Magnetization plateaux in periodically modulated 1D systems: effect of doping and disorder

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Abstract: We report results of theoretical investigations on the effect of doping and quenched disorder on the occurrence of plateaux in the magnetization curve of 1D systems with periodic modulations in the couplings. For single q-merized Hubbard chains, doping is shown to affect the position at which plateaux appear, leading to the emergence of plateaux at *irrational* values of the magnetization. For random bond antiferromagnetic Heisenberg chains with periodically modulated bond distributions, disorder generically removes the plateau structure, except in the case of discrete probability distributions. In the latter case, wide plateaux emerge at values of the magnetization dependent on the strength of disorder.

1. Introduction

In the past few years the occurrence of plateaux in the magnetization curve of quantum spin chains and ladders has attracted considerable interest, both theoretical and experimental.

From the theoretical side, it has been shown that plateaux can occur at *rational* fractions of the saturation magnetization. Such fractions are subject to a quantization condition whose most general form is the following:

$$qNS(1-m) = \text{integer} \ . \tag{1.1}$$

In the above equation m is the magnetization (normalized to 1 at saturation), S the spin, N the number of legs (for ladders, for chains $N = 1$) and q the number of sites to which one–site translational invariance is explicitly or spontaneously broken (see e.g. [1]–[5]). In particular, the condition (1.1) with $N = 1$ applies to pure spin chains with a q–periodic modulation in the coupling constants, whose magnetization curve indeed exhibits plateaux (see [5] and refs. therein).

From the experimental side, some investigations have indeed confirmed these predictions in few particular 1D cases, as for instance the dimerized spin–1 chain studied in [6], which exhibits a plateau at half the saturation magnetization, or the material NH_4CuCl_3 [7], which exhibits plateaux at 1/4 and 3/4 of the saturation magnetization.

In the case of materials with a ladder structure [8], due to the large coupling constants, plateaux with non–zero magnetization are predicted for very high values of magnetic field, which makes their observation very difficult with the present experimental tools. An attractive mechanism moving plateaux at lower field values may be provided by doping, as we have shown in refs. [9], [10] for the case of periodically modulated Hubbard chains and we expect to be the case for Hubbard ladders [11]. These models also provide the opportunity to investigate the effect of charge degrees of freedom on the physics of plateaux. Interestingly, for such systems plateaux are also predicted at *irrational* values of the magnetization, which depend continuously on doping. We review the results of refs. [9] and [10] in Sec. 2 .

A relevant question related to the appearance of magnetization plateaux is whether they survive or not in the presence of quenched disorder, which is almost inevitably present in ex-

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periments. We studied this issue in a disordered version of the periodically modulated XXZ antiferromagnetic chain [12]. We found that generically randomness in the exchange couplings removes the plateau structure. However, for some particular probability distributions, disorder instead of removing completely the plateaux, shifts the position of some of them by a precise amount, which depends on the strength of disorder. We review this and other results in Sec. 3 .

2. Effect of doping

In order to gain insights on the effect of doping on the occurrence of magnetization plateaux, we studied the concrete example of a *doped* Hubbard chain with a q–periodic modulation (q–merization for short) in the hopping amplitude[1] $t(x)$. The lattice hamiltonian is the following:

$$\begin{aligned} H \;=\; & -\sum_{x=1}^{L} t(x) \sum_{\sigma} \left(c^{\dagger}_{x+1,\sigma} c_{x,\sigma} + c^{\dagger}_{x,\sigma} c_{x+1,\sigma} \right) \\ & + U \sum_{x=1}^{L} n_{x,\uparrow} n_{x,\downarrow} + \mu \sum_{x=1}^{L} \left(n_{x,\uparrow} + n_{x,\downarrow} \right) \\ & - \frac{h}{2} \sum_{x=1}^{L} \left(n_{x,\uparrow} - n_{x,\downarrow} \right) \;, \qquad (2.1) \end{aligned}$$

where $t(x) = t$ if $x \neq lq$ and $t(lq) = t' = t + \delta$ (l is a generic integer). In the above equation $c^{\dagger}$ and c are electron creation and annihilation operators, $n_{x,\sigma} = c^{\dagger}_{x,\sigma} c_{x,\sigma}$ the number operator and $\sigma = \uparrow, \downarrow$ the two possible spin orientations. μ is the chemical potential and h an external magnetic field. There are various reasons for the choice of this model. The first is that at half–filling and in the limit of strong U it reduces exactly to the q–merized AF Heisenberg chain, which is among the simplest pure spin systems exhibiting magnetization plateaux [5]. The second reason is that it describes realistic situations, for instance the dimerized model is realized in a number of real compounds like the organic (super)conductors [13] and the ferroelectric perovskites [14]. There is finally a third, more technical, motivation, related to the fact that the uniform Hubbard chain is exactly solvable by

