a rigorous lower bound to the entropy $s > k_B N(.4812)$ by using a braiding technique.

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C. CLASSICAL LIMIT As $s \to \infty$, the singlet state is the ground state only as $\alpha \to \infty$. However, for arbitrary α, we have succeeded in determining the ground state exactly in the isotropic limit. We observe that the classical planar (i.e., x-y) and Heisenberg model share a ground state for the triangular Hamiltonian (5). Each triangle has a two-fold discrete "chiral" degeneracy, over and above the continuous degeneracy, of the sort discovered by Villain in similar systems [8]. The optimum twist angle between a spin at the base and apex of a triangle is $(\pi \pm \cos^{-1} 1/2\alpha)$ and the two chiralities correspond to the two choices of the sign. One may then assign arrows to the bonds indicating the direction along which rotations are anti-clockwise. The constraint on a square containing a diagonal bond is that the arrows on parallel sides be in the same direction. The constraints on empty squares is that the line integral of the arrows vanish (irrotational flow). There are precisely four degenerate ground states which satisfy these constraints. Each ground state contains one preferred direction, say one of the four points of the compass, such that there is an average flow of arrows in this direction. Thus, the spins exhibit helical ordering as we proceed in this preferred direction. for $\alpha < 1/2$, the Neel state is the ground state.

D. SUMMARY Our understanding of the model in the isotropic limit is summarized in the "phase diagram" (Fig. 2). The line bounding the Q.S.L. phase is the point of highest frustration in the Ising limit. In the Q.S.L. phase the Ising limit has macroscopic degeneracy but the quantum effects freeze this degeneracy out for arbitrarily small J_x and J_y. It is interesting that similar behavior is found in approximate treatments of similar systems [2,3,5].

Finally we would like to point out the remarkable property of the ground state $|\psi\rangle$ for $s = 1/2$ in the case $\alpha > 1$ and $J_x \neq J_y \neq J_z$. In this case the ground state possesses rotation invariance (being a singlet) even though the Hamiltonian does not. This is the only example of symmetry breaking in reverse that we are aware of. This provides an exmple in non-relativistic physics where the invariance of of the vacuum exceeds the invariance of the world [9].

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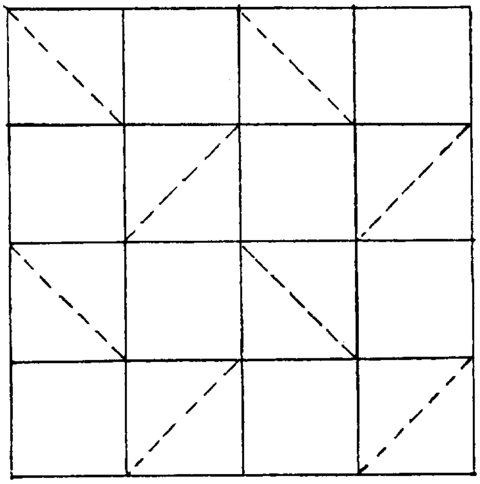

Fig. 1. The Lattice

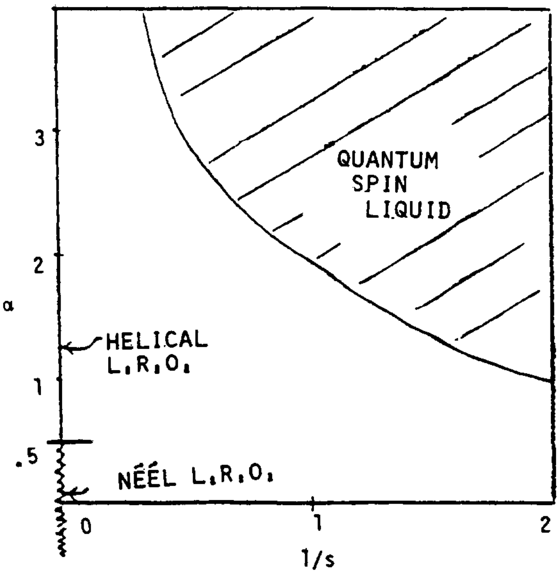

Fig. 2. The Phase Diagram