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Cite as: J. Math. Phys. **3**, 749 (1962); https://doi.org/10.1063/1.1724276
Submitted: 06 October 1961 . Published Online: 22 December 2004

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 3, NUMBER 4 JULY-AUGUST 1962

Ordering Energy Levels of Interacting Spin Systems

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(Received October 6, 1961)

The total spin S is a good quantum number in problems of interacting spins. We have shown that for rather general antiferromagnetic or ferrimagnetic Hamiltonians, which need not exhibit translational invariance, the lowest energy eigenvalue for each value of S [denoted $E(S)$] is ordered in a natural way. In antiferromagnetism, $E(S+1) > E(S)$ for $S \geq 0$. In ferrimagnetism, $E(S+1) > E(S)$ for $S \geq \mathbb{S}$, and in addition the ground state belongs to $S \leq \mathbb{S}$. $\mathbb{S}$ is defined as follows: Let the maximum spin of the A sublattice be S_A and of the B sublattice S_B; then $\mathbb{S} \equiv |S_A - S_B|$. Antiferromagnetism is treated as the special case of $\mathbb{S} = 0$. We also briefly discuss the structure of the lowest eigenfunctions in an external magnetic field.

INTRODUCTION

THE general Heisenberg Hamiltonian for interacting spins on a lattice (in any number of dimensions) is

$$H = 2 \sum J_{ij} S_i \cdot S_j. \tag{1}$$

This describes theories of ferromagnetism, ferrimagnetism, and antiferromagnetism, depending on the geometry of the lattice, the structure of the symmetric matrix J_{ij}, and the magnitude of the intrinsic spins (which may vary from site to site). In fact, it is conceivable that these factors be such that the spin system displays a mixture of the three magnetic properties. But we shall restrict the discussion to *ferrimagnetic* arrays, of which a special case is *antiferromagnetism*.

We consider only those arrays for which an A and a B sublattice can be defined. The definition of these two sublattices is circular, and perhaps not unique, for the only requirement in defining them is that there exist a constant $g^2 \geq 0$ such that for all sites $i(A)$ on one sublattice and $i(B)$ on the other,

$$J_{i(A),j(A)} \leq g^2, \qquad J_{i(B),j(B)} \leq g^2, \qquad \text{and} \quad J_{i(A),j(B)} \geq g^2. \tag{2}$$

In general, there might be several ways to decompose the lattice in such a way that (2) is obeyed, or there may be none. In the latter case, the system is not necessarily ferromagnetic, and only explicit solutions will reveal its properties. But if (2) is obeyed, we shall show that one is definitely dealing with ferrimagnetism or antiferromagnetism. Note that the number of sites in each sublattice and the magnitude of the intrinsic spin on each site is irrevalent, so that only the topology of the lattice and the structure of J_{ij} counts. Note also that for $g = 0$, and the A sublattice consisting of the nearest neighbors to the sites on (i.e., intermeshing with) the B sublattice, the requirement (2) gives a tendency for nearest neighbors to align antiparallel and next-nearest neighbors to align parallel, and therefore reduces to the usual definition of ferrimagnetism (when the spins are of unequal magnitude) and of antiferromagnetism (when all spins are equal).

The intrinsic spin of an electron is 1/2, but we may be dealing with various species of magnetized atoms or nuclei, so let the intrinsic spin angular momentum on each site be s_i. The maximum possible spin S_A on the A sublattice is therefore

$$S_A \equiv \sum_{i(A)} s_{i(A)}, \tag{3a}$$

and on the B sublattice

$$S_B \equiv \sum_{i(B)} s_{i(B)}. \tag{3b}$$

Defining

$$\mathbb{S} \equiv |S_A - S_B|, \tag{3c}$$

we shall prove that the ground state of H belongs *at most* to total spin $S = \mathbb{S}$. Moreover, if we denote by $E(S)$ the lowest energy eigenvalue belonging to total spin S, then we shall also prove

$$E(S+1) > E(S) \quad \text{for all} \quad S \geq \mathbb{S}, \quad \text{and} \quad E(S) > E(\mathbb{S}) \quad \text{for} \quad S < \mathbb{S} \quad \text{and} \quad g^2 = 0. \tag{4}$$

(Antiferromagnetism is when $\mathbb{S} = 0$, and the ground state belongs to total spin zero.) This can be regarded *either* as a theorem in ferri- or antiferromagnetism, *or* as a proof that the conditions in Eq. (2) and above eliminate the possibility of ferromagnetism (insofar as it costs energy to raise the total spin value over and above its ground-state value, and that this ground-state value is far from the maximum per-

missible value of $S_A + S_B$). It also indicates that a large class of apparently different Hamiltonians (1) have really a similar structure, as summarized in Eq. (4), and in the properties of the corresponding eigenfunctions which we shall find below.