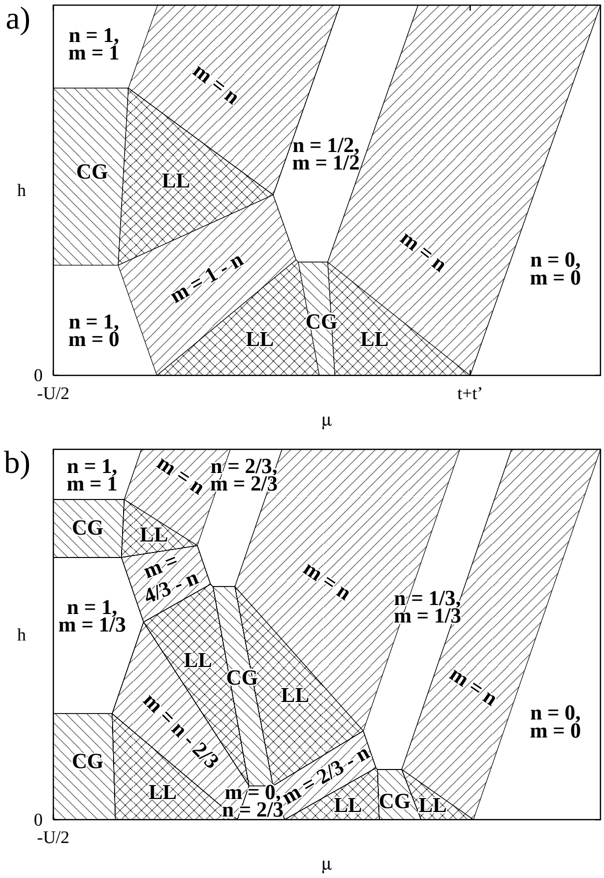

Figure 1: Schematic ground state phase diagram of a) the dimerized Hubbard chain ($q = 2$) and b) the trimerized chain ($q = 3$). For explanations compare the text.

means of the Bethe Ansatz [15]. The exact solution can be used to construct a *non–perturbative* bosonic representation of the low–energy sector of the Hubbard hamiltonian (even in non–zero magnetic field) [16], [17], providing a very efficient tool to study different generalizations of the model.

We studied the magnetic properties of model (2.1) by means of a variety of techniques: analytically, by means of abelian bosonization (which is appropriate for small q–merization, i.e. $t' \sim t$) and standard quantum mechanical perturbation theory (for small U); and numerically, by means of Lanczos diagonalization on finite size clusters. All results conspired to give the following scenario: There are several different phases in the $\mu - h$ plane (see Fig. 1 for a schematic illustration of the cases $q = 2$ and $q = 3$, based on the

[1] Similar results are found in the case of modulated on–site energy [10].

numerical results; abbreviations refer to the corresponding regions of these figures):

1. If both quantization conditions[2]

$$\frac{q}{2}\,(n \pm m) \in \mathbb{Z} \qquad (2.2)$$

are simultaneously satisfied, both spin and charge sectors are gapful (regions labeled by fixed n and m in Fig. 1). In this case, plateaux are found in the magnetization curve, since the presence of a spin gap is equivalent to the appearance of a plateau. Notice that (2.2) are simply the commensurability conditions for spin–up and spin–down electrons.

2. If only one of the conditions (2.2) is fulfilled (solutions are indicated in the corresponding regions of Fig. 1) and in addition the filling n is kept fixed, a magnetization plateau opens, *but one mode remains gapless*[3]. Thus, in contrast to the gapful magnetic behavior, charge transport remains metallic in this phase.

3. A charge gap ('CG') can open if the combination $qn \in \mathbb{Z}$ of the conditions (2.2) is satisfied. This case includes the well-known charge gap at half filling ($n = 1$) as well as the charge gap in the quarter-filled ($n = 1/2$) dimerized Hubbard chain ($q = 2$) [19].

4. In the remaining cases, both spin and charge sectors are massless, leading to Luttinger liquid ('LL') behaviour.

Notice that the plateaux predicted in **2.** have the particularly appealing aspect that they can appear at low magnetization (and thus at small magnetic field) if doping is suitably chosen. For instance, for the dimerized chain ($q = 2$) **2.** predicts a plateau at $m = 1 - n$.

