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Exact eigenstates of highly frustrated spin lattices probed in high fields

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Abstract. Strongly frustrated antiferromagnets such as the magnetic molecule $\{\text{Mo}_{72}\text{Fe}_{30}\}$, the kagome, or the pyrochlore lattice exhibit a variety of fascinating properties like low-lying singlets, magnetization plateaus as well as magnetization jumps. During recent years exact many-body eigenstates could be constructed for several of these spin systems. These states become ground states in high magnetic fields, and they also lead to exotic behavior. A key concept to an understanding of these properties is provided by independent localized magnons. The energy eigenvalue of these n -magnon states scales linearly with the number n of independent magnons and thus with the total magnetic quantum number $M = Ns - n$. In an applied field this results in a giant magnetization jump which constitutes a new macroscopic quantum effect. It will be demonstrated that this behavior is accompanied by a massive degeneracy, an extensive ($T = 0$)-entropy, and thus a large magnetocaloric effect at the saturation field. The connection to flat band ferromagnetism will be outlined.

1. Introduction

Geometric frustration of interacting spin systems is the driving force of a variety of fascinating phenomena in low-dimensional magnetism [1]. In this context the term *frustration* describes a situation where in the ground state of a classical spin system not all interactions can be saturated simultaneously. A typical picture for such a situation is a triangle of antiferromagnetically coupled spins, where classically the spins are not in the typical up-down-up configuration, but assume a ground state that is characterized by a relative angle of 120° between neighboring spins. This special classical ground state characterizes among others several frustrated spin systems which are built of corner-sharing triangles, among them the giant Keplerate molecule $\{\text{Mo}_{72}\text{Fe}_{30}\}$ which is a perfect icosidodecahedron [2] and the kagome lattice antiferromagnet. The pyrochlore lattice, which consists of corner-sharing tetrahedra and thus has a different structure, nevertheless shares several important properties with the above systems.

Research in this field is naturally focused on the low-energy, i.e. low-temperature, low-field behavior. A key observation is that the quantum spin systems possess many or even infinitely many singlet states below the first triplet state and the classical counterpart systems display a non-trivial ground state degeneracy [3]. Another important observation concerns a plateau in

the magnetization curve for $T = 0$, which for the systems made of corner-sharing triangles is at $\mathcal{M} = \mathcal{M}_{\text{sat}}/3$, see e.g. [4, 5], whereas for the pyrochlore it is at $\mathcal{M} = \mathcal{M}_{\text{sat}}/2$, see e.g. [6].

In this article we focus on special properties of these systems which arise at low temperatures but high magnetic fields. We will show that it is possible to construct exact many body states which are product states of independent one-magnon states. These states become ground states in high magnetic fields. In a wider perspective such an arrangement of independent single-particle objects can be understood as condensation of bosons [7, 8, 9]. The linear scaling of the minimal total energy with the number of these objects explains their unusual high-field behavior which is expressed in magnetization jumps [10, 11], non-zero ($T = 0$)-entropy [12, 13], and an enhanced magnetocaloric effect [14, 15].

2. Concept of independent magnons

In the following we assume that the spin systems under consideration are modeled by an isotropic Heisenberg Hamiltonian augmented with a Zeeman term, i.e.,

$$\tilde{H} = - \sum_{u,v} J_{uv} \tilde{\mathbf{s}}(u) \cdot \tilde{\mathbf{s}}(v) + g\mu_B B \tilde{S}_z . \quad (1)$$

$\tilde{\mathbf{s}}(u)$ are the individual spin operators at sites u and \tilde{S}_z is the z -component of the total spin. J_{uv} are the matrix elements of the symmetric coupling matrix. We will consider only antiferromagnetic couplings.

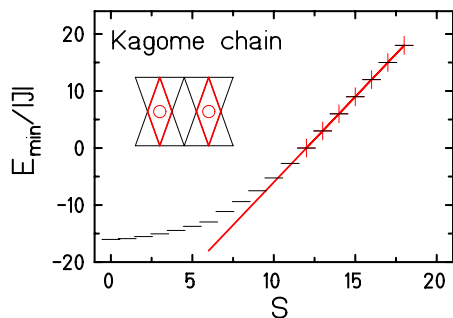


Figure 1. Minimal energies E_{\min} of a kagome chain with $N = 36$ and $s = 1/2$. The highest seven levels fall on a straight line. The highlighted diamonds in the structure are localized magnons.