W. Marshall was the first to show[1] that the ground state of an antiferromagnet is a singlet; Elsewhere,[2] we have commented on and strengthened his proof. In the present work, we succeed in removing the requirement of translational invariance, and also apply the method to identify the excited states. The M-subspace arguments presented here were previously found useful in the classification of the states of an electron system, and have been used to disprove the possibility of ferromagnetism in linear chains of atoms in s states.[3]

We shall now restrict the discussion to the special case $g^2 = 0$, until the end of the proof.

M SUBSPACES

With the help of the total spin operator

$$\mathbf{S} \equiv \sum \mathbf{s}_i$$

we can construct two operators which commute with each other and with H, namely, $\mathbf{S}^2$ and $\mathbf{S}_z$, which possess eigenvalues $S(S+1)$ and M, respectively. It is known from the theory of angular momentum that $S \geq |M|$. From the rotational invariance of the Hamiltonian we infer the $(2S+1)$-fold degeneracy of each energy level belonging to S, one degenerate level for each value of M in the range $-S \leq M \leq S$. It therefore follows that every energy eigenvalue has a corresponding eigenfunction (representative) in the $M = 0$ subspace of eigenfunctions; that every energy level except those belonging to $S = 0$ has a representative in the $M = 1$ subspace; similarly for all except $S = 0$ and $S = 1$ in the $M = 2$ subspace, and so forth. The theorem, Eq. (4), will be proved if we can show that the lowest energy in an M subspace belongs to $S = M$, for spin $S + 1$ also has a representative in that subspace and therefore $E(S) < E(S+1)$. If the ground state belongs to $S = S_0$ (we still have to prove that $S_0 \leq \mathcal{S}$), we need only consider the subspaces of $|M| \geq S_0$, for the ground states of the remaining subspaces will always belong to S_0.

The mechanics of the proof are this: The ground state of H in an M subspace is *not* orthogonal to the ground state of a soluble Hamiltonian in the same subspace, and the latter is *known* to belong to $S = M$ for $M \geq \mathcal{S}$; therefore, so does the former. Now let us go into more detail.

PROOF

In an M subspace, choose the basis set to consist of all distinct eigenfunctions of the $\mathbf{s}_i^z$ compatible with eigenvalue M. We denote each configuration in the set by ϕ_a, where a is an index which runs over all members of the set. Shortly, we shall specify a convenient choice of phase for each configuration. But first, perform a canonical transformation on H by letting

$$\mathbf{S}_{i(A)}^x \to -\mathbf{S}_{i(A)}^x, \qquad \mathbf{S}_{i(A)}^y \to -\mathbf{S}_{i(A)}^y, \qquad \mathbf{S}_{i(A)}^z \to +\mathbf{S}_{i(A)}^z \tag{5}$$

but leaving the spins on the B-sublattice invariant. In the *new* language, the Hamiltonian can be written as $H_0 + H_1$, where the diagonal part is

$$H_0 = 2 \sum J_{ij} \mathbf{S}_i^z \mathbf{S}_j^z, \tag{6}$$

and the nondiagonal part is

$$H_1 = -\{\sum |J_{ij}| \, S_i^+ S_j^- + \text{H.c.}\}. \tag{7}$$

We recall that g^2 of Eq. (2) is zero: the generalization for $g^2 > 0$ comes below.

