Exact results for a spin-1 lattice

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Abstract
We consider a lattice of spin-1 particles with a general pairwise interaction
$[(\cos \gamma)(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1}) + (\sin \gamma)(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1})^2]$. We show that, for a large class of lattices
with even numbers of sites, the ground state for the region $-\frac{3\pi}{4} < \gamma < -\frac{\pi}{2}$ has
total spin $S_{\text{tot}} = 0$, whereas the state of minimum excited energy but with finite
S_{tot} has $S_{\text{tot}} = 2$. These results are contrasted with the generalized Marshall
theorems, applicable to a bipartite lattice and for $-\frac{\pi}{2} < \gamma \leqslant 0$.

1. Introduction

In this paper, we consider a lattice consisting of $\mathcal{N}$ spins $S = 1$, interacting with each
other through a pairwise interaction. As an example, we consider the Hamiltonian for a
one-dimensional spin-1 chain with nearest-neighbour interaction:

$$\mathcal{H} = \sum_l [J(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1}) + K(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1})^2] \tag{1}$$

$$\equiv \sqrt{J^2 + K^2} \sum_l [(\cos \gamma)(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1}) + (\sin \gamma)(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1})^2] \tag{2}$$

where the sum is over the site labels l and the second relation defines γ. This Hamiltonian
has been of intense interest in theoretical studies of quantum magnetism [1–4]. Here we shall
demonstrate some exact properties of the ground states for this type of Hamiltonian. For
definiteness, we shall confine ourselves to the Hamiltonian (1) (or its slight generalization (3)
below) with $\mathcal{N}$ being even and finite unless otherwise stated. We shall be particularly interested
in the region $K < J < 0$, i.e., $-\frac{3\pi}{4} < \gamma < -\frac{\pi}{2}$.

In a recent paper [5], we have pointed out that this region of γ is relevant to spin-1
bosons trapped in an (optical) lattice in the regime of one particle, one orbital state per site, for
suitable interactions between the bosons. To see this, we generalize the standard derivation
of the Heisenberg (exchange) Hamiltonian from the Hubbard model [6] to spin 1. Let the
hopping between sites be t and the (repulsive) interaction for two particles on the same site
be U_0 (>0) if their total spin is 0, and U_2 (>0) if their total spin is 2. (Note that they
cannot have total spin 1 since we have identical bosons and there is only one orbital per site.)

Consider now two neighbouring sites (say 1 and 2) with one boson each. At $t = 0$ the states corresponding to different spin configurations are degenerate. For finite but small t we can perform perturbation to second order. The energies of the system can be classified according to the total spin S_{tot} for the two sites, and can be easily seen to be $-4t^2/U_0$, 0, and $-4t^2/U_2$ for total spin $S = 0, 1, 2$ respectively. Comparing these values with those of the general form of the spin Hamiltonian $\epsilon_0 + J(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2) + K(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2)^2$ for these two sites, and noting that $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 = -2, -1, 1$ for $S_{\text{tot}} = 0, 1, 2$ respectively, we find $J = -\frac{2t^2}{U_2}$, $K = -\frac{2}{3}\frac{t^2}{U_2} - \frac{4}{3}\frac{t^2}{U_0}$, and $\epsilon_0 = J - K$. Thus $K < J < 0$ if $0 < U_0 < U_2$. (ϵ_0 represents an energy shift independent of the spin configurations and can thus be dropped from our discussion.) The case $0 < U_0 < U_2$ is applicable to ^{23}Na atoms [7].

Our major results are collected as *theorems* and *corollaries* in section 2. In particular, we shall show that the ground state for the Hamiltonian (1) has zero total spin $S_{\text{tot}} = 0$. We also show that the excitation of lowest energy but with finite spin has $S_{\text{tot}} = 2$. Generalizations of our results to lattices other than one-dimensional chains are also possible. Some of them are mentioned in section 2.2.

