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Magnetization plateaux and jumps in frustrated four-leg spin tubes in magnetic fields

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Abstract. We study the ground state phase diagram of a frustrated spin-1/2 four-leg tube in an external magnetic field. We explore the parameter space of this model in the regime of all-antiferromagnetic exchange couplings by means of three different approaches: density matrix renormalization group (DMRG), a low-energy effective Hamiltonian (LEH) and a Hartree variational approach (HVA). We find that in the limit of weakly interacting plaquettes, singlet and triplet states play an important role in the formation of magnetization plateaux. We study the transition regions numerically and analytically, and find that they are described, at first order in a strong- coupling expansion, by an XXZ spin-1/2 chain in a magnetic field. These results are consistent with the DMRG and HVA calculations.

1. Introduction

Frustrated magnetism is a subject that has attracted much attention in the last decades and magnetic frustration is the key element in the search of exotics ground states[1]. Very often, low-energy effective models are used to get a better understanding of the physics of such frustrated systems[2]. In the last years there has been a growing interest to the phenomenon of magnetization plateaux in quasi one-dimensional spin systems, comprising chain, ladder and more involved magnetic structures spin systems. In a variety of models, the magnetization as a function of the applied magnetic field h exhibits plateaus at certain values; at those plateaux the magnetization in units of the saturation $m = M/M_s$ is locked at some rational number.

Recently, $Cu_2Cl_4{\cdot}D_8C_4SO_2$ has been established as a new spin 1/2 tube with an even number of legs [3] with diagonal coupling between adjacent legs. Recently in Ref.[4] this system has been studied at zero magnetic field revealing the existence of a gaped phase stable at a wide range of parameters. Motivated by this in this work, we study a frustrated four spin $\frac{1}{2}$ tube with a geometry depicted in Fig. 1 in a magnetic field and described by the following Hamiltonian:

$$\mathcal{H} = J_0 \sum_{n,a} \mathbf{S}_{n,a} \cdot \mathbf{S}_{n,a+1} + J_1 \sum_{n,a} \mathbf{S}_{n,a} \cdot \mathbf{S}_{n+1,a} + J_2 \sum_{n,a} \mathbf{S}_{n,a} \cdot \mathbf{S}_{n+1,a+1} - h \sum_{n,a} S^z_{n,a} \qquad (1)$$

with a lattice structure and exchange antiferromagnetic couplings $J_{0,1,2}$ as shown in Fig. 1. Here $a = 1, ..., 4$ (resp. $n = 1, ..., N$) is a chain (resp. site) index, J_0 is the coupling in each plaquette, $J_{1,2}$ the couplings along the chains and the site $(n, 5)$ is identified with the site $(n, 1)$. For $J_{1,2} \ll J_0$, the quantum properties of the frustrated four spin tube can be understood in terms of weakly coupled four-spin plaquettes.

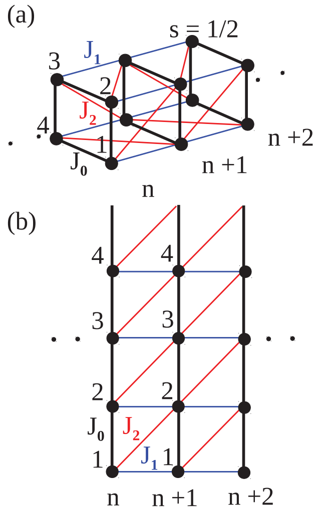

Figure 1. Diagram of the four spin tube studied. The four spins in the plaquette are indicated. Bonds mediated by J_0 are in red, by J_1 in blue and by J_2 in green. Figure taken from Ref. [4]

