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GAPS AND MAGNETIZATION PLATEAUS IN LOW-DIMENSIONAL QUANTUM SPIN SYSTEMS

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The Lieb-Schulz-Mattis theorem predicts the existence of "soft modes" (zero energy excitations) in quasi one-dimensional quantum spin systems exposed to an homogeneous external field. The soft modes appear as zeroes in the dispersion curve and as singularities in the static structure factors. The critical behavior at the (field dependent) soft mode momenta is described by conformal field theory. Breaking of translation invariance, e.g. by the modulation of the external field of the nearest-neighbor coupling, is shown to yield an efficient mechanism to generate gaps and plateaus in the magnetization curve. The plateaus appear at those magnetizations where the period of the modulation coincides with the soft mode momentum. Spin ladder systems develop a characteristic sequence of magnetization plateaus. Experimental results on plateaus in magnetization curves (so far in two- and three-dimensional compounds) are discussed.

1 Introduction

Gaps in the energy spectrum play a crucial role in condensed matter physics. Fundamental properties in superconductivity or in the fractional quantum Hall effect originate from the existence of a gap between the ground state and the excited states. The corresponding ground-state wave function describes cooperative phenomena, where infinitely many degrees of freedom act together for example to build the Bose condensate of Cooper pairs in the BCS theory or the condensate of composite fermions or bosons in the fractional quantum Hall effect.

In this report, I present recent results on the mechanisms, which lead to the formation of gaps in the energy spectrum of low-dimensional quantum

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spin systems. The corresponding Hamiltonians

$$H = \sum_l J_l H_l, \tag{1}$$

$$H_l = \sum_i \vec{S}_i \vec{S}_{i+l} \tag{2}$$

are built up from isotropic couplings of spin S operators $\vec{S}_i$ and $\vec{S}_{i+l}$ at sites i and $i+l$. Many exact and numerical results on the one-dimensional system with nearest-neighbor couplings have been accumulated during the last 70 years:

(1) The spin 1/2 system has been solved by Bethe [1] in 1931 with his famous ansatz which allows the computation of the energy eigenvalues. Quite recently an exact computation of the specific heat has been presented by Klümper [2]. An analytic derivation of the low lying excitations – the so called two-spinon spectrum – and their impact on the dynamical structure factor in the ground state has been achieved by Bougourzi, Karbach, and Müller [3]. The spin 1/2 system with nearest-neighbor couplings is gapless. The critical properties – coded in the η-exponents of the static structure factor – are well described by the predictions of conformal field theory [4], which relates η to the finite-size behavior of the energy eigenvalues [5,6].

(2) The spin 1 system is not solvable with the Bethe ansatz or similar techniques like the Yang-Baxter equations. Numerical results were obtained by exact diagonalization with a Lanczos or conjugate gradient algorithm and recently by means of the density matrix renormalization group (DMRG) [7]. Haldane [8] formulated in 1983 his famous conjecture that quantum spin chains with integer spin $S = 1, 2, \ldots$ have a gap, whereas chains with half integer spin $S = 1/2, 3/2, \ldots$ are gapless. Recent numerical results [9] for spin 1, spin 3/2 and spin 2 chains support the Haldane conjecture.

(3) During the last 10 years, also ladder systems [10] – quantum spin systems between one and two dimensions - have been studied with numerical methods like DMRG. Concerning the ground-state properties, the following peculiar property has been found: Ladder systems with an even number of legs ($l = 2, 4, 6, \ldots$) have a gap; those with an odd number ($l = 1, 3, 5, \ldots$) have no gap.

(4) The two-dimensional spin 1/2 system has been studied intensively after

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the discovery of high T_c superconductivity motivated by the following fact: The undoped material La_2CuO_4 shows antiferromagnetic order at low temperatures in the CuO planes. The corresponding order parameter - the "staggered" magnetization, given by the static structure factor at momentum $\vec{p} = (\pi, \pi)$ - is nonvanishing in two dimensions [11] in contrast to the one-dimensional case. We have studied the transition from two to one dimension in a model with different nearest-neighbor couplings $J_\parallel$ and $J_\perp$ along the horizontal and vertical directions. We find that the staggered magnetization is non-negative for all couplings $\alpha = J_\perp/J_\parallel > 0$ and vanishes with an infinite slope for $\alpha = 0$ (see Ref. [12]).

