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Exact eigenstates and macroscopic magnetization jumps in strongly frustrated spin lattices

J Richter^{1,5}, J Schulenburg², A Honecker³, J Schnack⁴ and H-J Schmidt⁴

¹ Institut für Theoretische Physik, Universität Magdeburg, PO Box 4120, D-39016 Magdeburg, Germany

² Universitätsrechenzentrum, Universität Magdeburg, PO Box 4120, D-39016 Magdeburg, Germany

³ Institut für Theoretische Physik, TU Braunschweig, Mendelssohnstr. 3, D-38106 Braunschweig, Germany

⁴ Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, D-49069 Osnabrück, Germany

E-mail: johannes.richter@physik.uni-magdeburg.de

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Abstract

For a class of frustrated spin lattices including for example the 1D sawtooth chain, the 2D Kagomé and checkerboard, as well as the 3D pyrochlore lattices, we construct exact product eigenstates consisting of several independent, localized one-magnon states in a ferromagnetic background. Important geometrical elements of the relevant lattices are triangles being attached to polygons or lines. Then the magnons can be trapped on these polygons/lines. If the concentration of localized magnons is small, they can be distributed randomly over the lattice. On increasing the number of localized magnons, their distribution over the lattice becomes more and more regular, and finally the magnons condense in a crystal-like state.

The physical relevance of these eigenstates emerges in high magnetic fields where they become groundstates of the system. As a result a macroscopic magnetization jump appears in the zero-temperature magnetization curve just below the saturation field. The height of the jump decreases with increasing spin quantum number and vanishes in the classical limit. Thus it is a true macroscopic quantum effect.

1. Introduction

The search for exact eigenstates of quantum spin systems has attracted continuous attention ever since the Heisenberg and related spin models have been studied. Of course we have

⁵ Author to whom any correspondence should be addressed.

the fully polarized ferromagnetic state as a trivial example. Furthermore, the one- and two-magnon states above the fully polarized ferromagnetic state can be calculated exactly (see, for example, [1]). A famous example for a very non-trivial eigenstate is Bethe's solution for the groundstate of the one-dimensional (1D) Heisenberg antiferromagnet (HAFM) [2].

The investigation of strongly frustrated magnetic systems surprisingly led to the discovery of several new exact eigenstates. Whereas in general the treatment of frustrated quantum magnets is even harder than that of unfrustrated systems, in some exceptional cases one finds eigenstates of quite simple nature. The interest in these eigenstates comes from the fact that often they become groundstates either for particular values of frustration or in magnetic fields. Furthermore, the spin correlation functions can be calculated analytically. Therefore these exact eigenstates play an important role either as groundstates of real quantum magnets or at least as reference states of idealized models for more complex quantum spin systems. There are two well known examples for simple eigenstates of strongly frustrated quantum spin systems, namely the Majumdar–Gosh state of the 1D J_1 – J_2 spin 1/2 HAFM [3] and the orthogonal dimer state in the Shastry–Sutherland model [4]. Both eigenstates are products of dimer singlets and become groundstates only for strong frustration. These eigenstates indeed play a role in realistic materials. While the Majumdar–Ghosh state has some relevance in quasi-1D spin–Peierls materials like CuGeO_3 (see, for example, [5]), the orthogonal dimer state of the Shastry–Sutherland model is the magnetic groundstate of the quasi-2D $\text{SrCu}_2(\text{BO}_3)_2$ [6]. Other frustrated spin models in one, two or three dimensions can be constructed, also having dimer singlet product states as groundstates (see, for example, [7–9]).

Less well known is the so-called uniformly distributed resonating valence bond state, which is the groundstate of the J_1 – J_2 chain with ferromagnetic nearest-neighbour (NN) bonds $J_1 < 0$ and frustrating antiferromagnetic next NN bonds $J_2 = -J_1/4$ [10].

Another striking feature of the dimer singlet product groundstates is the existence of magnetization plateaux at zero magnetization. These plateaux in quantum spin systems currently attract a lot of attention from the theoretical as well as experimental side. Recently it has been demonstrated for the 1D counterpart of the Shastry–Sutherland model, the so-called frustrated dimer-plaquette chain (also known as orthogonal dimer chain) [8, 11, 12], that more general product eigenstates containing chain fragments of finite length lead to an infinite series of magnetization plateaux [13].

In this paper we discuss a recently discovered [14] class of quite universal eigenstates of frustrated quantum antiferromagnets which become groundstates in strong magnetic fields and lead to macroscopic jumps in the magnetization curve close to saturation. In what follows we consider in more detail the sawtooth chain and the checkerboard lattice.