For comparison, we shall, in section 3, discuss the case where $J < K < 0$ ($-\pi < \gamma < -\frac{3\pi}{4}$). This case applies to spin-1 bosons in a lattice if the interaction among bosons is 'ferromagnetic' ($U_2 < U_0$), as would be the case for ^{87}Rb atoms trapped in an optical lattice [5]. It is worth remarking here that spin-polarized ^{87}Rb in an optical lattice in the (Mott) regime of one particle per site has already been obtained in a recent experiment [8].

Our work generalizes the corresponding results for the Heisenberg ($J \neq 0$, $K = 0$) Hamiltonian. For a bipartite lattice and $J > 0$ (the antiferromagnetic Heisenberg model), the results are usually referred to as the Marshall theorems [6]. The proofs here follow similar ideas, but the details are very different (in particular, our results here do not rely on a bipartite lattice). Section 4 below contains a comparison between the two cases. The main results are summarized in section 5.

2. The region $K < J < 0$

To simplify the presentation we shall first consider a linear spin chain (section 2.1). Then we shall discuss more general lattice types (section 2.2).

2.1. Linear spin chain

We shall consider, for definiteness, a generalized form of equation (1):

$$\hat{H} = \sum_l (1 - (-1)^l \delta)[J(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1}) + K(\boldsymbol{S}_l \cdot \boldsymbol{S}_{l+1})^2] \tag{3}$$

where $0 \leqslant \delta \leqslant 1$, i.e., with bond alternation (in strength but not in sign of the interaction). This is shown schematically in figure 1. For convenience we shall also define $\epsilon = 1 - \delta \geqslant 0$. ϵ is thus proportional to the strength of the weaker bonds. For $\delta = 0$ ($\epsilon = 1$), Hamiltonian (3) reduces to that of (1). For $\delta = 1$ ($\epsilon = 0$), the Hamiltonian can be solved trivially since we have a collection of spin pairs with no interaction among different pairs, a fact that we shall take advantage of.

We shall use the 'Ising configurations' as our basis set. Each of these configurations is defined by specifying the spin projection along the $\hat{z}$-direction for every site. Denoting the state at a site by $|+\rangle$, $|0\rangle$, $|-\rangle$ according as $S_z = 1, 0, -1$, a typical Ising configuration, which will be represented by $|\alpha\rangle$, is, e.g., $|+ - 0 + - - 00 \cdots\rangle$ etc. We shall express any many-body
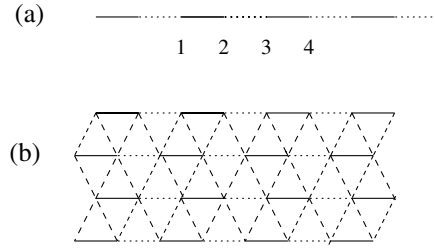
(a)

1 2 3 4

(b)

Figure 1. (a) A schematic representation of the spin-1 chain with Hamiltonian (3). Thick (dotted) lines represent stronger (weaker) bonds, with strengths proportional to $1+\delta$ $(1-\delta)$. (b) A schematic representation of a hexagonal spin-1 lattice.

state $|\Psi\rangle$ as a linear combination of these basis states, i.e.

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle \tag{4}$$

where the sum is over all $|\alpha\rangle$. We shall also introduce the rotated basis, defined by, for *all* sites,

$$\begin{aligned}
|+\rangle' &= |+\rangle \\
|-\rangle' &= |-\rangle \\
|0\rangle' &= i|0\rangle
\end{aligned} \tag{5}$$

and also use the expansion

$$|\Psi\rangle = \sum_{\alpha'} c_{\alpha'}|\alpha\rangle'. \tag{6}$$

The factor i in equation (5) should not alarm us. Since the z-component of the total spin $M \equiv S_{\text{tot},z}$ is conserved under $\mathcal{H}$, for each given M, the number of sites l with $S_{z,l} = 0$ in the expansions (4) or (6) must be either even or odd for all α (for given M, the number of these sites can be only changed by replacing $+-$ pairs (not necessarily nearest neighbours) by 00, or vice versa).

