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Spin Quantum Number in the Ground State of the Mattis–Heisenberg Model

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Total spin quantum number is rigorously calculated for a quantum version of the Mattis model of random spin systems. Crossover between three universality classes of the Ising model, the XY model, and the Heisenberg model is explicitly worked out in the presence of randomness. The randomness of the type of the Mattis model is shown to have no thermodynamic effects even in quantum systems.

KEY WORDS: Ground state; randomness; Mattis model; frustration; quantum effects.

1. INTRODUCTION

In the theory of spin glasses, the concept of frustration plays a central role in classifying randomness by relevance to thermodynamic properties.(1) The Mattis model,(2) for instance, is not considered to well describe observed characteristics of spin glass materials because it is free of frustration. However, the frustration is defined only for classical systems and is not applicable to quantum ones in a straightforward manner.(3) This is a contradiction in a sense, because the concept of frustration has its basis in the analysis of ground states of classical systems and the ground states of real materials need quantum mechanical treatment more than any other states do. Therefore it is necessary to investigate the ground states of random quantum systems to establish a sound foundation of the concept of frustration.

We calculate here the total spin quantum number in the ground state of a quantum version of the Mattis model (the Mattis–Heisenberg model). Quantum effects make this model different from a pure ferromagnet, in contrast to the classical case. But our analysis reveals that the symmetry

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properties of the model in the ground state can be interpreted as indicating irrelevance of the randomness of the Mattis type even in quantum systems. Of course, our investigation of the Mattis–Heisenberg model is still far from giving a definite picture of the effects of frustration in quantum systems, but it will serve as a starting point to construct a theory to describe quantum effects on frustrated systems.

In the next section we state an exact result on the symmetry of the ground state and give a proof of it. Physical discussions of the result are found in the last section.

2. STATEMENT AND PROOF

Let us consider the Hamiltonian

$$H = -\sum_{\langle ij\rangle} \tau_i \tau_j (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) \qquad (\tau_i = \pm 1) \tag{1}$$

Since we are interested in the ground state, the overall interaction constant J (> 0) is omitted here. The variables $\{\tau_i\}$ are arbitrarily fixed disordering variables, and Δ is an anisotropy parameter. Range of interactions and lattice structure are irrelevant to the following argument. If the spin variables in (1) are classical, this is the Mattis model. A simple redefinition of spins, $\tau_i S_i^x$, $\tau_i S_i^y$, $\tau_i S_i^z \to S_i^x$, S_i^y, S_i^z, brings (1) into a pure ferromagnet. But if the system is quantal, the above simple transformation is not allowed, because the transformation is not canonical when $\tau_i = -1$. Therefore, in contrast to the classical case, the randomness in (1) is a nontrivial one. We prove the following statement:

The ground state of (1) is unique, except for a trivial degeneracy, and the total spin quantum number is

(i) $-1 < \Delta < 1$:

$$M_z = \sum_i S_i^z = 0 \qquad \text{if } NS \text{ is an integer}$$

$$= \pm 1/2 \qquad \text{if } NS \text{ is a half-integer}$$

where N is the number of sites and S is the spin quantum number at a site.

(ii) $\Delta > 1$:

$$M_z = \pm\Big(\sum_i \tau_i\Big) S$$

(iii) $\Delta = 1$:

$$S_{\text{tot}} = \Big|\sum_i \tau_i\Big| S, \qquad M_z = -S_{\text{tot}}, -S_{\text{tot}} + 1, \cdots, S_{\text{tot}}$$

(iv) $\Delta = -1$:

$$S_{\text{tot}} = \Big|\sum_i \tau_i'\Big| S, \qquad M_z = -S_{\text{tot}}, -S_{\text{tot}} + 1, \ldots, S_{\text{tot}}$$

if the lattice is bipartite. The set $\{\tau_i'\}$ here is obtained from the original $\{\tau_i\}$ by changing the sign of all τ_i on one of the sublattices.

(v) $\Delta < -1$:

$$M_z = \pm\left(\sum_i \tau_i'\right)S$$

if the lattice is bipartite. The set $\{\tau_i'\}$ is the same one as described in (iv).

The proof below is a generalization of the arguments given by Lieb and Mattis[4] and Mattis[5]: We show that the ground state of (1) has the same symmetry property as a soluble model with long-ranged interactions. It is convenient to follow Lieb and Mattis[4] and Mattis[5] to perform two canonical transformations successively,

$$S_i^x \to \tau_i S_i^x, \qquad S_i^y \to S_i^y, \qquad S_i^z \to \tau_i S_i^z$$

and then

$$S_i^x \to S_i^x, \qquad S_i^y \to -S_i^z, \qquad S_i^z \to S_i^y$$

The Hamiltonian (1) acquires the expression

$$\begin{aligned} H &= -\sum_{\langle ij\rangle}(S_i^x S_j^x + \tau_i\tau_j S_i^z S_j^z + \Delta S_i^y S_j^y) \\ &= -\frac{1}{4}\sum_{\langle ij\rangle}\{(1-\Delta)(S_i^+S_j^+ + S_i^-S_j^-) + (1+\Delta)(S_i^+S_j^- + S_i^-S_j^+) \\ &\qquad + 4\tau_i\tau_j S_i^z S_j^z\} \end{aligned} \tag{2}$$