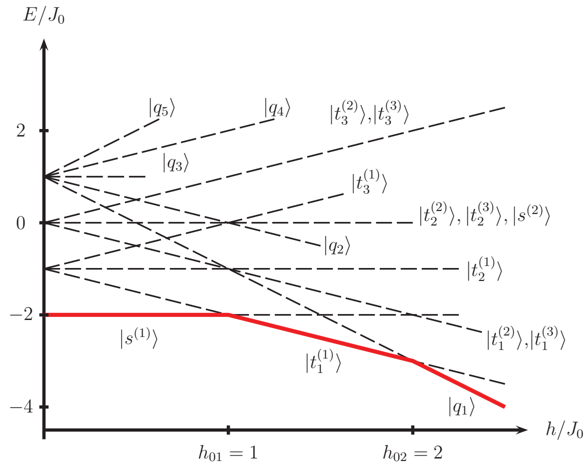

Figure 2. Energy of the states of a single plaquette of $S = 1/2$ as a function of the magnetic field. The lowest energy states and the values of the magnetic field where the energy is degenerate are indicated.

2. Low Energy Models

We treated the terms which contain interactions between plaquettes as a perturbation from the exactly solvable Hamiltonian of independent plaquettes $J_1, J_2 \ll J_0$. For $J_{1,2} = 0$, the system consists of independent plaquettes. The sixteen states of a given plaquette fall into a two spin-0 singlets ($|s^{(1)}\rangle$, $|s^{(2)}\rangle$), three spin-1 triplets ($|t_i^{(1)}\rangle$, $|t_i^{(2)}\rangle$ and $|t_i^{(3)}\rangle$ with $i = 1, ..., 3$) and one spin-2 quintuplet $|q_i\rangle$ (with $i = 1, ..., 5$). For no magnetic field, the ground state is not degenerate. When the magnetic field is switched on there are two particular values of the magnetic field $h_{01} = J_0$ and $h_{02} = 2\,J_0$ where two states cross (see Fig. 2). These two special fields define two separate regimes where we perform the perturbation expansion. For independent plaquettes, there are three magnetization plateaux, at $m = 0$, $m = 1$ and $m = 2$ corresponding to a singlet, a triplet and the quintuplet states. However the inclusion of interaction between plaquettes is expected to produce the emergence of other plateaux as well as the renormalization of existing ones.

In the first regime, when $|(h - J_0)| \ll J_0$ each plaquette can be found either in the singlet or in the triplet state. In the second regime, when $|(h - 2\,J_0)| \ll J_0$ each plaquette can be found either in the triplet or in the quintuplet state. Effectively, we can treat this as a system with only two states per site, using perturbation theory in J_1, J_2 to define a Hamiltonian that acts on this reduced Hilbert space. Defining the usual spin-1/2 matrices S^x, S^y and S^z acting on the reduced Hilbert space, one has at first order

$$\mathcal{H}_{\text{eff}} = \sum_{n=1}^{N} J_{xy}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + J_{zz}\, S_n^z S_{n+1}^z - h^{\text{eff}} \sum_{n=1}^{N} S_n^z \qquad (2)$$

where

$$h^{\text{eff}} = h - J_0 - \frac{J_1 + J_2}{4}, J_{xy} = \frac{4(J_1 - J_2)}{3}, J_{zz} = \frac{(J_1 + J_2)}{4}, \quad \text{for} \quad |(h - J_0)| \ll J_0 \tag{3}$$

$$h^{\text{eff}} = h - 2\,J_0 - \frac{3(J_1 + J_2)}{4}, J_{xy} = J_1 - J_2, J_{zz} = \frac{J_1 + J_2}{4}, \quad \text{for} \quad |(h - 2\,J_0)| \ll J_0 \tag{4}$$

