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Ground-State Symmetry in *XY* Model of Magnetism

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Numerical studies by Betts and Oitmaa have led those authors to conjecture that in the XY model the ground-state magnetization M_z is zero. This is a model of spins on a lattice with interactions $-J(S_n^xS_m^x+S_n^yS_m^y)$, that can also describe a hard-sphere boson fluid. In the present note I prove the conjecture for arbitrary spins $\mathcal{S}=\frac{1}{2}, 1, \frac{3}{2}, \ldots$ for positive J, and treat various generalizations.

In two recent papers,[1,2] Betts and Oitmaa have commented on the lack of a rigorous proof that the ground state of an infinite array of spins $\frac{1}{2}$, interacting *via* $-J(S_n^xS_m^x+S_n^yS_m^y)$ only, possesses magnetization $M_z=0$. This property is strongly implied by their various numerical experiments and is shared by other systems—notably the isotropic Heisenberg (XYZ) antiferromagnet—for which a variety of proofs already exist.[3] The classical-spin, two-dimensional, XY model has also been of extraordinary interest lately, because of conjectures by Kosterlitz and Thouless[4] concerning the unusual nature of the phase transition in this system, so that any certain knowledge concerning the ground state, especially for arbitrary spin magnitude $\mathcal{S}$, will be beneficial. For $J>0$ I have constructed a relatively simple proof valid in any number of dimensions on an arbitrary lattice, for arbitrary spins $\mathcal{S}_n$ (including the classical limit $\mathcal{S}_n\to\infty$) that M_z indeed vanishes (for integer total angular momentum) or has minimal magnitude $\frac{1}{2}$ (for half-integer total angular momentum) in the ground state. For $J<0$ the proof applies directly only to bipartite lattices, although Betts's latest studies[5] indicate that the result of minimal $|M_z|$ is always obtained. I confirm this by use of a "reference" Hamiltonian.

It should be noted that the theorem of minimal $|M_z|$ in the ground state does not preclude a phase transition in any number of dimensions, nor even the existence of long-range order. It merely confirms what should be evident upon minimal reflection, that M_z is not an appropriate order parameter in this problem.

Let

$$H=-J\sum(S_n^xS_m^x+S_n^yS_m^y),\qquad (n,m)=\text{neighbors}. \tag{1}$$

The coupling constant $J>0$ and the spins $\mathcal{S}_n$ are arbitrary. The magnetization operator is

$$M_z=\sum_{n=1}^{N}S_n^z. \tag{2}$$

We rotate in spin space $S_n^y\leftrightarrow -S_n^z$ at all sites. In the new representation, the Hamiltonian and magnetization operators are

$$H=-J\sum(S_n^xS_m^x+S_n^zS_m^z) \tag{3}$$

and

$$M_z=-\sum S_n^y=\tfrac{1}{2}i\sum(S_n^+-S_n^-), \tag{4}$$

respectively. The Hilbert space consists of $\prod(2\mathcal{S}_n+1)$ distinct configurations (e.g., 2^N for $\mathcal{S}_n$

$=\frac{1}{2}$) of two distinct types:

$$\psi_{\alpha,\mathrm{ev}} = C\prod (S_n^+)^{p_n}|0), \text{ with } \sum p_n = 0, 2, 4, \ldots \quad (5a)$$

and

$$\psi_{\alpha,\mathrm{od}} = C\prod (S_n^+)^{p_n}|0), \text{ with } \sum p_n = 1, 3, 5, \ldots . \quad (5b)$$

The Hamiltonian has no matrix elements to connect the "even" states to the "odd," therefore the two subspaces are decoupled and we must study the ground state of each. We further distinguish the two cases: $\sum \mathcal{S}_n$ = integer and $\sum \mathcal{S}_n$ = integer $+\frac{1}{2}$. In the latter case, minimal M_z will be $\pm\frac{1}{2}$ and a rotation of 180° about the S^x axis in spin space serves to interchange the even and the odd states, as well as to map $M_z \rightarrow -M_z$, while leaving H invariant. This implies an essential degeneracy of the two subspaces which is absent in the case of $\sum \mathcal{S}_n$ = integer, for which the minimal $|M_z|$ is zero. We shall return to these points shortly.