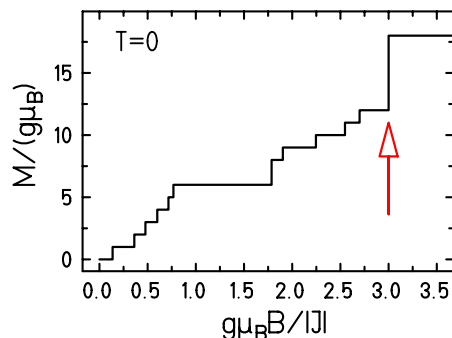


Figure 2. ($T = 0$)-magnetization curve of the kagome chain, Fig. 1 with $N = 36$. The magnetization jump of $\Delta M = 6$ is marked by an arrow.

One of the early unexpected results was that for the icosidodecahedron (e.g. $\{\text{Mo}_{72}\text{Fe}_{30}\}$) the minimal energies E_{\min} in each Hilbert subspace of $\mathcal{H}(M)$ of total magnetic quantum number M scale linearly with M close to the saturation [7]. Figure 1 shows as another example the minimal energy levels of a special kagome chain (introduced in [16]) where the seven highest levels are on a straight line. In an applied magnetic field this leads to a simultaneous crossing of the lowest Zeeman levels at the saturation field, which gives rise to an unusual magnetization jump, that for the kagome chain is shown in Fig. 2.

It turns out that the linear dependence of E_{\min} on M can be understood in terms of localized independent magnons. Figure 3 shows the structure of a localized magnon on a part of a model lattice as realized for instance in the kagome chain of Fig. 1. The one-magnon state is given by

$$\begin{aligned} |\text{localized magnon}\rangle &= \frac{1}{2} (|1\rangle - |2\rangle + |3\rangle - |4\rangle) , \quad \text{where} \quad (2) \\ |1\rangle &= \tilde{s}^-(1) |m_1 = s, m_2 = s, m_3 = s, m_4 = s, m_5 = s, \dots\rangle \quad \text{etc.} \end{aligned}$$

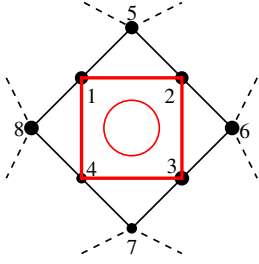


Figure 3. Localized one-magnon state on a model lattice.

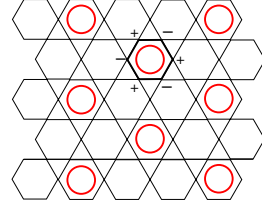


Figure 4. Independent localized magnons on the kagome lattice antiferromagnet. $N/9$ independent localized magnons can be placed on the kagome lattice.

It can be shown that this state is an eigenstate of lowest energy in one-magnon space $\mathcal{H}(M = Ns - 1)$. On an extended lattice such as the kagome chain, Fig. 1, or the two-dimensional kagome lattice, Fig. 4, many of these objects can be placed in such a way that they do not interact [7, 10]. Also in this case it can be shown that these states are eigenstates of lowest energy in their respective n -magnon space.