In this work, I will briefly review in Section 2 the Lieb-Schultz-Mattis theorem [13] and its implications on the existence of soft modes in one-dimensional quantum spin systems. Then I will demonstrate in Section 3 that breaking of translational invariance is a very efficient mechanism for the formation of gaps and magnetization plateaus. Section 4 is devoted to spin ladder systems. It turns out that each spin ladder system with l-legs possesses a characteristic sequence of magnetization plateaus. In section 5 I will report on some compounds where experimentalists have found plateaus in the magnetization curve. Unfortunately, these compounds seem to have a two- or higher-dimensional coupling structure.

2 The Lieb-Schultz-Mattis Theorem and the Appearance of Soft Modes in One-Dimensional Quantum Spin Systems

Let me specify first my notion of a ground-state gap: There is no unitary operator U, which creates, from the ground state $|0\rangle$, *new* states

$$|n\rangle = U^n|0\rangle \tag{3}$$

with energy expectation values

$$\langle n|H|n\rangle - \langle 0|H|0\rangle = O(N^{-1}), \tag{4}$$

coinciding with the ground-state energy $E_0 = \langle 0|H|0\rangle$ in the thermodynamical limit. Of course, the new states $|n\rangle$ should differ from the ground state by their quantum numbers. For translation invariant one-dimensional systems

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over a finite range L, the Hamiltonian is

$$H = \sum_{l=1}^{l=L} J_l H_l + B \sum_i S_i^{(3)}. \tag{5}$$

Lieb, Schultz, and Mattis [13] have proposed the following operator U:

$$U = \exp\left\{\frac{2\pi i}{N} \sum_{i=1}^{N} i S_i^{(3)}\right\}. \tag{6}$$

The Hamiltonian commutes with the total spin

$$S_3 = \sum_{i=1}^{N} S_i^{(3)} \tag{7}$$

and, in the presence of a magnetic field B, the ground state is magnetized: $M = S_3/N$. The magnetization $M = M(B)$ follows from the magnetization curve. Lieb, Schultz, and Mattis proved that the new states $|n\rangle = U^n|0\rangle$ obey Eq. (4). Following the argument of Affleck and Lieb [14], the quantum numbers of the new states can be seen by applying the translation operator

$$T|n\rangle = e^{i[nq(M)+p_0]}|n\rangle, \tag{8}$$

i.e. the momentum of the new states,

$$p_n(M) = nq(M) + p_0(M), \tag{9}$$

differs from the ground-state momentum $p_0(M)$ by

$$q(M) = \pi(1 - 2M), \tag{10}$$

unless $nq(M)$ is a multiple of 2π.

In the following, I will call the state $|n\rangle$ the n'th soft mode. Soft modes appear as zeros in energy differences defining the dispersion curve

$$\omega(q, M, N) = E(q + p_0, M, N) - E(p_0, M, N). \tag{11}$$

In Fig. 1 I show the dispersion curve for $M = 1/4$ in a model with nearest- and next-to-nearest-neighbor coupling with $\alpha = 0$ and $\alpha = 1/2$, where $\alpha = J_2/J_1$ (see Ref. [15]). The first soft mode ($n = 1$) is clearly visible at $q = \pi/2$. The second soft mode ($n = 2$) at $q = \pi$ still suffers from large finite-size effects.

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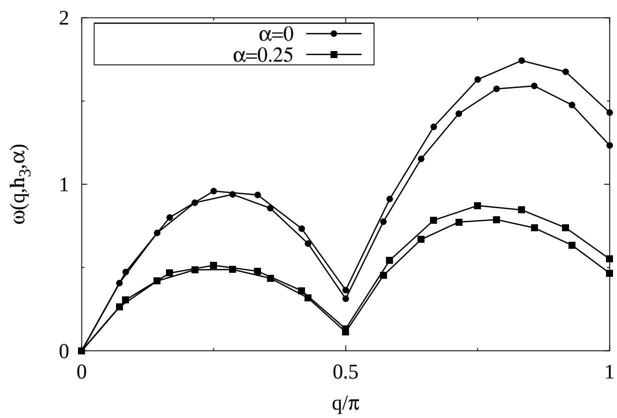

Figure 1. Dispersion curve (11) for $M = 1/4$, $\alpha = 0, 1/4$ on finite systems with $N = 24, 28$. The dips at $q = \pi/2, \pi$ occur at momenta of the first ($n = 1$) and second ($n = 2$) soft mode.