The conditions (2.2) are easily understood in the limit of large q–merization, i.e. $t' = 0$: the chain decomposes into clusters of q sites, the number of spin–up and spin–down electrons on a q–sites cluster must both be integer, which is equivalent to imposing both conditions (2.2). All these states are clearly fully gapped and they will remain fully gapped if one turns on a small perturbation $t' > 0$, only the transitions will soften.

[2]The density of particle or filling n and the magnetization m are normalized such that $0 \leq n \leq 2$ ($n = 1$ corresponds to half–filling) and $|m| \leq 1$.

[3]Similar observations have been made in other systems [4, 18].

As we mentioned above, in the opposite limit of small q–merization, i.e. $t' \sim t$, one can use abelian bosonization to analyze the model, as we sketch in the following (for the full and detailed discussion we refer the reader to ref. [10]).

The continuum low–energy effective hamiltonian of the uniform (i.e. $t' = t$) Hubbard chain in magnetic field is given by

$$\sum_{i=c,s} \frac{v_i}{2} \int dx \, \left[(\partial_x \phi_i)^2 + (\partial_x \theta_i)^2 \right] \,. \qquad (2.3)$$

The effective charge and spin fields $\phi_{c,s}$ are given by

$$\begin{pmatrix} \phi_c \\ \phi_s \end{pmatrix} = \frac{1}{\det\ Z} \begin{pmatrix} Z_{ss} & Z_{ss} - Z_{cs} \\ Z_{sc} & Z_{sc} - Z_{cc} \end{pmatrix} \begin{pmatrix} \phi_\uparrow \\ \phi_\downarrow \end{pmatrix} , \qquad (2.4)$$

where $\phi_{\uparrow,\downarrow}$ are the bosonic fields introduced as usual to bosonize the spin–up and spin–down electron operators (see e.g. [20]), $\theta_{c,s}$ are the duals of $\phi_{c,s}$ and Z_{ij} $(i,j = c,s)$ are the elements of the so–called dressed charge matrix given in ref. [16]. In zero magnetic field the transformation (2.4) simplifies and $\phi_{c,s}$ reduce to the usual charge and spin fields: $\phi_c = (\phi_\uparrow + \phi_\downarrow)/\xi$ and $\phi_s = (\phi_\uparrow - \phi_\downarrow)/\sqrt{2}$, where ξ is related to the standard Luttinger parameter K_c by $\xi^2 = 2K_c$.

In the presence of small q–merization, the hamiltonian (2.3) is perturbed by the following operators:

$$\begin{aligned} &\lambda_1 \sin[k_+/2 + qk_+x - \sqrt{\pi}\,(Z_{cc}\phi_c - Z_{cs}\phi_s)] \times \\ &\times \cos[k_-/2 + qk_-x - \\ &-\sqrt{\pi}\,((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s)] + \\ &+\lambda_2 \sin[k_+ + 2qk_+x - \sqrt{4\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s)] \end{aligned} \qquad (2.5)$$

where $k_+ = k_{F\uparrow} + k_{F\downarrow} = \pi n$ and $k_- = k_{F\uparrow} - k_{F\downarrow} = \pi m$ ($k_{F\uparrow,\downarrow}$ are the Fermi momenta for spin–up and spin–down electrons), and $\lambda_1,\ \lambda_2 \propto \delta$. If all operators in (2.5) are commensurate, which is achieved when both conditions (2.2) are simultaneously satisfied, both degrees of freedom are massive, since the perturbing operators are relevant. Thus one obtains magnetization plateaux with a charge gap.

Furthermore, since the λ_2 term in (2.5) contains only the proper charge field $\phi_\uparrow + \phi_\downarrow$, a charge gap opens for all values of the magnetization at the commensurate values of the filling, i.e. when the condition $qn \in \mathbb{Z}$ is satisfied.