The XXZ chain is gapped in the antiferromagnetic regime $J_{zz}/|J_{xx}| > 1$ and $h^{\text{eff}} = 0$, with zero magnetization in the ground state. The presence of the energy gap means that the magnetization remains exactly zero in a finite range of fields $-h_{\min} < h^{\text{eff}} < h_{\min}$. At $\pm h_{\min}$ the energy gap vanishes and the spinons condense. As $|h^{\text{eff}}|$ is increased further, the ground state becomes a sea of spinons with a growing magnetization. The system in this regime is a Luttinger liquid with continuously varying critical exponents. Finally, at $h^{\text{eff}} = \pm h_{\max}$ the magnetization of the XXZ chain saturates. The critical fields $h_{\min}$ and $h_{\max}$ of the XXZ chain are known exactly by Bethe ansatz solution[5].
To be more specific for the first regime around h_{01}, the effective S^z represents the plaquette $S^z = 0(1)$, corresponding to the singlet(triplet) state. So the plateaux in the curve of magnetization vs h^{eff} in the effective model at $M = -\frac{1}{2}$, 0 and $\frac{1}{2}$ translates into plateaux at $M = 0$, $\frac{1}{2}$ and 1 in the curve of magnetization vs h. The same idea applies to the field sector around h_{02}, where effective S^z represents plaquette $S^z = 1(2)$, corresponding to triplet(quintet) involved in the high field crossing. In this case, plateaux at $M = 0$, $\frac{1}{2}$ and 1 in effective model translate into $M = 1$, $\frac{3}{2}$ and 2 in plaquette model.

3. Variational approach

The simplest way to map out the phase diagram is to use a Hartree variational approach (HVA) for the wave function allowing a linear combination of low-energy states comprising of singlet, triplet and quintuplet states on each plaquette (we keep the plaquette wave function entangled), while we retain the product form over the bonds[6]

$$|\psi\rangle = \prod_{n=1}^{N/4} |\nu_n\rangle \tag{5}$$

where $|\nu_n\rangle = \sum_{i=1}^{Ne} \alpha_i |i\rangle$; $|i\rangle$ are the eigenstates of the plaquette and α_i are complex constants which satisfy $\sum_i |\alpha_i|^2 = 1$. The variational parameters α_i are then determined by minimizing the energy $E = \langle\psi|\mathcal{H}|\psi\rangle$. Replacing Eq. (5) in Eq. (1) we obtain

$$\begin{aligned} E \;\; = \;\; & J_0 \sum_n \vec{\alpha}_n^\dagger . M_d . \vec{\alpha}_n - h \sum_{n,a} \vec{\alpha}_n^\dagger \cdot M_a^z \cdot \vec{\alpha}_n + J_1 \sum_{n,\gamma,a} \left(\vec{\alpha}_n^\dagger \cdot M_a^\gamma \cdot \vec{\alpha}_n \right) \left(\vec{\alpha}_{n+1}^\dagger \cdot M_a^\gamma \cdot \vec{\alpha}_{n+1} \right) \\ & + J_2 \sum_{n,\gamma,a} \left(\vec{\alpha}_n^\dagger \cdot M_a^\gamma \cdot \vec{\alpha}_n \right) \left(\vec{\alpha}_{n+1}^\dagger \cdot M_{a+1}^\gamma \cdot \vec{\alpha}_{n+1} \right) \end{aligned} \tag{6}$$

The ground state is obtained using simulated annealing on lattices with periodic boundary condition and choosing the state with lowest energy per site. Simulations on each size were done by an exponential annealing schedule and the whole process was repeated many times to ensure stability of results. While the algorithm does not guarantee convergence to the ground state we nevertheless believe an accurate picture emerges since this method captures the main features of the low energy physics, compatible with the analytical calculations and DMRG simulations. In figures 3 and 4 we show typical magnetization curves obtained with HVA.

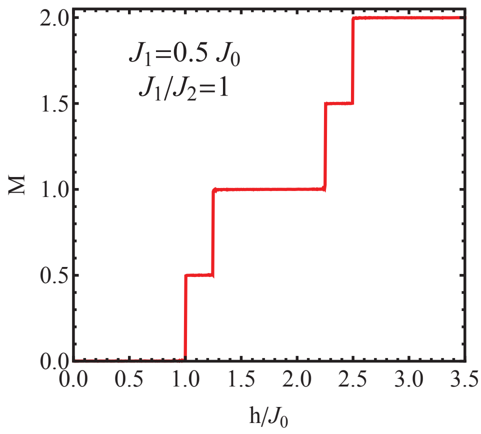

Figure 3. M vs h obtained by variational wave function approach for $J_1 + J_2 = 1$ and $J_2/J_1 = 1$.