Theorem 1. *For the lowest energy state of $\mathcal{H}$ of a given M, the coefficients $c_{\alpha'}$ are non-negative for all $|\alpha\rangle'$ (apart from an overall common phase factor, a caveat that we shall not repeat).*

Proof. The basic idea of the proof is similar to that of the Marshall theorem [6]. One regards the Schrödinger equation $\mathcal{H}|\Psi\rangle = E|\Psi\rangle$ as the corresponding one for a tight-binding (hopping) Hamiltonian with the lattice points labelled by $|\alpha\rangle$ $(|\alpha\rangle')$. Consider the general term in the Hamiltonian connecting sites l and $l + 1$:

$$H_{l,l+1} = (1 \pm \delta)[J(\mathbf{S}_l \cdot \mathbf{S}_{l+1}) + K(\mathbf{S}_l \cdot \mathbf{S}_{l+1})^2].$$

This term affects only the spins l and $l + 1$. When $H_{l,l+1}$ operates on an Ising configuration $|\alpha\rangle$, spin configurations for $l' \neq l, l + 1$ are unchanged. For simplicity, we shall suppress the configurations for all these l'. For the spin configurations of l and $l + 1$, $H_{l,l+1}$ only leads to 'hopping' among $|+-\rangle$, $|00\rangle$, $|-+\rangle$; between $|+0\rangle$ and $|0+\rangle$; and between $|-0\rangle$ and $|0-\rangle$. In the former subspace ($|+-\rangle$, $|00\rangle$, $|-+\rangle$), the matrix elements of $H_{l,l+1}$ are given by

$$(1 \pm \delta) \begin{pmatrix} -J + 2K & J - K & K \\ J - K & 2K & J - K \\ K & J - K & -J + 2K \end{pmatrix}. \tag{7}$$

In the latter subspace ($|+0\rangle$ and $|0+\rangle$), they are

$$(1 \pm \delta) \begin{pmatrix} K & J \\ J & K \end{pmatrix} \tag{8}$$

with identical matrix elements for the third subspace ($|-0\rangle$ and $|0-\rangle$). $H_{l,l+1}$ is diagonal in $|++\rangle$ and $|--\rangle$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

In the rotated basis, the matrix (7) transforms to

$$(1 \pm \delta) \begin{pmatrix} -J + 2K & -(J - K) & K \\ -(J - K) & 2K & -(J - K) \\ K & -(J - K) & -J + 2K \end{pmatrix} \tag{9}$$

while the matrix (8) is unchanged. In our γ-region of interest, $J - K > 0$, $K < 0$, $J < 0$; hence all hopping (off-diagonal) matrix elements are $\leqslant 0$. It follows that the lowest energy state must have $c'_\alpha \geqslant 0$ for all $|\alpha\rangle'$.

Corollary 1. *If $\delta \neq 1$, the lowest energy state for given M has $c_{\alpha'} > 0$ for all α'. It also follows that this state is unique for given M.*

Proof. If $\delta \neq 1$ ($\epsilon > 0$), all hopping matrix elements are negative (non-zero). As in the case of the Heisenberg Hamiltonian [6], all Ising configurations are connected by (albeit multiple) hopping. By the same reasoning as in [6], the lowest energy state must have all coefficients c'_α non-zero; and moreover there can be only one such state. $\qquad\qquad\qquad\qquad\qquad\qquad\square$

Remarks. For $\delta = 1$ ($\epsilon = 0$) the system becomes a collection of spin pairs, with no interaction among pairs. For one pair, the energies E_S only depend on the total spin S and are given by

$$\begin{aligned} E_0 &= 2[-2J + 4K] \\ E_1 &= 2[-J + K] \\ E_2 &= 2[J + K]. \end{aligned} \tag{10}$$

