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Ground state properties of the Schrödinger model of ferromagnetism

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Abstract. We consider a system described by the hamiltonian

$$\mathscr{H} = -\sum_{i,j} J_{ij}P_{ij} - \sum_{\substack{i,j,k,l\\ i\neq k,l;j\neq k,l}} J_{ijkl}P_{ij}P_{kl} - \ldots - g\mu_B H\sum_i S_{iz} + D\sum_i S_{iz}^2$$

where P_{ij} is the spin S Schrödinger exchange operator, H is an external magnetic field and D the single-ion anisotropy constant, and study its ground state properties. In particular for $S = 1$ at $T = 0$ we find that the magnetization $m = 0$ for $D > g\mu_B|H|$ while for $D < g\mu_B|H|$, $m = H/|H|$, the ground states being non-degenerate.

1. Introduction

Consider a system of N spin S particles on a lattice characterized by the hamiltonian

$$\mathscr{H} = \mathscr{H}_{SI} + \mathscr{H}_{EX}, \tag{1}$$

where

$$\mathscr{H}_{SI} = -g\mu_B H \sum_{i=1}^{N} S_{iz} + D\sum_{i=1}^{N} S_{iz}^2. \tag{2}$$

The latter two terms represent the Zeeman and single-ion anisotropy contributions, respectively. Let $|\phi\rangle = |m_1 m_2 \ldots m_N\rangle \equiv |\{m_i\}\rangle$ be a normalized state such that

$$\left.\begin{aligned} S_{iz}|\phi\rangle &= m_i|\phi\rangle \\ \langle\phi|\phi'\rangle &= \delta_{\phi\phi'} \end{aligned}\right\} \qquad i = 1, 2, \ldots, N. \tag{3}$$

m_i can take on the values $-S, \ldots, S$. We define a permutation operator p_r by

$$p_r|\phi\rangle = |p_r\phi\rangle \equiv |\phi'\rangle \tag{4}$$

where $p_r\phi$ means that the permutation p_r is performed on a sequence $\phi = \{m_i\}$ to give the new sequence $\phi' = \{m_i'\}$. We take for the operator $\mathscr{H}_{EX}$ the specific form

$$\begin{aligned} \mathscr{H}_{EX} &= -\sum_{p_r\in S_N} J_{p_r}(p_r - I) \equiv -\tilde{\mathscr{P}} \\ J_{p_r} &\geqslant 0 \end{aligned} \tag{5}$$

where S_N denotes the set of all permutations such that $p_r^2 = I$. If P_{ij} denotes the

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Schrödinger exchange operator (Schrödinger 1941) for spin S which permutes the spin states of the two spins i and j, equation (5) is equivalent to the form

$$\tilde{\mathscr{P}} = \sum_{i,j} J_{ij}P_{ij} + \sum_{\substack{i,j,k,l \\ i\neq k,l \\ j\neq k,l}} J_{ijkl}P_{ij}P_{kl} + \dots \quad (6)$$

If we were to set

$$J_{ij} = J \qquad \text{if } i,j \text{ are nearest neighbours}$$
$$= 0 \qquad \text{otherwise}$$
$$J_{ijkl} = 0 \qquad \dots,$$

then $\mathscr{H}$ reduces to the previously studied Schrödinger model of ferromagnetism (Kim and Joseph 1973a, b, 1974). In general P_{ij} is a polynomial of degree $2S$ in $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$.

The purpose of the present paper is to study rigorously the ground state ($T = 0$) properties of the system described by equations (1), (2) and (5). In § 2 general properties of the matrix $\tilde{\mathscr{P}}$ are studied while in § 3 these properties are used to consider the ground state energy of the system. In § 4 we conclude by showing for the case $S = 1$ that the magnetization $m = \langle \Sigma_i S_{iz} \rangle / N$ and quadrupolar order parameter $x = \langle \Sigma_i S_{iz}^2 \rangle / N$ are related by $x = |m|$. In particular for $D > g\mu_B|H|$, $m = x = 0$ while for $D < g\mu_B|H|$, $|m| = x = 1$. For these situations the ground state is non-degenerate. When $D = g\mu_B|H|$ no simple result is obtained due to a possible degeneracy in the ground state.