When instead only one of the conditions (2.2) is satisfied, say $q\,(n+m)\,/2 \in \mathbb{Z}$, one can show that the hamiltonian can be written as

$$H = \int dx \; \frac{v_\uparrow}{2} \; \left[(\partial_x \phi_\uparrow)^2 + (\partial_x \theta_\uparrow)^2 \right] + \lambda \cos 2\sqrt{\pi}\phi_\uparrow + \frac{v_\downarrow}{2} \; \left[(\partial_x \phi_\downarrow)^2 + (\partial_x \theta_\downarrow)^2 \right] \; . \tag{2.6}$$

Terms mixing derivatives of the up and down fields, which come from the U interaction, can be shown to be irrelevant. The massive field $\phi_\uparrow$ can be integrated out and one obtains an effective low–energy hamiltonian for $\phi_\downarrow$, with an effective Fermi velocity and Luttinger parameter K. This field is apparently massless but if the total filling is kept fixed, it is constrained to be in a particular topological sector. This global constraint can be shown to imply that changing the magnetization requires a finite amount of energy, which corresponds to a gap in the spectrum of magnetic excitations, i.e. a plateau. In order to support this conclusion, one can also compute the magnetic susceptibility for a finite size chain. Taking into account the global constraint imposed on the system, one finds a zero susceptibility, as expected in the presence of a plateau. This situation is somewhat exotic, because it combines gapful magnetic behavior (plateau at $q(n{+}m)/2 \in \mathbb{Z}$ for arbitrary, but fixed, value of n) with the algebraic decay of some correlation functions (due to the local massless dynamics of the down field).

A complementary derivation of the latter doping–dependent plateaux can be given in the limit of small on–site repulsion U by using quantum mechanical perturbation theory: for this we refer the reader to ref. [10].

3. Effect of disorder

We turn now to the issue of robustness of plateaux with respect to quenched disorder. In order to gain insights on this problem, we studied the magnetic behavior of a q–periodic spin–$1/2$ XXZ antiferromagnetic chain with a random distribution of exchange couplings. The hamiltonian of the model is

$$H = \sum_i J_i \; \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) \; , \tag{3.1}$$

where J_i are randomly distributed bonds. The occurrence of plateaux in this system turns out to depend largely on the probability distribution $P[J]$. To be specific, we considered two types of distributions: A binary distribution of strength p [4]:

$$P[J_i] = p\delta(J_i - J') + (1-p)\delta(J_i - J_0 - \gamma_i J) \; , \tag{3.2}$$

where $\gamma_i \equiv \gamma, \; (-\gamma)$ if $i/q \in \mathbb{Z}, \; (i/q \notin \mathbb{Z}\,)$ and a Gaussian distribution:

$$P[J_i] \propto \exp - \frac{(J_i - \overline{J_i})^2}{2\,\sigma_i^2} \; . \tag{3.3}$$

Both these distributions enforce q-merization.

To analyze the model (3.1) we adapted to our problem the arguments, based on the decimation procedure and real space renormalization group, used by Fisher to compute the low temperature zero field magnetic susceptibility of the AF XXZ chain in the random–singlet (strongly disordered) phase [21]. We will not give here details and refer the reader to ref. [12]. There, we essentially assume that all spins coupled by bonds stronger than the magnetic field[5] form singlets and do not contribute to the magnetization, whereas spins coupled by weaker bonds are completely polarized. Thus the magnetization at a given energy scale (i.e. magnetic field) is proportional to the fraction of spins remaining after decimation of all singlets formed at that energy scale. This argument happens to apply well to the binary distribution and can be used to study the magnetization process of (3.1). To start with, we consider the case of a dimerized chain ($q = 2$) with the binary distribution of bonds, and we assume that J' is the smallest coupling and $0 < \gamma < J_0/J$. At high enough magnetic field, all spins are polarized (saturation, $m = 1$). If we begin to decrease the magnetic field, the magnetization stays constant for a while, then decreases abruptly at $h \sim J_0 + \gamma J$ and after that a plateau occurs at $m = p$. The abrupt change happens because at $h \sim J_0 + \gamma J$ all spin pairs connected by the strongest bonds $J_0 + \gamma J$ form singlets and do not contribute anymore to the magnetization.

[4] $p = 0$ corresponds to the pure q-merized case, while $p = 1$ corresponds to the uniform chain.

[5] In our problem, which is at $T = 0$, the magnetic field provides the energy scale.