In the representation of Eqs. (3) and (4), the S_n^z are all diagonal, but the operators $S_n^x = \frac{1}{2}(S_n^+ + S_n^-)$ are not. The ground state in either subspace (ev) or (od) takes the form

$$\Phi_{0,r} = \sum F_\alpha^{(r)} \psi_{\alpha,r}, \quad \text{with } \sum |F_\alpha^{(r)}|^2 = 1 \quad (6)$$

and, according to a well-known theorem of Frobenius, has the property that all the $F_\alpha^{(r)}$, for r = ev or od, can be chosen real and positive. As connects all configurations within either subspace, no $F_\alpha^{(r)}$ vanishes nor is of opposite (negative) sign in the ground state. The proof is by contradiction: If some amplitude were not positive, the variational energy $E_{0,r} = (\Phi_{0,r}|H|\Phi_{0,r})$ could be decreased by making it so. However, $E_{0,r}$ is already the lowest possible energy for the respective subspace, hence all $F_\alpha^{(r)} > 0$. Finally, the ground state *in each subspace* is nondegenerate, as no other eigenstate of H can satisfy the condition of all positive amplitudes yet be orthogonal to $\Phi_{0,r}$. We note in passing that in the case $\sum \mathcal{S}_n$ = integer $+\frac{1}{2}$, these results imply $E_{0,\mathrm{ev}} = E_{0,\mathrm{od}}$, but not in the other case.

Now, Frobenius's theorem was already well known to Betts and Oitmaa[1,2] who, working with the "natural" operators (1) and (2), noted that within the subspace of a given M_z the ground state was nodeless and therefore unique, because M_z commutes with H and the eigenstates are chosen to be simultaneous eigenstates of both operators, this theorem gave them no indication of which eigenvalue m of M_z yields the lowest energy. The situation is quite different for the Heisenberg antiferromagnet,[3] of course, for which the eigenstates are also simultaneously eigenstates of $\vec{M}^2$ and where it therefore suffices to study the subspace $M_z = 0$. There is no corresponding simplification in the XY model.

Nevertheless, we can construct a rigorous proof of the stated theorem. We first recognize that M_z is now an imaginary (albeit Hermitean) operator, and that it commutes with H and therefore can be simultaneously diagonalized. However, M_z connects the two (ev, od) subspaces and therefore in the cases when the two ground states are not degenerate, the only possible eigenvalue of M_z is $m = 0$. In the case where there is the essential degeneracy, we can have $m = \pm\frac{1}{2}$, depending on the chosen linear combination of $\Phi_{0,\mathrm{ev}}$ and $\Phi_{0,\mathrm{od}}$. Now for a rigorous proof we shall construct two wave functions which we can, indeed, verify as belonging to minimal $|M_z|$ and which are not orthogonal to the ground states of Eq. (6). It will then follow that the latter also belong to minimal $|M_z|$.

Consider a "reference Hamiltonain"

$$H_{\mathrm{ref}} = -N^{-1}[(\sum S_n^x)^2 + (\sum S_n^z)^2] \quad (7)$$

in which *every* spin on the same lattice as before interacts with every other spin. On the one hand, the ground states in the even and odd subspaces $\Phi_{0,r}^{\mathrm{ref}}$ have all positive amplitudes, by Frobenius's theorem. They are therefore *not orthogonal* to their counterparts in Eq. (6), and therefore share the same quantum number m. On the other hand, the energy levels of (7) are immediately obtained as $E = -N^{-1}[I(I+1) - m^2]$, with $I_{\max} \equiv \sum \mathcal{S}_n$, $I = I_{\max}$, $I_{\max} - 1$, $I_{\max} - 2$, ... and $m = I_{\max}$, $I_{\max} - 1$, $I_{\max} - 2$, ... Evidently, the ground states belong to $I = I_{\max}$ and $m = 0$ ($I_{\max}$ = integer) or $m = \pm\frac{1}{2}$ ($I_{\max}$ = integer $+\frac{1}{2}$). Q.E.D.

