Quasiperiodic spin chains in a magnetic field

M. Arlego,¹ D. C. Cabra,^{1,2} and M. D. Grynberg¹

¹*Departamento de Física, Universidad Nacional de La Plata, C.C. 67, (1900) La Plata, Argentina*

²*Facultad de Ingeniería, Universidad Nacional de Lomas de Zamora, Cno. de Cintura y Juan XXIII, (1832) Lomas de Zamora, Argentina*

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We study the interplay between a (quasi) periodic coupling array and an external magnetic field in a spin- $\frac{1}{2}$ XXZ chain. A new class of magnetization plateau is obtained by means of Abelian bosonization methods which gives rise to a sufficient quantization condition. The investigation of magnetic phase diagrams via exact diagonalization of finite clusters finds a complete agreement with the continuum treatment in a variety of situations.

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The magnetic properties of quasicrystals have become a fundamental issue of study since their discovery in 1984.¹ A variety of theoretical efforts, ranging from renormalization group (RG) analysis of Ising models in Penrose lattices² to exact solutions of both Ising and XY Fibonacci spin chains^{3–5} have revealed fairly intricate magnetic orderings associated with the quasiperiodicity of these structures. The nonmetallic spin-exchange mechanism implicit in those studies has been evidenced in recently synthesized rare-earth (RE) ZnMg-RE quasicrystals (see, e.g., Ref. 6) whose RE elements have well localized $4f$ magnetic moments.

Bolstered by these latter findings and as a further step within the line of the local moment descriptions referred to above, here we consider the ordering of quasiperiodic spin- $\frac{1}{2}$ XXZ chains in a magnetic field to elucidate the quantization conditions of massive spin excitations or magnetization plateaus. In periodic systems, this issue has received systematic attention in the last few years from both experimental and theoretical points of view (see, e.g., Ref. 7). In this paper, we are specifically interested in studying the antiferromagnetic system

we focus on the combined effect of a quasiperiodic exchange modulation under a uniform magnetic field.

Of particular importance are the rational frequencies of Eq. (1), not only as a way to approach the quasiperiodic limit, but also because they allow for a thorough numerical verification of a novel situation (see Refs. 13–15 for related work). As we shall see, although the allowed fractional plateaus predicted in the present case fall into the classification provided by the generalized Lieb-Schultz-Mattis theorem,¹⁶ a bosonization approach to Eq. (1) yields an alternative scenario not envisaged in previous studies.^{17,18} This will be reflected in the appearance of magnetization plateaus associated to each of the frequencies present in Eq. (1). To strengthen the potential interest of our results, we show how a simple two frequency model exhibits a magnetization curve with two wide plateaus at $1/4$ and $3/4$ of saturation, a situation which is highly reminiscent of that observed in magnetization experiments on NH_4CuCl_3 .¹⁹

Following the standard bosonization procedure (see, e.g., Ref. 20), the continuum limit of the XXZ Hamiltonian in the presence of an external magnetic field h is given by the Tomonaga-Luttinger Hamiltonian

$$H_{qp} = J \sum_n (1 + \epsilon_n) (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) - h \sum_n S_n^z, \quad (1)$$

where S^x, S^y, S^z denote the spin- $\frac{1}{2}$ matrices involved in the standard XXZ Hamiltonian ($\epsilon_n = 0$) in a magnetic field h applied along the anisotropy direction ($|\Delta| \leq 1$). Here, the coupling modulation is introduced via the ϵ_n parameters defined as $\epsilon_n = \sum_\nu \delta_\nu \cos(2\pi\omega_\nu n)$, so quasiperiodicity arises upon choosing an irrational subset of frequencies ω_ν with amplitudes δ_ν .

The interest of Eq. (1) stems partly from the widespread applications of $1d$ Hamiltonians in the description of artificially grown quasiperiodic heterostructures,⁸ quantum dot crystals,⁹ and magnetic multilayers.¹⁰ Also, recent investigations of quasiperiodicity involving either the couplings¹¹ or the magnetic field,¹² have been addressed using Abelian bosonization along with RG and numerical techniques. Here

$$H = \frac{1}{2} \int dx \left(v K (\partial_x \tilde{\phi})^2 + \frac{v}{K} (\partial_x \phi)^2 \right). \quad (2)$$