2. Matrix elements of $\tilde{\mathscr{P}}$

By its definition, p_r changes the configuration $\{m_i\}$ into the new configuration $\{m_i'\}$ but it preserves the quantities $\Sigma_i m_i$ and $\Sigma_i m_i^2$. Hence we have

$$\left[p_r, \sum_i S_{iz}\right] = \left[p_r, \sum_i S_{iz}^2\right] = 0$$

so that the hamiltonian commutes with both $\Sigma_i S_{iz}$ and $\Sigma_i S_{iz}^2$.

Let $S(Q, M)$ be the finite set of all the $\phi = \{m_i\}$ with the constraints $M = \Sigma_i m_i$, $Q = \Sigma_i m_i^2$. We then have

$$\left.\begin{aligned} \sum_i S_{iz}|\phi\rangle &= M|\phi\rangle \\ \sum_i S_{iz}^2|\phi\rangle &= Q|\phi\rangle \end{aligned}\right\} \qquad \text{when } \phi \in S(Q, M). \quad (7)$$

Furthermore we have that

$$\langle \phi' | \mathscr{H} | \phi \rangle \neq 0 \quad (8)$$

only when ϕ, ϕ' both belong to the same set $S(Q, M)$ since $p_r|\phi\rangle = |\phi'\rangle \in S(Q, M)$ if $|\phi\rangle \in S(Q, M)$ for any p_r. Consequently we may restrict our attention to the quantities $\langle \phi' | \tilde{\mathscr{P}} | \phi \rangle$ where both $\phi \in S(Q, M)$ and $\phi' \in S(Q, M)$.

Now if $\phi \neq \phi'$ we have

$$\begin{aligned}\langle\phi'|\tilde{\mathscr{P}}|\phi\rangle &= \langle\phi'|\sum_{p_r\in S_N} J_{p_r}(p_r - I)|\phi\rangle \\ &= \sum_{p_r\in S_N} J_{p_r}\langle\phi'|p_r|\phi\rangle \\ &= \sum_{p_r\in S_N} J_{p_r}\langle\phi'|p_r\phi\rangle. \end{aligned} \tag{9}$$

But $\langle\phi'|p_r\phi\rangle = 1$ if $p_r|\phi\rangle = |\phi'\rangle$, otherwise it is zero. Hence we immediately have the result

$$\langle\phi'|\tilde{\mathscr{P}}|\phi\rangle \geqslant 0 \qquad \text{if } \phi' \neq \phi. \tag{10}$$

Consider now the quantity $P_{ij}\,\Sigma_{\phi\in S(Q,M)}|\phi\rangle$ where P_{ij} is any transposition (i,j). Suppose that $\phi \in S(Q,M)$ and let $P_{ij}|\phi\rangle \equiv |\phi'\rangle$. Then $\phi' \in S(Q,M)$ also. Furthermore we see that $P_{ij}|\phi'\rangle = P_{ij}^2|\phi\rangle = |\phi\rangle$. Here ϕ' and ϕ may or may not be the same depending upon whether m_i and m_j are the same or not. Therefore we can always regroup the quantity $\Sigma_{\phi\in S(Q,M)}|\phi\rangle$ into the form

$$\sum_{\phi}|\phi\rangle = \sum_{\phi_0}|\phi_0\rangle + \sum_{\phi_1}(|\phi_1\rangle + |\phi_2\rangle) \tag{11}$$

where ϕ_0 denotes those $|\phi\rangle$ which remain unchanged under the P_{ij} operator and $|\phi_2\rangle = P_{ij}|\phi_1\rangle$ with $\phi_1 \neq \phi_2$. Applying the operator P_{ij} to this form we see that

$$P_{ij}\sum_{\phi\in S(Q,M)}|\phi\rangle = \sum_{\phi\in S(Q,M)}|\phi\rangle \qquad \text{for any } i, j. \tag{12}$$