The reference Hamiltonian also shows clearly the tendency of the order parameter (total spin in this case) to be maximal in the XY plane, as observed in numerical calculations. The spontaneous magnetization is never in the z direction in the ground state, because there is no energetic advantage for the spins to lie along the axis devoid of interactions.

On a bipartite lattice, the above proofs apply even if $J < 0$, for we can rotate the spins on the A sublattice by 180° along some appropriate axis and effectively reverse the sign of J.

It is therefore challenging to see what happens on a *non*-bipartite lattice with $J < 0$. In fact, Betts[5] has made some preliminary studies of spins $\frac{1}{2}$ on a cluster of triangular cells. The triangular lattice is the prototype "frustrated" lattice[6] for antiferromagnetic couplings, one in which it is impossible to satisfy all the bonds in the ground state. Surprisingly, Betts once again finds that the ground state belongs to minimum $|M_z|$! However, the ground state is now highly degenerate, in contrast to the previous case where Frobenius's theorem applies. Similarly, our reference Hamiltonian (7) will, after change of sign, have not only a unique (or doublet) ground state belonging to $I=0$ and $m=0$ (or $I=\frac{1}{2}$, $m=\pm\frac{1}{2}$) but a dense spectrum of low-lying states, *almost* degenerate with the ground states (in the limit $N\to\infty$, $I_{\max}\propto N$).

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Critical Correlation Function and Exponent η: A Sum Rule

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A sum rule is derived from the connection of the critical specific heat with the critical correlation function in the disordered symmetric state. The "Ornstein-Zernike hole" which appears above the critical point must, by virtue of this sum rule, be canceled exactly by the "Fisher-Langer tail." It follows that the anomalous dimension index η is fixed by the shape of the spectral function. A spectral function satisfying certain general properties yields $\eta\approx 0.04$.

The order-parameter–order-parameter correlation function, $G(r,\kappa)$, and its Fourier transform, $g(k^2,\kappa^2)$ describe correlation in configuration and wave-number space, respectively. The critical-region temperature dependence enters through the inverse correlation length κ and is expressed by the differences $\Delta G(r,\kappa)\equiv G(r,\kappa)-G(r,0)$ and $\Delta g(k^2,\kappa^2)\equiv g(k^2,\kappa^2)-g(k^2,0)$. In many cases a sufficiently accurate approximation is the Ornstein-Zernike[1] formula

$$g_{\rm OZ}(k^2,\kappa^2)=C_{\rm OZ}/(k^2+\kappa^2), \qquad (1)$$

where $C_{\rm OZ}$ is a positive constant. In this approximation the critical variation is given by the negative-definite expression

$$\Delta g_{\rm OZ}=-\frac{C_{\rm OZ}\kappa^2}{k^2(k^2+\kappa^2)}\,. \qquad (2)$$

But with the experimental precision which can presently be achieved,[2] a more accurate representation of $g(k^2,\kappa^2)$ is needed. This is also true in theoretical calculations where $g(k^2,\kappa^2)$ enters as an essential ingredient. An accurate form for $g(k^2,\kappa^2)$ is especially important in calculations where fluctuations of large k enter in an essential way, such as in studies of the critical viscosity[3] and of the critical attenuation of sound. For $k\gg\kappa$ the correlation function must asymptotically approach its $\kappa=0$ Green[4]-Fisher[5] form

$$g(k^2,0)=C_{\rm GF}k^{-2+\eta} \qquad (3)$$

assuming that k is still small enough to be in the critical region. Here $C_{\rm GF}$ is a constant and η is the anomalous dimension index. η is the most basic of the critical indices and its calculation is one of the central problems in the theory of phase transitions. A related problem, generally studied independently is the detailed k^2 and κ^2 dependence of $g(k^2,\kappa^2)$, i.e., the "shape" of the function. In this Letter we discuss a sum rule which is equivalent to a certain identity in Lagrangian field theory.[6] This sum rule imposes an intimate con-