Simultaneously, the constant of motion M_z of (1) is transformed into $\sum_i \tau_i S_i^y$. Next we notice[5] that the space of states decouples into two subspaces spanned by

$$\phi_{\text{even}} = C\prod_i (S_i^+)^{p_i}|0\rangle, \qquad \sum_i p_i = \text{even}$$

and

$$\phi_{\text{odd}} = C\prod_i (S_i^+)^{p_i}|0\rangle, \qquad \sum_i p_i = \text{odd} \tag{3}$$

Here $|0\rangle$ is the state with $\sum_i S_i^z = -NS$ in the representation (2). Since the Hamiltonian (2) has no matrix elements between these two spaces, we may look for the ground state in each space. The ground state wave function is expressed by a linear combination of (3) as

$$\Psi = \sum_\nu a_\nu \phi_\nu \qquad \left(\sum_\nu |a_\nu|^2 = 1\right) \tag{4}$$

where ν runs over all basis states in either subspace. A necessary condition for (4) to be a ground state is obtained by minimizing the expectation value of the Hamiltonian (2),

$$E = \langle \Psi | H | \Psi \rangle$$
$$= -\sum_{\nu} \sum_{\mu}{}' \frac{1}{4}(1-\Delta)|a_\nu|\,|a_\mu| \cos(\theta_\nu - \theta_\mu)$$
$$-\sum_{\nu} \sum_{\lambda}{}' \frac{1}{4}(1+\Delta)|a_\nu|\,|a_\lambda| \cos(\theta_\nu - \theta_\lambda) + \text{(diagonal term)} \quad (5)$$

Here θ_ν is the phase of a_ν ($a_\nu = |a_\nu| \exp i\theta_\nu$), ν runs over all states, μ is a state obtained from ν by the operation of $S_i^+ S_j^+$ or $S_i^- S_j^-$, and λ is a state obtained by operating $S_i^+ S_j^-$ or $S_i^- S_j^+$ on ν. The sums over μ and λ in (5) are restricted to such states. Since the energy is real, only the real part has been left in (5). By "diagonal term" we mean the expectation value of the term $S^z S^z$ in (2) and hence the diagonal term is a function only of the absolute value of a_ν, independent of the phase θ_ν. We seek a necessary condition to minimize (5) by varying θ_ν arbitrarily. Accordingly the diagonal part plays no role in our game. The necessary condition thus obtained will prove to determine the total spin uniquely. Now examine each value of Δ.

(i) $-1 < \Delta < 1$. To minimize (5), it is necessary to take all θ_ν equal to a common value if $-1 < \Delta < 1$.[2] As an overall phase factor is irrelevant, we choose $\theta = 0$ and thus any a_ν is real and positive. This necessary condition of the ground-state wave function is shared by a long-ranged system as follows. Consider a reference Hamiltonian[(5,10)]

$$H_{\text{ref}} = -N^{-1}\left\{\left(\sum_i S_i^x\right)^2 + \left(\sum_i S_i^z\right)^2\right\} \quad (6)$$

This model is solved as

$$H_{\text{ref}} = -N^{-1}\left[I(I+1) - m^2\right]$$

where $I = I_{\max}, I_{\max} - 1, \ldots$ and $m = I_{\max}, I_{\max} - 1, \ldots$ with $I_{\max} = NS$. The quantum number m is the eigenvalue of $\sum_i S_i^y$. In the ground state it is evident that $m = 0$ (if NS is an integer) or $\pm 1/2$ (if NS is a half-integer). Therefore, by applying a canonical transformation $S_i^y \to \tau_i S_i^y, S_i^z \to \tau_i S_i^z$ to (6), we find that another reference system

$$H_{\text{ref}} = -N^{-1}\left[\left(\sum_i S_i^x\right)^2 + \left(\sum_i \tau_i S_i^z\right)^2\right] \quad (7)$$

[2] This fact is nothing but the Frobenius theorem.[(5)] Since the off-diagonal terms in (2) connect all states in a subspace (even or odd), a common value of the phase factor θ (independent of ν) is assumed by all states in the subspace under consideration.

has the ground state quantum number $\sum_i \tau_i S_i^y = 0$ or $\pm 1/2$. On the other hand, we can again evaluate the expectation value of (7) by the wave function (4) and minimize it. By rewriting (7) as

$$H_{\text{ref}} = -N^{-1} \frac{1}{4} \sum_{i,j} (S_i^+ S_j^+ + S_i^- S_j^- + S_i^+ S_j^- + S_i^- S_j^+) + (\text{diagonal term})$$

one can readily convince oneself that all coefficients a_ν in the expansion (4) can be chosen to be real and positive. This is a necessary condition on the ground state of (7). We now observe that the same necessary condition, positive definiteness of the coefficients, is shared by both ground state wave functions, those of (2) and (7). Consequently these wave functions are never orthogonal to each other, indicating that they share the same quantum number for $\sum_i \tau_i S_i^y$. This completes the proof of the statement (i). Uniqueness also follows from the positive definiteness of the coefficients; no other eigenstates of the Hamiltonian (2) can satisfy the same necessary condition yet be orthogonal to Ψ.