Now any p_r can be decomposed into products of the transpositions, e.g. equation (6), and for each of these transpositions, equation (12) holds. Hence we have

$$p_r\sum_{\phi\in S(Q,M)}|\phi\rangle = \sum_{\phi\in S(Q,M)}|\phi\rangle \tag{13}$$

or upon performing the sum $p_r \in S_N$ and using the definition of the operator $\tilde{\mathscr{P}}$,

$$\tilde{\mathscr{P}}\left(\sum_{\phi\in S(Q,M)}|\phi\rangle\right) = 0.$$

This immediately gives us the result

$$\sum_{\phi\in S(Q,M)}\langle\phi'|\tilde{\mathscr{P}}|\phi\rangle = 0 \qquad \text{for all } \phi'. \tag{14}$$

We know that

$$\langle\phi'|p_r|\phi\rangle = \begin{cases} 1 & \text{if } p_r|\phi\rangle = |\phi'\rangle \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

and that

$$\langle\phi|p_r|\phi'\rangle = \begin{cases} 1 & \text{if } p_r|\phi'\rangle = |\phi\rangle \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

But since $p_r^2 = \boldsymbol{I}$ we have

$$\langle\phi|p_r|\phi'\rangle = \begin{cases} 1 & \text{if } p_r|\phi\rangle = |\phi'\rangle \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

Hence we find that

$$\langle\phi'|p_r|\phi\rangle = \langle\phi|p_r|\phi'\rangle = \begin{cases} 1 & \text{if } p_r|\phi\rangle = |\phi'\rangle \\ 0 & \text{otherwise.} \end{cases} \tag{18}$$

Therefore

$$\begin{aligned} \langle\phi'|\tilde{\mathscr{P}}|\phi\rangle &= \langle\phi'| \sum_{p_r \in S_N} J_{p_r}(p_r - \boldsymbol{I})|\phi\rangle \\ &= \sum_{p_r \in S_N} J_{p_r}(\langle\phi'|p_r|\phi\rangle - \langle\phi'|\phi\rangle) \\ &= \sum_{p_r \in S_N} J_{p_r}(\langle\phi|p_r|\phi'\rangle - \langle\phi|\phi'\rangle) \\ &= \langle\phi| \sum_{p_r \in S_N} J_{p_r}(p_r - \boldsymbol{I})|\phi'\rangle \\ &= \langle\phi|\tilde{\mathscr{P}}|\phi'\rangle. \end{aligned} \tag{19}$$

Hence we see that $\langle\phi|\tilde{\mathscr{P}}|\phi'\rangle$ is a real, symmetric, finite (with dimension equal to the number of elements in $S(Q, M)$) matrix with non-negative off-diagonal elements and that the sum of the elements in any row (or column) is zero.

3. Ground state energy

In order to study the ground state energy of the system we make use of the following theorem.

Theorem. Let A be a real, symmetric matrix of dimension n whose elements a_{ij} satisfy the following conditions:

$$a_{ij} \geqslant 0 \qquad \text{if } i \neq j \tag{20}$$

$$\sum_{j=1}^{n} a_{ij} = 0 \qquad \text{for all } i. \tag{21}$$

Then the largest eigenvalue of A is zero. The vector $\hat{x} = n^{-1/2}(1, 1, \ldots, 1)$ is an eigenvector (not necessarily unique) of A corresponding to the eigenvalue zero.

Proof. The maximum eigenvalue of A is equal to the greatest value which the quadratic form

$$A(x, x) \equiv \sum_{i,j=1}^{n} a_{ij} x_i x_j \tag{22}$$

can take subject to the condition

$$\sum_{i=1}^{n} x_i^2 = 1. \tag{23}$$

Furthermore the unit vector $\hat{x}$ which gives this maximum is the corresponding eigenvector†. Equation (22) can be rewritten in the identical form

$$A(x, x) = -\tfrac{1}{2}\sum_{i,j=1}^{n} a_{ij}(x_i - x_j)^2 + \tfrac{1}{2}\sum_{i,j=1}^{n} a_{ij}(x_i^2 + x_j^2). \tag{24}$$