The bosonic field ϕ and its dual $\tilde{\phi}$ are given by the sum and difference of the light-cone components, respectively. The constant $K = K(\langle M \rangle, \Delta)$ governs the conformal dimensions of the bosonic vertex operators and can be obtained exactly from the Bethe-Ansatz solution of the XXZ chain (see, e.g., Ref. 18 for a detailed summary). One has $K = 1$ for the $\text{SU}(2)$ symmetric case ($\Delta = 1$) and it is related to the radius R of Ref. 18 by $K^{-1} = 2\pi R^2$. In terms of these fields, the spin operators read

$$S_x^z = \frac{1}{\sqrt{2\pi}} \partial_x \phi + a : \cos(2k_F x + \sqrt{2\pi} \phi) : + \frac{\langle M \rangle}{2}, \quad (3)$$

$$S_x^\pm = (-1)^x : e^{\pm i\sqrt{2\pi}\tilde{\phi}} [b \cos(2k_F x + \sqrt{2\pi}\phi) + c] :, \quad (4)$$

where the colons denote normal ordering with respect to the ground state with magnetization $\langle M \rangle$. The Fermi momentum

k_F is related to the magnetization of the chain as $k_F = (1 - \langle M \rangle)\pi/2$. Either the XXZ anisotropy or an external magnetic field modify the scaling dimensions of the physical fields through K and the commensurability properties of the spin operators, as can be seen from Eqs. (3) and (4). The nonuniversal constants a , b , and c can be in general computed numerically (see, e.g., Ref. 21, for the case of zero magnetic field) and in particular the constant b has been obtained exactly in Ref. 22.

For the sake of clarity, let us first consider the effect introduced by a *single* frequency term in Eq. (1), i.e., $\epsilon_n = \delta \cos(2\pi\omega n)$. Thus using Eqs. (3) and (4) it follows that the relevant part of the interaction term in $H_{qp} = H + H_{int}$ reads

$$H_{int} = \sum_x \cos(2\pi\omega x) [\lambda_1 (\partial_x \tilde{\phi})^2 + \lambda_2 (\partial_x \phi)^2 + \lambda_3 \cos(2k_F x + \sqrt{2\pi}\phi) + \lambda_4 \sin(2k_F x + \sqrt{2\pi}\phi)], \quad (5)$$

where $\lambda_i \propto \delta$, $i = 1, \dots, 4$.

As in previous analysis^{16–18} one can readily obtain the necessary quantization condition for the appearance of a plateau by looking at the commensurability of the relevant operators. In the present case we need only to consider the vertex operators $\exp \pm i\sqrt{2\pi}\phi$ of scaling dimension $d = 1/(4\pi R^2)$. Therefore we obtain that $\langle M \rangle$ should satisfy

$$\langle M \rangle = \pm(2\omega - 1), \quad (6)$$

in order for a plateau to be present. The fulfillment of this condition opens a spin-gap excitation since the operator in question is relevant at least for $0 < \Delta < 1$. In the region $-1 < \Delta < 0$ a critical curve appears which can be determined from the Bethe-Ansatz solution for $R(\langle M \rangle, \Delta)$.¹⁸ Furthermore, the gap width can be easily computed to scale as $\delta^{1/(2-d)}$. Notice that the perturbations $\lambda_{1,2}$ do not play a role here since they are incommensurate whenever Eq. (6) holds.

In fact, these expectations turn out to apply well above the weak-coupling regime discussed so far. In Fig. 1 we show the magnetization phase diagram resulting from exact diagonalization of fairly large XX chains (10^5 spins) by setting $\omega = 13/21$ through a wide range of couplings. Notice that for rational frequencies, $\omega \in \mathbb{Q}$ and $\delta \rightarrow \delta_c$, for some appropriate value of δ_c which depends on ω , the chain breaks up into a periodic collection of *finite* segments which naturally yield additional plateaus of rational values. Being the unit cell composed of 21 spins one would naively expect plateaus to appear for values of $M = (2n+1)/21$, $n = 0, \dots, 10$, but as can be seen from Fig. 1 this is not the case due to the non-trivial structure of the unit cell and only some of these values are indeed observed. Interestingly, Eq. (6) yet remains robust all the way through the decoupling point and the corresponding plateau corresponds to the most prominent.

These observations were also corroborated on XXZ chains. However, owing to the large spaces involved in their diagonalization now we content ourselves with moderate lengths L (up to 24 spins). After resorting to the Lanczos method²³ in each of the magnetization subspaces with $S^z \in \{0, 1, \dots, L/2\}$, we built up the magnetization contours

FIG. 1. Critical fields (in bold lines) of the XX chain with $\omega = 13/21$ and 10^5 spins. At $\delta = 0.9$ these fields conform the standard magnetization curve displayed in the inset. Vertical lines denote regions of massless spin excitations where the magnetization increases continuously with h . Empty zones in ascending order represent plateaus appearing at $\langle M \rangle = 1/21, 5/21$ [central region expected by Eq. (6)], $9/21, 11/21$, and $15/21$ before saturation (top zone).

shown in Fig. 2 using $\omega = 5/8$ for $L = 8, 16, 24$. As expected, the massless XXZ excitations around $\langle M \rangle = 1/4$ render size effects rather noticeable within small coupling regions. Nevertheless, already for $\delta > 0.2$ they clearly become less pronounced, thus lending our results further support to the bosonization picture.