For $K < J < 0$, $E_0 < E_2 < E_1$. The minimum energy state is given by: for $M = 0$, $\frac{1}{\sqrt{3}}[|+-\rangle + |-+\rangle - |00\rangle] = \frac{1}{\sqrt{3}}[|+-\rangle' + |-+\rangle' + |00\rangle']$; for $M = 1$, $\frac{1}{\sqrt{2}}[|+0\rangle + |0+\rangle] = -\frac{i}{\sqrt{2}}[|+0\rangle' + |0+\rangle']$; and for $M = 2$, $|++\rangle = |++\rangle'$. The first state has $S = 0$ and the latter two both have $S = 2$. These states obviously obey the sign rules stated in theorem 1.

For $\mathcal{N} = 2N$ spins, the ground state has $S_{\text{tot}} = M = 0$ and is a collection of singlet pairs. For $M = 1$ (2), the lowest energy states have one pair of spins in the $S = 2$, $S_z = 1$ (2) state with the rest in the singlet states. These states are not unique due to the freedom of choice of which pair is the $S = 2$ pair.

Theorem 2. *For a given M, the lowest energy state for $0 \leqslant \delta \leqslant 1$ has the same S_{tot} independently of δ.*

Proof. For any given $\delta \neq 1$ we have already seen that the minimum energy state has $c_{\alpha'}(\delta) > 0$ for *all* Ising configurations α'. For $\delta = 1$, we have $c_{\alpha'}(1) \geqslant 0$. Their overlap, given by $\sum_{\alpha'} c_{\alpha'}(1) c_{\alpha'}(\delta)$, is non-vanishing. Hence they must have the same S_{tot}. $\qquad\qquad\square$

From the *remarks* following *corollary* 1, it follows that, for our region of γ:

(i) The lowest energy state in the $M = 0$ sector has $S_{\text{tot}} = 0$.
(ii) The lowest energy state in the $M = 1$ sector and the lowest energy state in the $M = 2$ sector both have $S_{\text{tot}} = 2$.

Since the M-sector contains states with $S_{\text{tot}} \geqslant M$, we have:

Corollary 2. *(a) The ground state for our region ($K < J < 0$) has $S_{\text{tot}} = 0$.*
(b) The spin excitation ($S \neq 0$) with the smallest excited energy has $S_{\text{tot}} = 2$.
(c) Any state with $S_{\text{tot}} = 1$ has energy higher than the state mentioned in (b) if $\delta \neq 1$ ($\epsilon > 0$).

The lines of reasoning above can also applied to deduce some properties concerning states of large S_{tot}. The sector $M = 2N - 1$ has one state with $S_{\text{tot}} = 2N$ and one with $S_{\text{tot}} = 2N - 1$. The former state can be written down trivially and has $c_{\alpha'} \geqslant 0$. Hence we conclude that $E_{2N} \leqslant E_{2N-1}$, and this latter expression becomes a strict inequality if $\epsilon \neq 0$.

For odd $\mathcal{N}$, considerations similar to the above show that the ground state has $S_{\text{tot}} = 1$.

The conclusions in this corollary agree with known numerical results (e.g. [3]).

2.2. Other lattice types

As may already have been obvious, our *theorems* and *proofs* in the last subsection can be generalized to other lattice types. Moreover, these lattices need not be bipartite. A particularly interesting case is that shown in figure 1(b). Here we are again considering a spin-1 lattice with pairwise interactions $J(S_1 \cdot S_2) + K(S_1 \cdot S_2)^2$ with the strengths of the bonds proportional to, for full lines, 1, for dashed lines, ϵ_1, and, for dotted lines, ϵ_2. ($\epsilon_1, \epsilon_2 \geqslant 0$ but not necessarily equal.) The case where all bond strengths are equal is contained in $\epsilon_1 = \epsilon_2 = 1$. The arguments leading to *theorem* 1 and *corollary* 1 go through unchanged. If $\epsilon_1 = \epsilon_2 = 0$, the system again reduces to the collection of pairs, and the *remarks* subsection following *corollary* 1 applies. By comparing the system of interest (with ϵ_1, ϵ_2 both finite) with that with $\epsilon_1 = \epsilon_2 = 0$, we can again prove *theorem* 2 and *corollary* 2 as before. It is worth mentioning that a triangular optical lattice can also be formed by three suitable laser beams propagating at angles $\pi/3$ with respect to each other; thus the discussion here is applicable also to a physical system.