It follows directly from equation (21) together with the fact that $a_{ij} = a_{ji}$ that the last sum in this equation is zero whence we have

$$A(x, x) = -\tfrac{1}{2}\sum_{i,j=1}^{n} a_{ij}(x_i - x_j)^2 = -\sum_{i>j} a_{ij}(x_i - x_j)^2. \tag{25}$$

Hence from equation (20) we have the result

$$A(x, x) \leqslant 0. \tag{26}$$

If $x_i = x_j$ for all i, j, we have that $A(x, x) = 0$ which by equation (26) is the maximum value of $A(x, x)$. By the normalization condition (equation (23)) the vector $x = n^{-1/2}(1, 1, \ldots, 1)$ is the eigenfunction corresponding to the eigenvalue zero. Note however that this eigenfunction is not necessarily the only eigenfunction corresponding to eigenvalue zero since depending upon what the a_{ij} are, this eigenvalue zero may be degenerate.

The matrix $\langle\phi|\tilde{\mathscr{P}}|\phi'\rangle$ satisfies all the requirements of this theorem whence we conclude that its largest eigenvalue is zero and one possible state associated with this eigenvalue is proportional to $\Sigma_{\phi\in S(Q,M)}|\phi\rangle$.

Let $|Q, M, \psi_i\rangle$ denote the eigenstates of $\tilde{\mathscr{P}}$ in the Q, M subspace associated with the eigenvalue $\lambda_{\psi_i} \leqslant 0$. Here i takes on the values $1, 2, \ldots, |S(Q, M)|$ where $|S(Q, M)|$ is the number of elements in the set $S(Q, M)$. In particular

$$|Q, M, \psi_1\rangle \equiv |S(Q, M)|^{-1/2} \sum_{\phi\in S(Q,M)} |\phi\rangle \tag{27}$$

denotes the eigenfunction corresponding to the maximum eigenvalue $\lambda_{\psi_1} = 0$. In other words we have

$$\left(\sum_{i=1}^{N} S_{iz}\right)|Q, M, \psi_i\rangle = M|Q, M, \psi_i\rangle \tag{28}$$

$$\left(\sum_{i=1}^{N} S_{iz}^2\right)|Q, M, \psi_i\rangle = Q|Q, M, \psi_i\rangle \tag{29}$$

$$\tilde{\mathscr{P}}|Q, M, \psi_i\rangle = \lambda_{\psi_i}|Q, M, \psi_i\rangle. \tag{30}$$

Hence $|Q, M, \psi_i\rangle$ is an eigenstate of $\mathscr{H}$ with eigenvalue

$$E(Q, M, \psi_i\rangle = -\lambda_{\psi_i} - g\mu_B HM + DQ. \tag{31}$$

In particular we have

$$E(Q, M, \psi_1) = -g\mu_B HM + DQ \tag{32}$$

and

$$E(Q, M, \psi_i) \geqslant E(Q, M, \psi_1). \tag{33}$$

† For a proof of this statement see for example Courant R and Hilbert D 1953 *Methods of Mathematical Physics* vol 1 (New York and London: Interscience) pp 23–7.

Thus far our results have been valid for general S. Let us now for concreteness restrict our attention to the case $S = 1$ (where $P_{ij} = -1+\boldsymbol{S}_i.\boldsymbol{S}_j+(\boldsymbol{S}_i.\boldsymbol{S}_j)^2$). The number of elements in the set $S(Q, M)$ is then just

$$|S(Q, M)| = \binom{N}{Q}\binom{Q}{\frac{1}{2}(Q+M)}. \tag{34}$$

Q can take the values $0, 1, 2, \ldots, N$ and M the values $-Q, -Q+2, \ldots, Q-2, Q$ for fixed Q. Alternatively M can take the values $-N, \ldots, N$ and Q the values $|M|$, $|M|+2, \ldots, N$ or $N-1$ for fixed M. In terms of the $|\phi\rangle = |\{m_i\}\rangle$ notation we have