Conformal field theory makes a prediction on the finite-size dependence at the soft mode

$$\omega(q = q(M), M, N) \stackrel{N\to\infty}{=} \frac{\Omega(M)}{N}, \tag{12}$$

which can be verified numerically. Moreover the coefficient $\Omega(M)$ is related to the critical η-exponent

$$\eta(M) = \frac{\Omega(M)}{\pi v(M)}, \tag{13}$$

where $v(M)$ is the spin wave velocity

$$v(M) = \lim_{N\to\infty} \left[E\left(p_0 + \frac{2\pi}{N}, M, N\right) - E\left(p_0, M, N\right) \right]. \tag{14}$$

For the nearest-neighbor model ($\alpha = 0$), the energy differences, which enter on the right hand side of Eq. (13) can be computed by means of the Bethe ansatz on very large systems ($N = 10^4$). Therefore, in this case, the field dependence of the critical exponent $\eta = \eta(M)$ is very well known (see Fig. 2) [16]. The η-exponent describes the divergence in the static structure factor at the soft mode $q = q(M)$. The latter are defined as ground-state expectation values

$$S_0(q, M) = \langle 0|O(q)O(-q)|0\rangle \tag{15}$$

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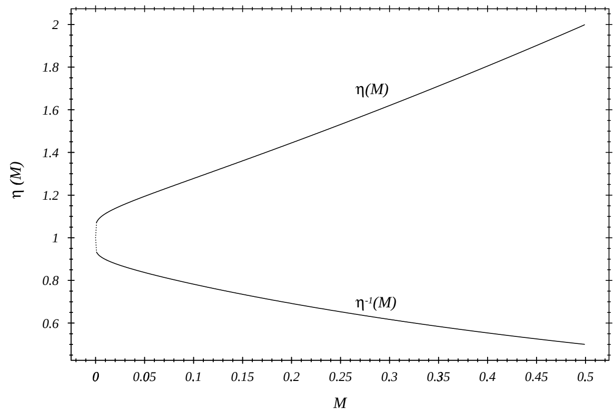

Figure 2. The critical η-exponent (13) versus magnetization M for $\alpha = 0$. The energy differences (12) and (14) were computed with the Bethe ansatz on large systems ($N = 10^4$).

of appropriate Fourier transformed operators

$$O(q) = \sum_j e^{iqj} O_j, \tag{16}$$

$$O_j =: S_j^{(3)},\ \left(\vec{S}_j \vec{S}_{j+1}\right), \ldots, \tag{17}$$

$$S_0\left(q\left(M\right), M, N\right) \stackrel{N\to\infty}{\longrightarrow} N^{1-\eta(M)}. \tag{18}$$

Figure 3 shows the q-dependence of the static structure factor for the dimer operator $\vec{S}_j \vec{S}_{j+1}$ [15]. A clear singularity is seen at the first soft mode ($q = \pi/2$). No singularity is visible at the second soft mode ($q = \pi$). According to the Lieb-Schultz-Mattis theorem, the position of the soft modes does not depend on the couplings (e.g. on $\alpha = J_2/J_1$). The critical exponents $\eta(M, \alpha)$, however, do depend on α. For α large enough, the singularity at the first soft mode is weakened and the second soft mode becomes visible.

3 Breaking of Translation Invariance: A Mechanism for the Formation of Gaps and Magnetization Plateaus

Translation invariance is essential for the validity of the Lieb-Schultz-Mattis theorem. Breaking of translation invariance is a vital attack against the soft modes. It has severe consequences.