2. Localized magnon states

We consider N quantum spins of 'length' s described by the Heisenberg Hamiltonian

$$\hat{H} = \sum_{ij} J_{ij} \{s_i^x s_j^x + s_i^y s_j^y + s_i^z s_j^z\} - h S^z. \quad (1)$$

$S^z = \sum_i s_i^z$ is the z -component of the total spin, h is the magnetic field, and the J_{ij} are the exchange constants.

If the magnetic field h is sufficiently strong ($h \geq h_s$), the groundstate of (1) becomes the fully polarized ferromagnetic state (magnon vacuum state) $|0\rangle = |\uparrow\uparrow\uparrow\dots\rangle$ where all spins assume their maximal s_i^z -quantum number and $M = \langle S_z \rangle = Ns$. The lowest excitations for $h > h_s$ are one-magnon states $|1\rangle$ with $M = Ns - 1$. They can be written as $|1\rangle \sim \frac{1}{c} \sum_i^N a_i s_i^- |0\rangle$, where in general the excitation is distributed over the whole system.

However, for highly frustrated magnets having special bond geometry it turns out that the excitation can be localized over a restricted area L of the system, i.e. we have

$$|1\rangle \rightarrow |1\rangle_L = \frac{1}{c} \sum_{i \in L} a_i s_i^- |0\rangle = |\Psi_L\rangle |\Psi_R\rangle, \quad (2)$$

where $|\Psi_L\rangle$ is the wavefunction of the magnon localized on area L and $|\Psi_R\rangle$ the wavefunction of the fully polarized ferromagnetic remainder R containing all sites not belonging to L . In (2) the constant c is chosen to normalize $|1\rangle_L$. To demonstrate this we split the Hamiltonian into three parts $\hat{H} = \hat{H}_L + \hat{H}_{L-R} + \hat{H}_R$, where \hat{H}_L (\hat{H}_R) contains only spins belonging to the local area L (remainder R) and \hat{H}_{L-R} is the interaction term between L and R . We restrict our consideration to the case that the wavefunction $|\Psi_L\rangle$ is an eigenstate of \hat{H}_L and has lowest one-magnon energy. Of course, the wavefunction $|\Psi_R\rangle$ is an eigenstate of \hat{H}_R . Now we demand that the total wavefunction (2) is an eigenstate of the full Hamiltonian $\hat{H}_L + \hat{H}_{L-R} + \hat{H}_R$. After some manipulation one finds that the exchange couplings in the interaction term \hat{H}_{L-R} have to fulfill two conditions⁶, namely

$$\sum_{l \in L} J_{rl} a_l = 0 \quad \forall r \in R \quad (3)$$

and

$$\sum_{r \in R} J_{rl} = \text{constant} \quad \forall l \in L. \quad (4)$$

The first one comes from the xx and yy terms in \hat{H}_{L-R} and the second one from the zz term (i.e. condition (4) is not relevant for the pure xy model). Equation (3) leads to a condition on the bond geometry, whereas equation (4) is a condition for the bond strengths and is automatically fulfilled in uniform lattices with equivalent sites. Indeed one finds that the above conditions are fulfilled for remarkably many different lattices/models such as the Kagomé and the sawtooth chain, the 2D Kagomé, square-Kagomé or checkerboard lattices, and the 3D pyrochlore lattice, and also for a fractal lattice like the Sierpinski gasket.

In figure 1 we illustrate the localized magnon states on the sawtooth chain with $J_2 = 2J_1$ and on the checkerboard lattice. Both systems currently attract a lot of attention as examples for novel low-energy physics in quantum systems (see, for example, [15, 16]). We show in the figures only the localized magnons of minimum size. On the checkerboard lattice localized magnons can sit on the four sites of an ‘empty’ square and also on the \sqrt{N} sites of a vertical, horizontal or sloping (45°) line. On the sawtooth chain a magnon can sit on the three neighbouring sites forming ‘V’ and also on the $N/2$ sites on the base line.