$$\begin{aligned}
|0, 0, \psi_1\rangle &= |0, 0, 0, \ldots, 0\rangle \\
|N, N, \psi_1\rangle &= |1, 1, 1, \ldots, 1\rangle \\
|N, -N, \psi_1\rangle &= |-1, -1, -1, \ldots, -1\rangle \\
|1, 1, \psi_1\rangle &= N^{-1/2}(|1, 0, 0, \ldots, 0\rangle+|0, 1, 0, \ldots, 0\rangle+|0, 0, 1, 0, \ldots, 0\rangle \\
&\quad +\ldots+|0, 0, 0, \ldots, 0, 1\rangle)
\end{aligned} \tag{35}$$

and so on. For this case we have

$$\begin{aligned}
E(0, 0, \psi_1) &= 0 \\
E(N, N, \psi_1) &= (D-g\mu_B H)N
\end{aligned} \tag{36}$$

and so on. It then follows from equations (32) and (33) that

$$E(Q, M, \psi_i) \geqslant E(Q, M, \psi_1) = -g\mu_B HM+DQ. \tag{37}$$

The equality may hold for several ψ_i other than $i = 1$ due to the possible degeneracy of the eigenvalue zero of $\tilde{\mathscr{P}}$. Let us consider equation (37) for the following situations.

(i) $D > g\mu_B H > 0$. Then

$$E(Q, M, \psi_i) \geqslant -g\mu_B HM+DQ = (-g\mu_B H+D)Q+g\mu_B H(Q-M) \geqslant Q(D-g\mu_B H) \geqslant 0. \tag{38}$$

Hence

$$E(Q, M, \psi_i) \geqslant E(0, 0, \psi_1) = 0 \tag{39}$$

with equality holding only when $|Q, M, \psi_i\rangle = |0, 0, \psi_1\rangle$ and there is no degeneracy in the ground state.

(ii) $g\mu_B H > 0, D < g\mu_B H$. Then

$$\begin{aligned}
E(Q, M, \psi_i) &\geqslant -g\mu_B HM+DQ \\
&\geqslant DQ-g\mu_B HQ = Q(D-g\mu_B H) \\
&\geqslant -(g\mu_B H-D)N = E(N, N, \psi_1).
\end{aligned} \tag{40}$$

Therefore

$$E(Q, M, \psi_i) \geqslant E(N, N, \psi_1) = (D-g\mu_B H)N \tag{41}$$

with equality holding only when $|Q, M, \psi_i\rangle = |N, N, \psi_1\rangle$ and there is no degeneracy in the ground state.

(iii) If $H < 0$, similar arguments lead to the unique ground state $|0, 0, \psi_1\rangle$ for $D > g\mu_B|H|$ and $|N, -N, \psi_1\rangle$ for $D < g\mu_B|H|$.

4. Conclusion

When $T = 0$ the free energy per particle, f, is equal to the ground state energy per particle. In this case the magnetization m and quadrupolar order parameter x become

$$m \equiv \frac{1}{N}\left\langle \sum_i S_{iz} \right\rangle = \left\langle 0 \left| \frac{1}{N} \sum_i S_{iz} \right| 0 \right\rangle \tag{42}$$

and

$$x \equiv \frac{1}{N}\left\langle \sum_i S_{iz}^2 \right\rangle = \left\langle 0 \left| \frac{1}{N} \sum_i S_{iz}^2 \right| 0 \right\rangle \tag{43}$$

where the symbol $|0\rangle$ means we consider the non-degenerate ground state. Hence for $S = 1$ we have from the results of the previous section that:

(i) $D > g\mu_B|H|$

$$f = 0, \qquad m = x = 0 \tag{44}$$

since the ground state is just $|0, 0, \ldots, 0\rangle$.

(ii) $D < g\mu_B|H|$

$$f = -N(g\mu_B|H| - D), \qquad m = \frac{H}{|H|}, \qquad x = 1 \tag{45}$$

since the ground state is $|1, 1, \ldots, 1\rangle$ for $H > 0$ and $|-1, -1, \ldots, -1\rangle$ for $H < 0$. If $D = g\mu_B|H|$ there is a possible degeneracy in the ground state, so that no simple result holds for the values of x and m. However, for this situation it follows directly that $x = |m|$ since $E(Q, M, \psi_i) \geqslant 0$ with equality holding only when $Q = M$ for $H > 0$, $Q = -M$ for $H < 0$.

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