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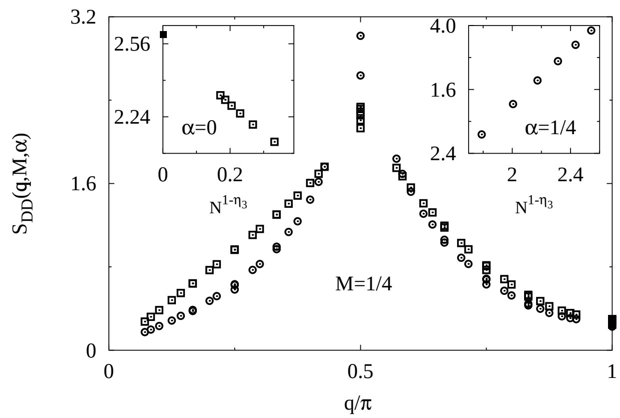

Figure 3. The static dimer structure factor (15) for $M = 1/4$, $\alpha = 0, 1/4$ on finite systems with $N = 24, 28$. A peak occurs at the first soft mode $q = \pi/2$. No peak is visible at the second soft mode $q = \pi$. The insets demonstrate the validity of (18) derived from conformal field theory.

Let us consider the nearest-neighbor model

$$H = H_1 + BS^{(3)}(0) + \delta \left(S^{(3)}(q) + S^{(3)}(-q) \right) \tag{19}$$

in a homogenous field B and a modulated field of strength δ:

$$S^{(3)}(q) = \sum_{j=1}^{N} S_j^{(3)} e^{iqj}. \tag{20}$$

In Fig. 4(a) we see what happens if one switches on the perturbation δ with wave number $q = \pi/2$. For $\delta = 0$ we see a smooth magnetization curve $M = M(B)$. Indeed this curve has been computed at the beginning of the sixties by C.N. Yang and C.P. Yang [17]; they used the Bethe ansatz to compute the energy eigenvalues in the sectors with given magnetization

$$B(M) = E\left(M + \frac{1}{N}, p_0\right) - E(M, p_0). \tag{21}$$

If we now look at $\delta > 0$ [18]; we see the emergence of a plateau at $M = 1/4$. For this magnetization the wave number of the perturbing field $q = \pi/2$ coincides with the first soft mode:

$$q = \pi(1 - 2M) \Rightarrow M = \frac{1}{2} - \frac{q}{2\pi}. \tag{22}$$

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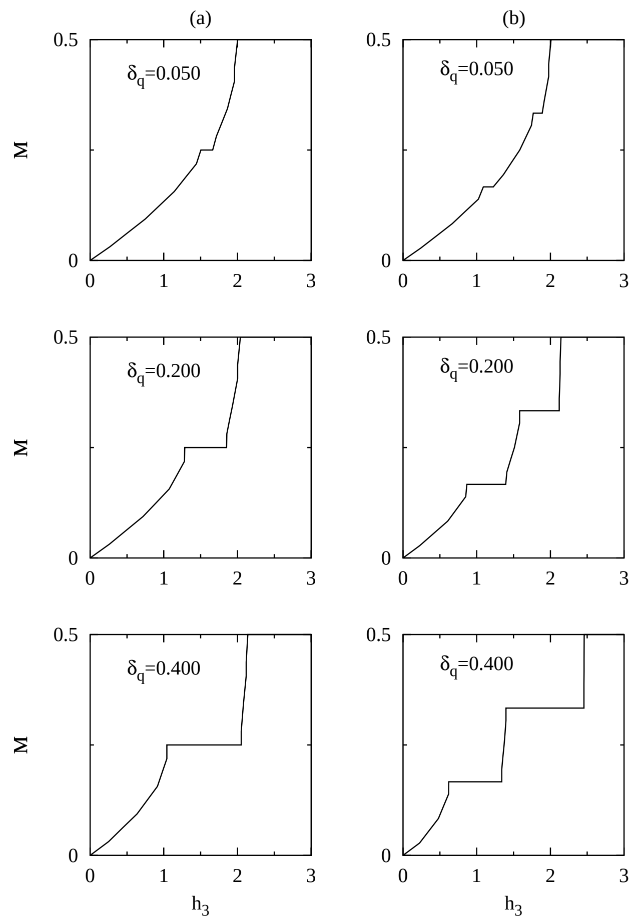

Figure 4. The magnetization curve for the nearest-neighbor Hamiltonian H_1 with a periodic perturbation: (a) of the external magnetic field with wave number $q = \pi/2$ (cf. Eq. (19)): Plateau at $M = 1/4$, and (b) of the nearest-neighbor coupling with wave numbers $q = \pi/3$ and $q = 2\pi/3$ (cf. Eq. (26)): Plateaus at $M = 1/6, 1/3$.

