The band structure of two-magnon excitations for a finite 2D lattice

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Abstract. The energy bound structure and the distribution of the states over the first Brillouin zone of two-magnon excitations for finite spin systems has been investigated. It was shown that the energy spectrum of the eigenstates could be arranged into rarefied bands determined by the symmetry types of the spin configurations. It was demonstrated that the elaborated classification of eigenstates is equivalent to splitting of the first Brillouin zone into sub-zones depending on the parity of vector $k$, exactly in the same way as was obtained within a continuum model approach.

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1. Introduction

The magnetic properties of low-dimensional ferromagnetic and antiferromagnetic quantum spin systems have been a subject of many theoretical studies in recent years. These studies are motivated by the recent progress in nanotechnology devices involving spin degrees of freedom [1]. In this article, we shall investigate the two-dimensional Heisenberg ferromagnetic with the nearest-neighbor exchange interaction and with periodic boundary conditions, defined by the Hamiltonian [2]

$$ H = - \sum_{p,q \in \tilde{N}} J_{pq} \left[ \frac{1}{2} \left( S_p^+ S_q^- + S_p^- S_q^+ \right) + S_p^z S_q^z \right] $$

where $\tilde{N}$ is the set of lattice nodes, $J_{pq} = J_0 > 0$ for nearest neighbors, and $J_{pq} = 0$ otherwise.

We shall only consider the two-magnon excitations over the ground state of the model in the form

$$ |\psi\rangle = \sum_{p,q \in \tilde{N}} c_{pq} S_p^- S_q^- |0\rangle $$

where $|0\rangle$ is the ferromagnetic ground state with all spins aligned up. The symmetry of the Hamiltonian guarantees that the number of spin deviations is preserved under the action of the Hamiltonian (1). This enables us to restrict the problem of diagonalization of the Hamiltonian to the subspace spanned by configurations with a fixed number of spin deviations. The set of all possible configurations

$$ |p, q\rangle = S_p^- S_q^- |0\rangle $$

forms a basis in the magnetic configuration space $\Omega$. The dimension of the spaces is given by the formula

$$ \dim \Omega = \frac{(N - 1)N}{2}, $$
First, we analyze the action of the translation group in the configuration space and arrange the orbits to the actually obtained configurations (members of the orbits). For the “border” orbits where $|O| \neq 2$, the configuration space $\mathcal{O}$ is invariant under some nontrivial translations then the orbit is irregular and contains $N/|T|$ elements, where $|O| \neq 2$.

### Table 1. Orbit classes and their stability groups $T_r$

| $r$         | $T_r$       | $|O_r|$ |
|-------------|-------------|--------|
| $(0, \frac{N}{2})$ | $\{t(0,0), t(0, \frac{N}{2})\}$ | $\frac{N}{2}$ |
| $(\frac{N}{2}, 0)$ | $\{t(0,0), t(\frac{N}{2}, 0)\}$ | $\frac{N}{2}$ |
| $(\frac{N}{2}, \frac{N}{2})$ | $\{t(0,0), t(\frac{N}{2}, \frac{N}{2})\}$ | $\frac{N}{2}$ |
| other       | $\{t(0,0)\}$ | $N$    |

where $N = |\mathcal{N}| = L^2$ is the number of nodes of the square $L \times L$ lattice. It is easy to notice that when $N$ is even, the dimension of the space is not divisible by the number of points in the first Brillouin zone. It means that the distribution of the eigenstates of the Hamiltonian (1) over the Brillouin zone could not be uniform. The main task of this work is to investigate the distribution of the eigenstates over the Brillouin zone. We carry out this analysis in two stages. First, we analyze the action of the translation group in the configuration space and arrange the configurations into orbits. Next, we introduce symmetry adopted basis and carry out numerical calculations for all invariant subspaces.