A word of caution should be added here, namely, the importance of periodic boundary conditions (PBC's) in testing

FIG. 2. Magnetization contours of the isotropic ($\Delta = 1$) XXZ chain for $\omega = 5/8$. Solid, dashed, and dotted lines stand, respectively, for the critical fields of $L = 24, 16$, and 8 . The middle empty region corresponds to the $\langle M \rangle = 1/4$ plateau expected by Eq. (6). The inset shows one of the typical magnetization curves upon setting $\delta = 0.5$.

FIG. 3. Magnetization curves of a dimerized Heisenberg chain ($\omega = 1/2$ with $\delta = 0.4$), using *open* boundary conditions displaying a plateau at $\langle M \rangle = 2/L$. Solid, dashed, and dotted lines denote, respectively, the results of $L = 24, 20$, and 16 .

the analytic approach via exact diagonalization of small systems. Already at the level of a simple dimerized chain ($\omega = 1/2$), PBC's become crucial. In fact, the numerical analysis of this latter situation using *open* boundary conditions shows that the well-known $\langle M \rangle = 0$ plateau expected in the large length L limit actually emerges at $\langle M \rangle = 2/L$. Figure 3 illustrates this observation for $L = 24, 20$, and 16 and should emphasize the essential role of PBC's in all our subsequent numerical checks.

By construction, the bosonization approach can be straightforwardly extended to the case in which more than one frequency is present in ϵ_n . It turns out that whenever condition (6) is satisfied *for each frequency*, a magnetization plateau shows up. This extension is simple since each operator (corresponding to each frequency) is commensurate separately, and hence the different perturbations can be treated separately. Of course the situation changes in the case of a dense multifrequency spectrum (such as in the Fibonacci potential that we discuss below) and a more complete analysis has to be carried out.¹¹

In order to test the reliability of these predictions, we have analyzed numerically both XX and XXZ chains using double frequency couplings. In Fig. 4 we display the magnetization curves obtained for $\omega_1 = 5/8, \omega_2 = 7/8$ with amplitudes $\delta_1 = 0.2$ and $\delta_2 = 0.3$, respectively. As we mentioned before, the rather robust plateaus emerging at $\langle M \rangle = 1/4$ and $3/4$ not only confirm the correctness of our extended bosonization prediction, but also pave the way to an alternative description of the massive spin excitations observed in NH_4CuCl_3 ; a quasi-one-dimensional $S = \frac{1}{2}$ compound which is attracting both theoretical and experimental attention and whose magnetization behavior yet remains unexplained.^{19,24,25} Of course, a more realistic description of this material must start from the microscopic structure observed by x-ray spectroscopy, which points to a two-leg zigzag ladder. Still, it is quite encouraging to obtain a magnetization curve qualitatively similar with the simple two-frequency model we considered here.

In studying irrational frequencies or other quasiperiodic modulations, it is natural to check our analysis with the pro-

FIG. 4. Double frequency magnetization curve of the isotropic ($\Delta = 1$) XXZ chain for $\omega_1 = 5/8, \omega_2 = 7/8$ with amplitudes $\delta_1 = 0.2$ and $\delta_2 = 0.3$. Solid and dashed lines denote, respectively, the magnetizations of $L = 24$ and 16 . The inset shows the magnetization curve of the corresponding XX chain with 10^5 spins.

totype Fibonacci sequence, a coupling array $J_A = J(1 + \delta)$, $J_B = J(1 - \delta)$ generated by iterating the substitution rules $B \rightarrow A$ and $A \rightarrow AB$.^{3-5,11} Here we discuss the general XXZ situation (a related model has been studied in Ref. 26), and compare our results with the already well-known magnetization curve of the XX case.^{4,5} Before continuing with the bosonization approach, we pause to discuss the *strong* coupling regimes of this system ($\delta \rightarrow \pm 1$) in the context of a simple decimation procedure (see, e.g., Ref. 27). To evaluate the magnetization of the widest plateaus, there are two different cases to consider, according to $\delta \approx -1$, i.e., $J_B \gg J_A$, and the opposite situation for $\delta \approx 1$.