The connection between q and M is a special case of a more general rule established by Oshikawa, Yamanaka, and Affleck [19] on the position of possible magnetization plateaus. For small perturbations δ, the length Δ of the plateaus, i.e. the difference between the upper and lower critical fields, is

$$\Delta = B_U - B_L \sim \delta^{\epsilon}, \tag{23}$$

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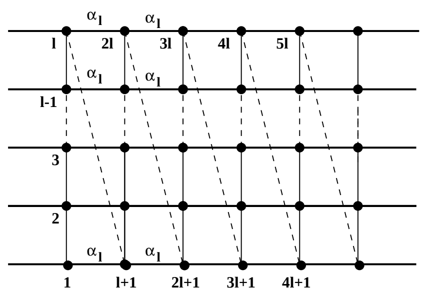

Figure 5. Mapping of the l-leg ladder on a one-dimensional system with modulated nearest-neighbor couplings.

i.e. scales with a power δ^ϵ, where ϵ is given by the critical η-exponent

$$\epsilon(M) = \frac{2}{4 - \eta(M)}. \tag{24}$$

Breaking of translation invariance can be achieved in many ways, e.g. instead of modulating the external magnetic field we can modulate as well the nearest-neighbor coupling

$$\bar{D}_1(q) = \frac{1}{2}\left(D_1(q) + D_1(-q)\right) = \sum_{i=1}^{N} \cos(q \cdot i)\vec{S}_i\vec{S}_{i+1}. \tag{25}$$

In Fig. 4(b) we can see the effect of a superposition of two modes:

$$\bar{D}_1\left(q = \frac{2\pi}{3}\right) + \bar{D}_1\left(q = \frac{\pi}{3}\right). \tag{26}$$

According to the rule (22) we observe two plateaus at

$$M = \frac{1}{6}, \quad M = \frac{1}{3}. \tag{27}$$

4 Gaps and Magnetization Plateaus in Spin Ladder Systems

A spin ladder system with l legs - as shown in Fig. 5 - can be viewed as a one-dimensional system

$$H = H_1 + \alpha_l H_l + D_1^{(l)}, \tag{28}$$

with nearest-neighbor coupling and couplings over l sites [15]. The translation invariant ring H_1, however, also contains "diagonal" couplings $l \to l+1$,

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$2l \to 2l+1$ (dashed lines in Fig. 5), which are absent in a normal ladder. We subtract these couplings using the term

$$D_1^{(l)} = \sum_{n=1}^{N} J_n^{(l)} \vec{S}_n \vec{S}_{n+1}, \tag{29}$$

$$J_n^{(l)} = \begin{cases} 0, & n = 1, \dots, l-1, \\ \delta, & n = l, \end{cases} \tag{30}$$

$$J_{n+l}^{(l)} = J_n^{(l)}. \tag{31}$$

The periodicity of the couplings,

$$J_n^{(l)} = \sum_{j=0}^{l/2} \cos\left(\frac{2\pi n j}{l}\right) \delta\left(q = \frac{2\pi j}{l}\right), \tag{32}$$

leads to a Fourier decomposition of the "unwanted" couplings:

$$D_1^{(l)} = \sum_q \delta_q^l \bar{D}_1(q). \tag{33}$$

The "unwanted" couplings induce a modulation of the nearest-neighbor couplings with certain wave numbers q, which again generate magnetization plateaus at $M = 1/2 - q/2\pi$ provided that the first soft mode is active. This consideration leads to the following prediction of magnetization plateaus for l leg ladders:

l	2	3	4	5	6
M	0	1/6	0; 1/4	1/10; 3/10	0; 1/6; 1/3

Note, that the even l ladders have a plateau at $M = 0$. This means they have a gap in the absence of a magnetic field. The odd l ladders do not have such a gap. (I mentioned this phenomenon [10] in the introduction.) The table means that one can associate a characteristic sequence of plateaus to each ladder.