The next step is to construct eigenstates containing $n > 1$ localized magnons on different localized areas L_α , $\alpha = 1, \dots, n$. If these localized areas are separated from each other one can still fulfill both conditions (3) and (4). This way one can find a whole class of product eigenstates of the form $|\Psi\rangle = |\Psi_{L_1}\rangle |\Psi_{L_2}\rangle \cdots |\Psi_{L_n}\rangle |\Psi_R\rangle$, where the $|\Psi_{L_\alpha}\rangle$ and $|\Psi_R\rangle$ are defined in analogy to (2). The system can be filled with separated magnons as long as the magnons do not interact. The maximum number of localized magnons depends on the lattice geometry. The state with maximum filling corresponds to a ‘magnon crystal’, i.e. to a state with a regular arrangement of magnons (see figure 1). The ‘crystalline’ magnon state of the sawtooth chain (checkerboard lattice) is twofold (fourfold) degenerate and breaks spontaneously the translational symmetry of the lattice. Maximum filling for the checkerboard lattice is reached if magnons sit on every fourth ‘empty’ square and for the sawtooth chain if magnons sit on every second ‘V’. Each

⁶ The second condition is not a necessary one, i.e. one can find models with eigenstates of form (2) violating (4); see [14]. This more general case appears if $|\Psi_L\rangle |\Psi_R\rangle$ is not an individual eigenstate of both \hat{H}_L and \hat{H}_{L-R} but of $(\hat{H}_{L-R} + \hat{H}_L)$.

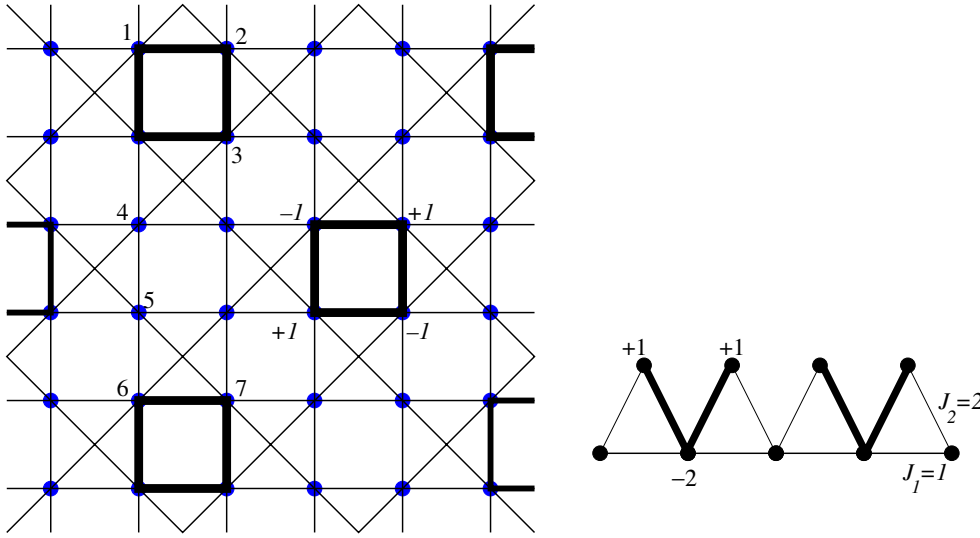


Figure 1. Localized magnon states on the checkerboard lattice and on the sawtooth chain with $J_2 = 2J_1$. The positions of the localized magnons are indicated by extra thick lines. The numbers $+1$, -1 , -2 at the corners represent the coefficients a_i (see equation (2)).

(This figure is in colour only in the electronic version)

localized magnon lowers the magnetic quantum number M of total S_z by one, i.e. one has $M = Ns - n$ for a state with n localized magnons. Hence the corresponding quantum number of the ‘magnon crystal’ is $M = Ns - N/8$ (checkerboard) and $M = Ns - N/4$ (sawtooth).

Due to the simple product form of the eigenstates one can calculate the spin–spin correlation functions explicitly. They depend on the parameters a_i . One has three different types of correlations, namely within R, within L, and between L and R. As an example we give the correlations for the checkerboard lattice with localized magnons on ‘empty’ squares: $\langle \vec{s}_1 \vec{s}_2 \rangle = -1/4$; $\langle s_1^z s_2^z \rangle = 0$; $\langle \vec{s}_1 \vec{s}_3 \rangle = 1/4$; $\langle s_1^z s_3^z \rangle = 0$; $\langle \vec{s}_1 \vec{s}_4 \rangle = \langle s_1^z s_4^z \rangle = 1/8$; $\langle \vec{s}_1 \vec{s}_6 \rangle = \langle s_1^z s_6^z \rangle = \langle \vec{s}_1 \vec{s}_7 \rangle = \langle s_1^z s_7^z \rangle = 1/16$ and $\langle \vec{s}_4 \vec{s}_5 \rangle = \langle s_4^z s_5^z \rangle = 1/4$ (the numbers correspond to those given in figure 1). Other correlation functions can be obtained by symmetry arguments, bearing in mind that there is no real distance dependence of correlations within R and between L and R.