3. The region $J < K < 0$

Arguments similar to the above can easily be generalized to the region $J < K < 0$ ($-\pi < \gamma < -\frac{3\pi}{4}$) for Hamiltonian (3). In this case with $0 \leqslant \delta < 1$, all hopping matrix elements are negative in the original (unprimed) basis, and thus the ground state for each M-sector has $c_\alpha > 0$. This result is in agreement with the common wisdom expressed in the literature (e.g., [4]) that the ground state here has $S_{\text{tot}} = 2N$. These states, obtainable from $|{+}{+}{+}{+}\cdots\rangle$ by suitable number of lowering operators, indeed has $c_\alpha > 0$ for all $|\alpha\rangle$.

4. Comparison with Marshall theorems

For the antiferromagnetic Heisenberg ($J > 0$, $K = 0$) model *on a bipartite lattice*, the Marshall theorems hold. The basis employed in these theorems is defined by, for the A sublattice,

$$
\begin{aligned}
|{+}\rangle_\mathcal{M} &= |{+}\rangle \\
|0\rangle_\mathcal{M} &= |0\rangle \\
|{-}\rangle_\mathcal{M} &= |{-}\rangle
\end{aligned}
\tag{11}
$$

and, for the B sublattice,

$$
\begin{aligned}
|{+}\rangle_\mathcal{M} &= -|{+}\rangle \\
|0\rangle_\mathcal{M} &= |0\rangle \\
|{-}\rangle_\mathcal{M} &= -|{-}\rangle.
\end{aligned}
\tag{12}
$$

For our more general Hamiltonian (3), the matrix elements of $H_{l,l+1}$ in this basis is given also by (9) for the $|+-\rangle$, $|00\rangle$, $|-+\rangle$ subspace while that for $|+0\rangle$ and $|0+\rangle$ (or $|-0\rangle$ and $|0-\rangle$) becomes

$$(1 \pm \delta) \begin{pmatrix} K & -J \\ -J & K \end{pmatrix}. \tag{13}$$

Thus, for $J > 0$, $K < 0$ ($J - K > 0$ trivially), all 'hopping' elements are negative. Thus the Marshall theorems can be generalized to the region $-\frac{\pi}{2} < \gamma < 0$ with the results (arguing as in [6] or as in section 2; note that in this region, for a system with two spins, one has $E_0 < E_1 < E_2$):

(a$\mathcal{M}$) The ground state of (3) has $S_{\text{tot}} = 0$ and is unique (if $\delta \neq 1$).

(b$\mathcal{M}$) The spin excitation with lowest energy has $S_{\text{tot}} = 1$.

(c$\mathcal{M}$) Any state with $S_{\text{tot}} = 2$ has energy higher than that of the state mentioned in (b$\mathcal{M}$) if $\epsilon > 0$.

For $\gamma = -\frac{\pi}{2}$, some hopping matrix elements vanish ($J = 0$). There are in general degeneracies for the minimum energy states for a given M. This fact can also be seen from the work of Parkinson [2].

5. Concluding remarks

We have proven some exact properties of lowest energy states for Hamiltonian of the type (3) with $K < J < 0$. We demonstrated that, for a large class of lattices (not necessarily bipartite) with even numbers of sites, the ground state has total spin $S_{\text{tot}} = 0$, whereas the state of minimum excited energy but with finite S_{tot} has $S_{\text{tot}} = 2$. The results derived here are relevant to spin-1 bosons trapped in an optical lattice in the regime of one particle per site for suitable interaction between the bosons.

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