We have tested this prediction by a numerical calculation of the magnetization curve in ladder systems with $l = 3, 4$ and 5 legs by means of the density matrix renormalization group (DMRG). The gap in the two leg ladder had been discussed before in the context of the compound $CuGeO_3$, which shows a spin Peierls transition [20].

The plateaus at $M = 1/3$ in the three leg ladder have been discovered by Honecker and collaborators [21]. In Fig. 6 you see this magnetization

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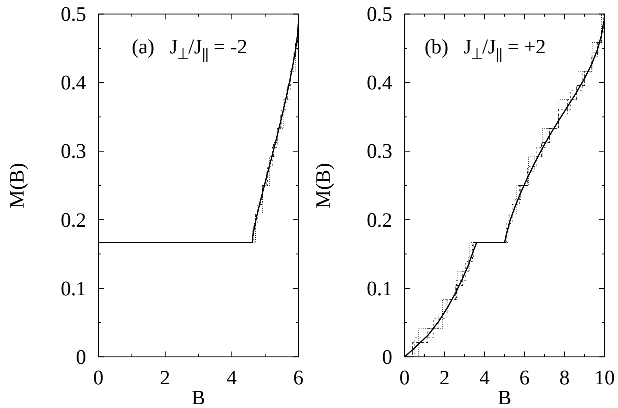

Figure 6. Magnetization curve of a three leg ladder with plateau at $M = 1/4$: (a) Couplings along the legs and rings are ferro- and antiferromagnetic respectively: ferrimagnetism. (b) Both couplings are antiferromagnetic.

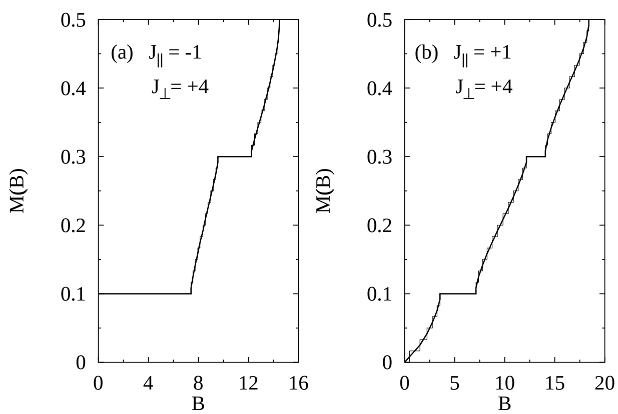

Figure 7. The same magnetization curve as Fig. 6, for a five leg ladder.

curve [15]. In the right picture both couplings $J_\perp$, $J_\|$ along the rings and the legs are antiferromagnetic (i.e. positive). In the left, the ring coupling is antiferromagnetic, the leg coupling ferromagnetic; here the plateau extends to a zero magnetic field, which means that the ground state at $B = 0$ is not a singlet, but a state with total spin $S = M \cdot N = N/3$. Such a phenomenon is often called "ferrimagnetism". The five leg ladder is shown in Fig. 7. The two predicted plateaus at $M = 1/10$ and $M = 3/10$ are clearly visible. Switching

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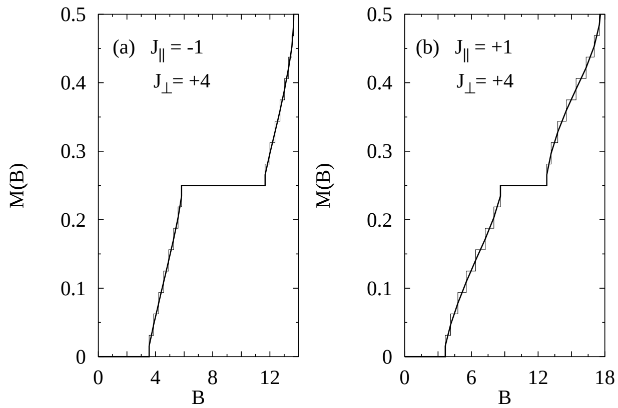

Figure 8. The same magnetization curve as Fig. 6 for a four leg ladder. But: No ferrimagnetism.

the leg coupling from antiferromagnetic to ferromagnetic, the phenomenon of ferrimagnetism appears again.