Starting from saturation, in the first case the magnetic field is lowered until it reaches the value $h_c \approx J_B$ at which the type- B bonds experience a transition from the state of maximum polarization to the singlet state. The magnetization at this plateau is then obtained by decimating the B bonds. This simply yields $\langle M \rangle = 1 - 2N_B/(N_B + N_A)$, where $N_{A,B}$ denotes the number of bonds of type A and B , respectively. For a large iteration number of the rules referred to above ($L \rightarrow \infty$), N_A/N_B approaches the golden mean $\gamma = (1 + \sqrt{5})/2$ and therefore we find $M_1 = (\gamma - 1)/(\gamma + 1) \approx 0.236\,068$.

In the second case, $J_A \gg J_B$, we have to distinguish two different unit cells since type- A bonds can appear either in pairs (forming trimers) or isolated (forming dimers). It can be readily checked that when lowering the magnetic field from saturation the first spins to be decimated correspond to those forming trimers. We then find two plateaus at $M_2 = 1 - 2/\gamma^3 \approx 0.527\,864$ (after decimating trimers) and, like the case $\delta \approx 1$, at M_1 (after decimating the remaining dimers). Since the decimation procedure applies for generic XXZ chains,²⁷ we conclude that the emergence of these strong coupling plateaus is a generic feature, at least with an antiferromagnetic anisotropy parameter $0 < \Delta < 1$.

For intermediate regimes $0 < |\delta| < 1$ the magnetization curve has a much richer structure which can be easily understood from our bosonization analysis in a multifrequency case. Evidently, the self-similar hierarchy of frequencies re-

FIG. 5. Fibonacci magnetization for $\delta=0.5$ and $F(25)=75025$ XX spins (bold line). Here, $F(25)$ denotes the 25th Fibonacci number defined as $F(n+1)=F(n)+F(n-1)$ with $F(1)=F(2)=1$. Dotted and solid lines stand, respectively, for the single and double frequency approximants to the M_1 and M_2 plateaus referred to in the text. The slopes compared in the inset show the gap width of M_2 and M_1 , in ascending order. Bold lines denote the Fibonacci gaps whereas solid lines represent the double approximant widths.

sulting from the Fourier transform of the Fibonacci exchanges (see, e.g., Ref. 11) along with the quantization condition studied so far, enables us to reconstruct the whole spin gap structure of the Fibonacci chain, at least for $|\delta| \ll 1$ and as long as the operator responsible for the plateaus is relevant. Actually, it turns out that one can obtain a fair approximation to the latter showing the most important plateaus by keeping just a few numbers of main spectrum frequencies, even beyond weak-coupling regimes. Interestingly, when the constraint (6) is applied to the dominant Fibonacci frequencies $\omega_1=1/\gamma$ and $\omega_2=2(1-1/\gamma)$ it yields precisely the M_1 and M_2 plateaus arising from the strong-coupling decimation. These results are shown in Fig. 5 where both single and double frequency approximations are dis-

played. Moreover, using the Fourier spectrum to set $\delta_2/\delta_1 \approx 0.36237$, the Fibonacci gap widths exhibit a remarkable agreement with the scaling exponents $1/(2-d)$ referred to above. This can be observed in the inset over more than three decades in δ . In turn, this supports the observation that *all* gap widths of the XX Fibonacci chain scale simultaneously with δ , as for $\Delta=0$ the compactification radii comprehended in the scaling exponents are independent of the magnetization [$R \equiv 1/(2\sqrt{\pi})$] (see, e.g., Ref. 18).

Finally, we point out that for the Fibonacci chain (which has a dense Fourier spectrum), it was shown by solving the one-loop RG equations at zero magnetic field¹¹ (see also Ref. 12) that the critical value of R at which the Kosterlitz-Thouless transition occurs is moved to $R_c = 1/\sqrt{4\pi}$, in contrast to $R_c = 1/\sqrt{8\pi}$ for the single, or more generally non-dense frequency case. Hence, for $0 < \Delta < 1$ and arbitrary magnetization, the operator responsible for spin gap openings at each of the Fibonacci frequencies is relevant. Therefore the magnetization curve of the XXZ case with antiferromagnetic anisotropy is of the same form as that of the XX situation (see Fig. 5), though with different plateau widths.

To summarize, we have studied the interplay between quasiperiodic exchanges and uniform magnetic fields in strongly correlated antiferromagnetic chains using both bosonization and numerical techniques. The former were tested and complemented by the latter in a variety of nonperturbative scenarios. Our calculations suggest the possibility to observe rather stable magnetization plateaus [Eq. (6)] on artificially grown arrays of quantum dots⁹ according to the (controlled) spatial distribution of their exchange integrals. We trust this work will convey an interesting motivation for further experimental studies in these material technologies.

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