3. Consequences

An immediate consequence of the independence of the localized one-magnon states and thus of the linear dependence of the minimal energies E_{\min} on M is the magnetization jump at the saturation field B_{sat} as well as the high degeneracy of levels at this field value. In an infinite lattice such as the kagome or pyrochlore lattice both quantities are macroscopic [10, 11, 12, 13], although it turns out that it is rather involved to evaluate the exact degeneracy at the saturation field due to possible relations between the n -magnon product states [17]. The ground-state degeneracy at B_{sat} is related to a finite ($T = 0$) entropy per site, i.e. $S(T = 0)/N > 0$ (for the kagome chain one obtains $S(T = 0)/N \approx 0.1604039$ [12]). In the context of magnetocalorics such a residual entropy gives rise to large adiabatic cooling rates $(\frac{\partial T}{\partial B})_S = -\frac{T}{C} (\frac{\partial S}{\partial B})_T$ in the vicinity of the saturation field [14, 15]. In a real compound, e.g. $\{\text{Mo}_{72}\text{Fe}_{30}\}$, the perfect degeneracy at B_{sat} would be lifted by residual, e.g. dipolar or Dzyaloshinskii-Moriya interactions. Consequently, the magnetization jump would be smeared out, compare Ref. [18] for $\{\text{Mo}_{72}\text{Fe}_{30}\}$. Nevertheless, the low-lying density of states remains large at B_{sat} , which would still be clearly visible in magnetocaloric investigations.

4. Relation to flat bands

It is clear that the energetically degenerate independent localized one-magnon states on translationally symmetric lattices can be superimposed to form eigenstates of the translation operator with the same energy which leads to a flat band. Figure 5 shows the three energy bands of the kagome chain introduced in Fig. 1. We observe that one third of all one-magnon states form independent magnons or equally well belong to the flat band. Therefore a jump of one third of the saturation magnetization occurs at B_{sat} for $s = 1/2$, see Fig. 2.

The emergence of flat bands has been already noted in the context of *line graphs* and *flat-band ferromagnetism*, see e.g. [19, 20, 21, 22, 23, 24, 25]. A connection can be made by replacing the Heisenberg model by a Hubbard model [13]. The roles of the magnetic exchange J and the applied magnetic field are then played by the hopping integral t the chemical potential μ , respectively. If the flat band is the lowest band, then non-interacting localized excitations can be constructed for such fermionic systems in a manner very similar to the Heisenberg model, and these fermionic systems exhibit similar thermodynamic properties, but now as function of temperature and chemical potential. An example is given by Fig. 6 where the isentropes for free

spinless fermions [13] on the kagome chain (Fig. 1) are displayed. At $\mu = 2t > 0$ the ground state is degenerate with an extensive ($T = 0$) entropy $S(T = 0)/N = \ln(2)/3 = 0.231049\dots$. The value $\mu = 2t$ corresponds to the saturation field B_{sat} of the Heisenberg model, and a very similar behavior would be observed in its vicinity, e.g. the slopes of the isentropes correspond to the adiabatic cooling rates [15]. However, at lower values of μ (B) there are qualitative differences: free spinless fermions (whose dispersion is essentially given in Fig. 5) have no band gaps, while the magnetization curve of the $s = 1/2$ Heisenberg model presumably has plateaus (corresponding to gaps) at least at one third and two thirds of the saturation magnetization (see Fig. 2). It may be remarked here that flat-bands on partial line graphs do not need to be ground-state bands [25].

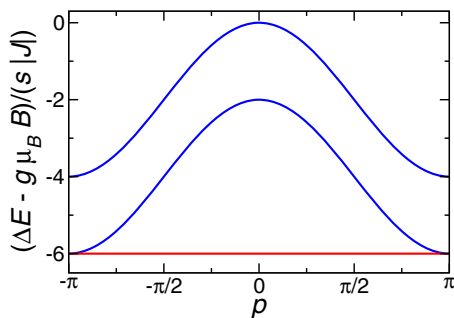


Figure 5. One-magnon excitation energies ΔE for the kagome chain; the flat band consists of $N/3$ degenerate levels.

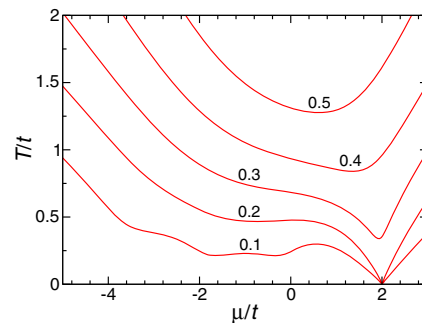


Figure 6. Lines of constant entropy for free spinless fermions on the kagome chain. The value of the entropy per site $S(T)/N$ is indicated next to each line.

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