Finally, we mention that the existence of localized magnon states in regular spin lattices is related to the existence of flat bands in the magnon dispersion [14].

3. Macroscopic magnetization jump

The interest in the above-described eigenstates is not only an academic one. One can show rigorously that these eigenstates under certain conditions become groundstates in a magnetic field [17]. This is true for instance in many systems with translational symmetry. We define as magnetization $m = \langle S^z \rangle / Ns = M/M_0$, i.e. m is normalized to unity for the fully polarized ferromagnetic state $|0\rangle$. Since the z component of the total spin commutes with the Hamiltonian, one can calculate the magnetization from the lowest zero-field energies $E(M)$ in each sector of M , i.e. $E(M, h) = E(M) - hM$ and $h(M) = \Delta E / \Delta M$. The eigenstates discussed in section 2 contain localized noninteracting magnons and have therefore well defined energies $E(M = Ns - n) = E_{\text{FM}} - n\varepsilon_1$, where ε_1 is the energy difference between the magnon vacuum

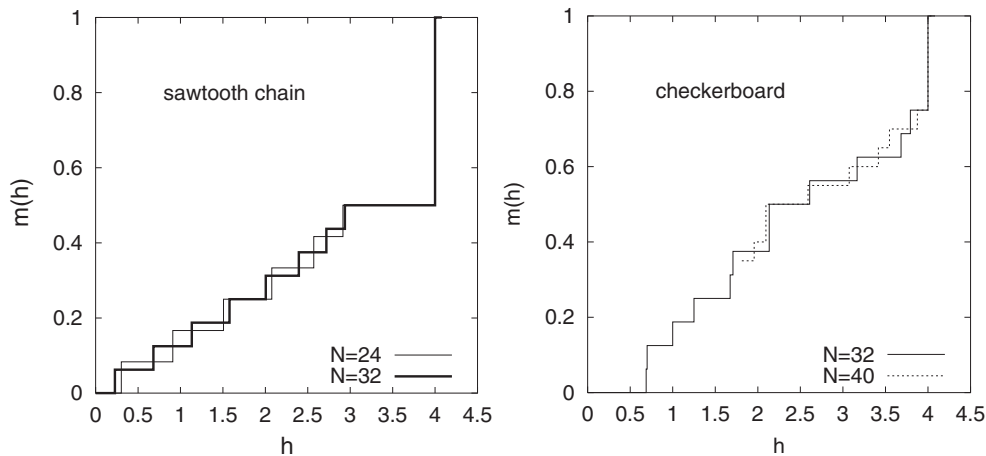


Figure 2. Magnetization m versus magnetic field h of the spin-half Heisenberg antiferromagnet on the sawtooth chain ($J_2 = 2J_1$, cf figure 1) and on the checkerboard lattice. For the finite checkerboard lattice of $N = 40$ only the upper part of the curve was calculated.

and the state with *one* magnon, and n is the number of localized magnons. Hence we have a straight part in the E versus M curve close to saturation leading to a jump in the $m(h)$ curve. The height of the jump Δm is determined by the maximal number n_{\max} of localized magnons in the system and on the spin ‘length’ s , $\Delta m = n_{\max}/Ns$. Obviously the jump is a true quantum effect and vanishes for $s \rightarrow \infty$.

In figure 2 we show magnetization curves for the sawtooth chain and the checkerboard lattice for $s = 1/2$ calculated with exact diagonalization for finite lattices. The height of the jump for the sawtooth chain is $\Delta m = 1/2$, and for the checkerboard lattice $\Delta m = 1/4$. We emphasize that Δm does not depend on the size of the system provided that the periodic boundary conditions of the finite lattice fit to the translational symmetry of the ‘magnon crystal’. For the sawtooth chain we see a well-pronounced plateau preceding the jump. This plateau belongs to the ‘magnon crystal’ state. Though such a plateau is less pronounced for the checkerboard lattice there are general arguments [18] that such a crystalline magnon state should have gapped excitations and may therefore be connected with a magnetization plateau at $m = 1 - \delta m = 1 - n_{\max}/Ns$. We mention that the plateaux fulfill the condition of Oshikawa *et al* [19] derived for plateaux in 1D systems not only for the sawtooth chain but also for the 2D checkerboard lattice.

To our knowledge the jump has not yet been observed experimentally. To see the jump and the preceding plateau in experiments one needs highly frustrated magnets with small spin quantum number s and sufficiently small exchange coupling strength J to reach the saturation field.

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