In a given state ϕ_a, S_i^z has eigenvalue m_i. Choose the phase of ϕ_a in the following manner:

$$\phi_a = C(S_1^+)^{S_1+m_1}(S_2^+)^{S_2+m_2} \cdots (S_N^+)^{S_N+m_N}\chi, \tag{8}$$

where χ is the state in which $m_i = -S_i$, and C is a positive normalization constant. With this definition in mind, it is clear that if we define $K_{\beta a}$ to be

$$K_{\beta a} = \langle \phi_\beta \, | H_1 | \, \phi_a \rangle, \tag{9}$$

then

$$K_{\beta a} \leq 0, \quad \text{or equivalently,} \quad K_{\beta a} = -|K_{\beta a}|. \tag{10}$$

The ground state in the M subspace is denoted ψ, belongs to the ground-state energy E_M, and can be expanded in our complete set in terms of the amplitudes f_a,

$$\psi = \sum f_a \phi_a. \tag{11}$$

Since H_0 is diagonal, denote its eigenvalues by e_a,

$$H_0 \phi_a = e_a \phi_a, \tag{12}$$

and therefore the Schrödinger equation reads

$$-\sum_\beta |K_{\beta a}| \cdot f_\beta + e_a f_a = E_M f_a. \tag{13}$$

The variational energy of any trial function exceeds E_M, unless it is also a ground-state eigenfunction.

[1] W. Marshall, Proc. Roy. Soc. (London) **A232**, 48 (1955).
[2] E. Lieb, T. Schultz, D. Mattis, Ann. Phys. **16**, 407 (1961), particularly Appendix B.
[3] E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).

But

$$\psi' = \sum |f_\alpha| \phi_\alpha \tag{14}$$

is a trial function with variational energy E_M, and therefore

$$-\sum |K_{\beta\alpha}| \, |f_\beta| + e_\alpha |f_\alpha| = E_M |f_\alpha|. \tag{15}$$

Moreover,

$$e_\alpha - E_M > 0, \quad \text{for all} \quad \alpha \tag{16}$$

(otherwise, some *one* ϕ_α would be the ground state, which is in general impossible.) Therefore, taking the absolute value of $(e_\alpha - E_M)f_\alpha$ as given be Eq. (11) and combining with Eq. (15), we obtain

$$|(\sum |K_{\beta\alpha}| \, f_\beta)| = \sum |K_{\beta\alpha}| \, |f_\beta|. \tag{17}$$

This is a contradiction unless

$$f_\beta \geq 0 \quad \text{for all} \quad \beta. \tag{18}$$

In general, we have a slightly stronger result,

$$f_\beta > 0, \quad \text{for all} \quad \beta. \tag{19}$$

For, if some f_α vaaished, then Eq. (15) would read:

$$\sum K_{\beta\alpha} |f_\beta| = 0,$$

and by succeeding applications of the Hamiltonian, one could establish that *all* the amplitudes vanished, unless the Hamiltonian splits into sets of noninteracting spins in which case only the weaker result (18) holds. Therefore, in general, all amplitudes are positive and nonvanishing, and hence E_M in nondegenerate. This last statement follows from the impossibility of constructing states orthogonal to ψ without some changes of sign, and consequent violation of the ground-state property (19).

Next consider the special Hamiltonian where $J_{i(A)j(A)} = J_{i(B)j(B)} = 0$ and $J_{i(A)j(B)} = J$, a positive constant. The eigenvalues are readily calculated. The lowest energy belonging to each spin is given by $E(S)$, for $S \geq \mathcal{S}$, and the ground state belongs to $S = \mathcal{S}$.

$$E(S) = J\{S(S+1) - S_A(S_A+1) - S_B(S_B+1)\} \quad \text{for} \quad S \geq \mathcal{S}. \tag{20}$$

By the previous arguments, the ground-state eigenfunctions of this special Hamiltonian in a given M subspace satisfy Eq. (18) or (19) and are therefore not all orthogonal to the corresponding ground state of H. The special Hamiltonian has an $S = M$ ground state in each M subspace, provided $M \geq \mathcal{S}$. Therefore, so does H and this completes the proof for $g^2 = 0$.

When $g^2 > 0$, we have proved the theorem (4) for $H - g^2\mathbf{S}^2$ and it is therefore true *a fortiori* for H. However, the lowest ground state no longer necessarily belongs to $\mathcal{S}$, but belongs to $S \leq \mathcal{S}$.

MAGNETIC FIELD

A magnetic field in the z direction but of arbitrary and variable amplitude B_i modifies H_0 but not H_1, and therefore (18) or (19) are still valid for the ground state in an M subspace. The absolute ground state of the system is no longer necessarily in the $M \leq \mathcal{S}$ subspace nor is S a good quantum number in the presence of such a magnetic field.

ACKNOWLEDGMENT

It is a pleasure to thank Dr. T. D. Schultz for helpful discussion.