### 2. The configuration space

Let $|p, q\rangle$ defined by (2) be a magnetic configuration with two spin deviations at nodes $p, q \in \mathcal{N}$, where $p \neq q$ and $|p, q\rangle = |q, p\rangle$. The translational symmetry of Hamiltonian (1) enables us to introduce the symmetry adopted basis in the space $\Omega$. In order to construct such a basis for all representations $\Gamma_k$ of the translation group $T$, it is convenient to split the configurations into orbits $O_r$ of the action of the translation group

$$O_r = \{\hat{t} |0, r\rangle, \hat{t} \in T\}$$  \hspace{1cm} (3)

where $|0, r\rangle$ is a configuration with spin deviations at nodes $(0,0)$ and $(r_x, r_y)$ respectively, chosen to be the representative configuration of the orbit $O_r$. All other configurations of the orbit are obtained by translation $\hat{t}$ of the representative configuration $|0, r\rangle$. If a configuration $|0, r\rangle$ is invariant under some nontrivial translations then the orbit is irregular and contains $N/|T|$ elements, where $T_r \subset T$ is the stability group of the configuration. For the case of two spin deviations we get four orbit classes characterized by the stability group as shown in Table 1. The set of all orbits and their representatives is presented in picture 1. The result of the action of the Hamiltonian (1) on configuration $|p, q\rangle$ can be written in the form

$$H|0, r\rangle = \frac{1}{2} \left( \hat{t}_{-01}|0, r_{-01}\rangle + \hat{t}_{01}|0, r_{01}\rangle + \hat{t}_{-10}|0, r_{-10}\rangle + \hat{t}_{10}|0, r_{10}\rangle \right) + \varepsilon|0, r\rangle,$$  \hspace{1cm} (4)

where $|0, r_d\rangle$ are representatives of orbits which are nearest-neighbors in the schematic graph 2, obtained from the diagram in picture 1 by join the points according to the action of the Hamiltonian. The translations $\hat{t}_q$ are some translations that transform the representatives of orbits to the actually obtained configurations (members of the orbits). For the “border” orbits in diagram 1 only some terms of (4) do occur.

### 3. The distribution of eigenstates over the Brillouin zone

For each orbit (3) we can build a basis vector $|k, r\rangle$ that transforms according to the irreducible representation $k$ of the translation group.

$$|k, r\rangle = c \sum_{\hat{t} \in T} \exp(i\mathbf{k} \cdot \mathbf{t}) \hat{t} |0, r\rangle$$  \hspace{1cm} (5)
Figure 1. The representatives of orbits (the three distinguished ones correspond to irregular orbits).

Figure 2. The graph generated by the action of the Hamiltonian in the orbit space.

| $k_x$ | $k_y$ |
|------|------|
| odd  | odd  |
| odd  | even |
| even | odd  |
| even | even |

Table 2. The classification of $k$ vectors

All vectors (5) for fixed $k$ span a subspace $\Omega_k$, which is invariant under the action of the Hamiltonian $H$. The dimension of the subspace $\Omega_k$ depends on $k$ because for some $k$, vectors (5) spanned on irregular orbits collapse to zero, which is the case if the representation $\Gamma_k$ of $T$ restricted to the stability subgroup $T_r$ gives the antisymmetric representation $1, -1$. Taking into account all four possible stability groups presented in table 1 we get four different types of subspaces $\Omega_k$ depending on the parity of components $k_x$ and $k_y$ of the vector $k = (k_x, k_y)$ (see table 2). Such classification of representations leads to splitting of the first Brillouin zone into four sub-zones. That classification of states over the first Brillouin zone is in accordance with the classification based on investigating of the inverse symmetry of the continuum model [5, 6, 7]. By direct diagonalization of the Hamiltonian matrix in all subspaces $\Omega_k$ we get the distribution of states over the first Brillouin zone. If we form an energy band by choosing n-th eigenstate for each $k$ and plot the surface determined by the corresponding eigenvalues we get a picture like that shown in picture 3, however if we restrict the choice of surface points only to one of the four sub-zones then we get quite smoothly looking energy band (picture 4). All such bands are rarefied (i.e. do not contain states for all points in Brillouin zone [8, 9, 10]), similarly as in the case of two-magnon excitations for linear chain [3, 4].

4. Concluding remarks
The existence of irregular orbits of the action of the translation group in the configuration space leads to inhomogeneous distribution of the eigenstates over the first Brillouin zone. In the case of two spin deviation we get four different types of the orbits, characterized by their stability group (see table 1). Introducing symmetry adopted basis we notice that for some representations $\Gamma_k$ of the translation group $T$ some basis vectors spanned on irregular orbits decay, what leads to lowering of the dimension of the invariant subspace $\Omega_k$. As a result, we get four different classes of eigenstates characterized by parity of vector $k$ (see table 2). This result coincidence with the classification of states obtained in [5, 6, 7] for the improved continuum approach.
Figure 3. The distribution of energy over the first Brillouin zone for a fixed energy level.

Figure 4. The distribution of the same energy level, restricted to one of the four sub-zones.

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