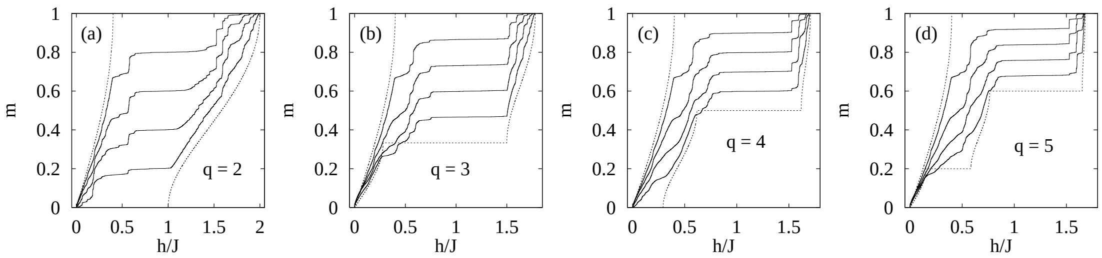

Figure 2: Magnetization curves of modulated XX spin chains with $q = 2$ (a), 3 (b), 4 (c) and 5 (d), immersed in disordered binary backgrounds of strength p. Solid lines represent averages over 100 samples with 5×10^4 sites, $J'/J_0 = 0.2$, $\gamma J = 0.5$ and $p = 0.2, 0.4, 0.6, 0.8$ in ascending order. The left and rightmost dotted lines denote respectively the pure uniform and pure modulated cases $p = 1$ and $p = 0$.

Since the number of remaining (completely polarized) spins is $N - 2 \times (1-p)N/2 = pN$, a plateau occurs at

$$m = p \,. \tag{3.4}$$

The appearance of this plateau, then, is due to the fact that the remaining strongest bonds have values $J_0 - \gamma J$, and all spins left from the first step remain polarized (and thus the magnetization constant), until the magnetic field decreases to $h \sim J_0 - \gamma J$ [6]. Following this reasoning, a second plateau is found at magnetization

$$m = p - p^2 + p^3 \ . \tag{3.5}$$

These arguments can be easily generalized to a q-merized chain with a binary distribution. One finds that the first plateau appears at

$$m = 1 + \frac{2}{q}\,(p-1) \ . \tag{3.6}$$

Notice that this result locates correctly the plateaux appearing in a pure q-merized Heisenberg chain ($p = 0$) [5].

Since the decimation procedure applies for generic XXZ chains [21], we conclude that the emergence of the plateaux predicted in (3.6) is a generic feature, at least for discrete probability distributions.

To support these assertions, we also studied the model (3.1) by means of exact numerical diagonalization. For the sake of simplicity, we considered only the case $\Delta = 0$. In Figs. 2(a), 2(b), 2(c) and 2(d) we show respectively the magnetization curves obtained for $q = 2$, 3, 4 and 5 after averaging over 100 samples of $N = 5 \times 10^4$ sites with binary distribution (3.2). The numerical curves clearly exhibit robust plateaux, precisely at the positions predicted by eq. (3.6). The secondary plateaux (the extension of (3.5) for arbitrary q), though narrower, are still visible in Figs. 2 .

It is important to stress that the derivation of our results eqs. (3.4), (3.5), (3.6) relies strongly on the discreteness of the binary probability distribution and would not apply to a continuous distribution. Indeed, for the Gaussian case referred to above, it turns out that no traces of plateaux can be observed in the numerical curves.

We also studied the behavior of the magnetic susceptibility at low magnetic field. Without entering here into the details, we found that the susceptibility exhibits an interesting even–odd effect. In fact, for q odd we found the same kind of universal singularity (independent of the probability distribution) as for the homogeneously disordered case (i.e. $q = 1$) [21], namely

$$\chi_z \propto \frac{1}{h(\ln h^2)^3} \,, \tag{3.7}$$

whereas the even q modulations yield a generic non-universal power law behavior, as the one found in [22] for $q = 2$,

$$\chi_z \propto h^{\alpha - 1} \,, \tag{3.8}$$

where the non–universal exponent α turns out to depend on the probability distribution parameters [12]. The numerical data give further support to these results [12].

[6] In fact, this depends on the values of J', J_0, γJ. This is generically true for $J_0 + \gamma J > J_0 - \gamma J > J'$ which is satisfied by the values used in the numerical diagonalizations.

4. Conclusions

To conclude, the main results we want to emphasize are first, that plateaux can appear at irrational values of the magnetization in doped systems. Doping can indeed be used as a tool to study experimentally irrational plateaux in systems whose half-filled parent compounds exhibit plateaux only at prohibitively high magnetic fields. A natural candidate are ladder systems, where doping can indeed be controlled. A theoretical investigation on doping-dependent magnetization plateaux in Hubbard ladders is in progress [11]. The second result is the observation that disorder affects the plateau structure in a very peculiar way, namely by shifting the position of some of them with respect to the pure case by an amount precisely related to the periodicity q and the strength of disorder.

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