(ii) $\Delta > 1$. If Δ exceeds unity, the sign of the first term in (5) changes while that of the second term does not. Minimization of (5) is then achieved by choosing $\theta_\nu = \theta_\mu + \pi$ and $\theta_\nu = \theta_\lambda$. Two states ν and μ differ in $\sum_i S_i^z$ by ± 2 (because μ is obtained from ν by $S^+S^+ + S^-S^-$). And the states ν and λ have the same value of $\sum_i S_i^z$ (because λ is obtained from ν by $S^+S^- + S^-S^+$). Accordingly the phases of the coefficients a_ν must now be changed by π in passing from a state ν with a value of $\sum_i S_i^z$ to another state μ with a value of $\sum_i S_i^z$ different from that of ν by ± 2. Within a space of definite $\sum_i S_i^z$, θ_ν assumes a constant value because of the second term in (5). This is a necessary condition of the ground state when $\Delta > 1$. The appropriate reference Hamiltonian is

$$H_{\text{ref}} = -N^{-1} \Big(\sum_i S_i^y \Big)^2 \tag{8}$$

This Hamiltonian is already diagonal in S_i^y, and so the operator $\sum_i \tau_i S_i^y$ is a good quantum number. Equation (8) may be cast into another form:

$$H_{\text{ref}} = (4N)^{-1} \sum_{i,j} (S_i^+ S_j^+ + S_i^- S_j^- - S_i^+ S_j^- - S_i^- S_j^+) \tag{9}$$

The signs of coefficients of terms in (9) are just the same as the corresponding ones in (2) (if $\Delta > 1$). Thus the same rule for the phases of a_ν in (4) follows, implying the nonorthogonality of two ground state wave functions of (2) and (9). Since both (2) and (8) commute with $\sum_i \tau_i S_i^y$, we conclude that (2) and (8) share the same quantum number in their ground states. In the ground state of (8), $\sum_i \tau_i S_i^y$ is evidently $\pm \sum_i \tau_i S$ and we have proved the statement (ii). Nondegeneracy (except a trivial ± symmetry) is also a consequence of the phase rule for a_ν; quite the same argument as in (i) applies and we do not bother to repeat it here.

(iii) $\Delta = 1$. The total spin for $\Delta = 1$ has already been obtained by Lieb and Mattis.[(4)] They do not mention explicitly the relevance of their result to the present random system (1), but their formula for the ground state total spin is easily rewritten into the expression (iii) of our statement.[3]

(iv), (v) $\Delta \leqslant -1$. If the lattice is bipartite, it is straightforward to show the equivalence of negative and positive Δ: On one of the sublattices we perform the canonical transformation $S_i^x \to -S_i^x$, $S_i^y \to -S_i^y$, $S_i^z \to S_i^z$. This transformation makes (1) into

$$H = \sum_{\langle ij \rangle} \tau_i \tau_j (S_i^x S_j^x + S_i^y S_j^y + |\Delta| S_i^z S_j^z)$$

Then we change the sign of all τ_i on either sublattice, $\tau_i \to -\tau_i$. Since the lattice is bipartite,

$$H = -\sum_{\langle ij \rangle} \tau_i \tau_j (S_i^x S_j^x + S_i^y S_j^y + |\Delta| S_i^z S_j^z)$$

Therefore a system with negative Δ is equivalent to a system with positive $|\Delta|$ but with the sign of all τ changed on a sublattice. If the lattice is not bipartite and Δ is less than or equal to -1, the system (1) is said to have competing interactions and we have nothing to say about this case.

3. DISCUSSION

The total spin obtained in the previous section indicates irrelevance of randomness of the Mattis type. For $-1 < \Delta < 1$, the randomness changes nothing of the ground state symmetry. For $\Delta \geqslant 1$, the total spin is modified in a manner shown in the statement, but this modification is compatible with the naive classical picture: Spins at sites with $\tau = -1$ are down and other spins are up. Of course a down-spin is not just on the site with $\tau = -1$ but has some probability to reside on nearby sites owing to quantum fluctuations.[(6)] Nevertheless the value of M_z and the uniqueness of the ground state strongly support the picture that the effect of the randomness does not prevail in a macroscopic scale but is localized around the impurities. Although the Mattis–Heisenberg model (1) is not rigorously equivalent to a pure ferromagnetic system, in contrast to the classical case, its randomness is concluded to have no essential effects on the macroscopic system.

[3] In their formula, $S_A - S_B$ is equal to $\sum_i \tau_i S$ of our expression.

As for systems with competing interactions [not expressed by (1)], our method of analysis breaks down and no definite statements can be made. Several preliminary results are reported[7–9] but the present state of understanding is far from illuminating.

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