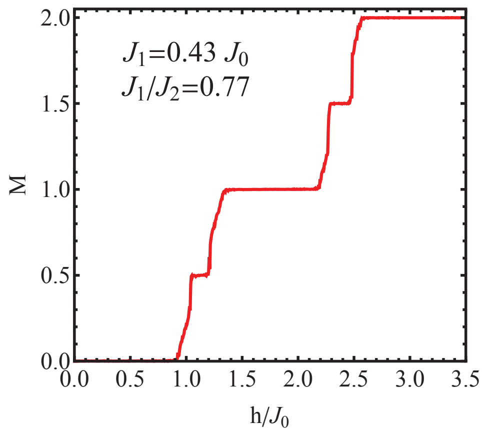

Figure 4. M vs h obtained by variational wave function approach for $J_1 + J_2 = 1$ and $J_2/J_1 = 0.77$.

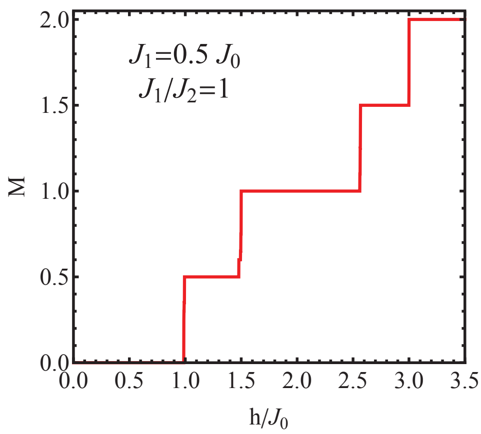

Figure 5. M vs h obtained by DMRG for $N = 4 \times 20$ sites and $J_1 + J_2 = 1$ and $J_2/J_1 = 1$.

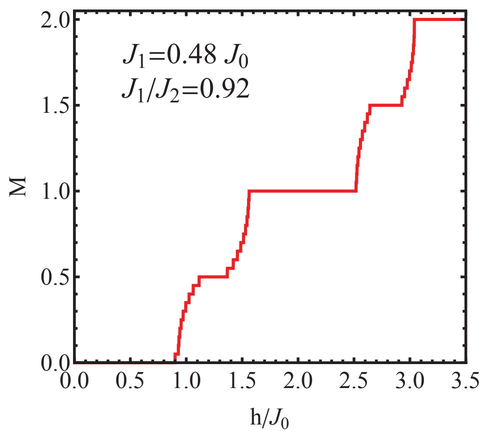

Figure 6. M vs h obtained by DMRG for $N = 4 \times 20$ sites and $J_1 + J_2 = 1$ and $J_2/J_1 = 0.48$.

4. DMRG analysis

In previous sections we provide the perturbative and qualitative picture expected when the couplings $J_1 - J_2$ connect the plaquettes. To have a complete picture we study the system using extensive DMRG computations. More specifically, we compute the ground state energy $E(S^z_{total}, h = 0)$ of Eq. (1) in the complete set of S^z_{total} subspaces using periodic boundary conditions, and keeping just 500 states was shown to be enough to assure the accuracy of the calculation. As usual, adding the Zeeman term, we solve the equation $E(S^z_{total}, h) = E(S^z_{total} + 1, h)$ to obtain the normalized magnetization where the plateaux are showing up. This procedure allows us to compute the actual width of the plateaux. From the DMRG data, we confirm the presence of two fractional plateaux at $M = 1/2$ and $M = 3/2$ in a wide range of parameter space J_1-J_2. In figures 5 and 6 we show typical magnetization curves obtained numerically which confirm those obtained by HVA and perturbation analysis.

5. Conclusion

In this paper, we have shown that frustrated interactions in a system consisting of non-frustrated plaquettes of spins-1/2 leads to the formation of rational plateaux that are not present in the non-frustrated case. With our analisys based in degenerate perturbation theory, a variational wave function approach and DMRG simulations show that the phases of plateaux are robust and hold up to large values of the coupling between plaquettes.

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