Finally, the four leg ladder is shown in Fig. 8. Two plateaus can be seen at $M = 0$ and $M = 1/4$, however the change from antiferromagnetic to ferromagnetic leg coupling does not change the magnetization curves substantially. In particular, there is no ferrimagnetism.

5 Experimental Evidence for Plateaus in Magnetization Curves

The following compounds have been synthesized and investigated by several groups:

(1) NH_4CuCl_3:
The authors of Ref. [22] found plateaus at $M = 1/8, 3/8$. It is suggested that this compound forms a two-dimensional structure of coupled zig zag ladders with two legs [23]. However, two leg zig zag ladders alone cannot explain the observed plateaus.

(2) $CsCuCl_3$:
The authors of Ref. [24] found a plateau at $M = 1/6$. They consider the compound as a three-dimensional structure built up from coupled three leg ladders. This would easily explain the position of the plateau [25], if the coupling between the three leg ladders does not change the situation.

(3) $SrCu_2(BO_3)_2$:
The authors of Ref. [26] found plateaus at $M = 1/6, 1/8, 1/16$. They

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suggest [27] that the compound has a two-dimensional coupling structure à la Shastry-Sutherland [28].

6 Perspectives

In this report I have restricted the discussion on the existence of magnetization plateaus in isotropic spin 1/2 systems. The considerations presented here can be extended to higher spin systems. Our next project is to consider a quite general class of systems with three states at each site. Spin 1 systems are included as well as lattice systems with spin 1/2 particles carrying charge, like the $t - J$ model. The $t - J$ model is a Hubbard model for electrons on a lattice with a constraint preventing two electrons, one with spin up, the other with spin down, to sit on the same site. The symmetry structure of three-state systems becomes apparent if we express the couplings between sites x and y in terms of the 8 generators of the $SU(3)$, the so called Gell-Mann matrices λ_A, $A = 1, \ldots, 8$:

$$H(x, y) = \sum_{A=1}^{8} \lambda_A(x)\lambda_A(y)J_A. \tag{34}$$

The Gell-Mann matrices are just the $SU(3)$ analogue of the Pauli matrices for $SU(2)$. For the $t-J$ model the coupling parameters J_A are related to the parameters t and J via

$$J_1 = J_2 = J_3 = \frac{J}{4}, \quad J_4 = J_5 = J_6 = J_7 = -\frac{t}{2}, \quad J_8 = -\frac{J}{12}. \tag{35}$$

The Cartan subalgebra of SU(3) contains two elements. In case of the $t - J$ model we choose the 3-component of the spin (λ_3) and the charge (λ_8) of the state at site x. Total spin and total charge are conserved quantities in the $t-J$ model. In one-dimensional models the whole line of arguments developed by Lieb, Schultz, and Mattis [13] in the spin sector can be repeated as well as in the charge sector of the $t - J$ model. In other words there are soft modes with momenta $q(\rho) = 2\pi\rho$ which move with the charge density ρ as long as translation invariance and the finiteness of the range of the couplings is guaranteed. We expect that a breaking of translation invariance by means of a perturbation with wave number q will produce a plateau at $\rho = q/2\pi$ in the curve $\rho = \rho(\mu)$, which describes the dependence of the electronic density ρ (or filling factor) as function of the chemical potential μ for the electrons.

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Moreover, the $t - J$ model on a ladder system with l legs should evolve a characteristic sequence of plateaus in $\rho(\mu)$. Plateaus in the filling factor $\rho(\mu)$ for the two-dimensional Hall system yield indeed the explanation for the integer and fractional quantum Hall effect. In these systems one can tune the chemical potential μ for the electrons by means of the perpendicular magnetic field.

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