Competing interactions in the *XYZ* model

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We study the interplay between an *XY* anisotropy γ, exchange modulations, and an external magnetic field along the *z* direction in an *XYZ* chain using bosonization and Lanczos diagonalization techniques. We find an Ising critical line in the space of couplings which occur due to competing relevant perturbations that are present. More general situations are also discussed.

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I. INTRODUCTION

The competition between different relevant perturbations that can render a system critical in a certain domain of the couplings space has been studied by many authors.[1–8] Within a low-energy description of many different one-dimensional (1D) lattice models, one often finds the double-frequency sine-Gordon model,[3] that is, a U(1) scalar field with two perturbations of different frequencies. In the case where both perturbations are relevant and for a certain frequency ratio, it has been conjectured that an Ising criticality can arise.[3] Such a situation has been found in the study of different lattice systems (see, e.g., Ref. 6, and references therein). More recently, the so-called self-dual sine-Gordon model has been studied in Ref. 6.

A simple realization of this situation is found in an exactly solvable case, i.e., in the dimerized *XY* chain[8,9] and a qualitative analysis of the phase diagram has been presented for more general cases in a field.[8] The effect of an *XY* anisotropy has also been studied for the Fibonacci *XY* chain in a magnetic field where it was shown that the rather involved staircase structure of the magnetization curve gradually disappears by increasing the anisotropy of the spin-exchange interactions.[10]

In the present paper, we present a unified picture of the above-mentioned effects and describe, by using bosonization as well as numerical techniques, generic situations in which a spin gap opening mechanism[11] competes with an *XY* anisotropy to render Ising criticality. This issue was studied first in Refs. 7 and 8. In Ref. 8, the interplay between a gap-opening perturbation and *XY* anisotropy was analyzed, and a qualitative phase diagram was proposed. In this paper, we focus on the Hamiltonian

$$H=\sum_n [(1+\gamma)S_n^xS_{n+1}^x+(1-\gamma)S_n^yS_{n+1}^y+\delta(-1)^n \times(S_n^xS_{n+1}^x+S_n^yS_{n+1}^y)+\Delta S_n^zS_{n+1}^z]-h\sum_n S_n^z, \quad (1)$$

which captures most of the essential aspects referred to above, and provide quantitative results that support the statements made in Ref. 8. A more general situation, as that arising in the Fibonacci *XYZ* chain in a magnetic field, is discussed in the conclusions.

II. FREE FERMION RESULTS

In preparation for the analysis of more general situations, first we discuss the *XY* or $\Delta=0$ case that already bears some generic features. In this case, the model is exactly solvable as it reduces to a bilinear fermionic form. As is well known, after the usual (1D) Jordan-Wigner transformation, the Hamiltonian can be readily diagonalized by means of the Bogoliubov transformation, leading to

$$H=\sum_{k=1}^{N/4}\{E_{k,0}(\delta,\gamma,h)(d_{k,0}^\dagger d_{k,0}+1)+E_{k,1}(\delta,\gamma,h)\times(d_{k,1}^\dagger d_{k,1}+1)\}, \quad (2)$$

where

$$E_{k(0,1)}=\frac{1}{\sqrt{2}}[1+\cos(k)+(\delta^2+\gamma^2)[1-\cos(k)]+2h^2 \pm f(\delta,\gamma,k,h)]^{1/2} \quad (3)$$

and

$$f(\delta,\gamma,k,h)=2(\delta^2\gamma^2[1-\cos(k)]^2+2h^2\{1+\cos(k)+\delta^2[1-\cos(k)]\})^{1/2}. \quad (4)$$

The mean value of the magnetization is thus given by

$$\langle M\rangle=\frac{\partial\langle H\rangle_{GS}}{\partial h}=\frac{1}{L}\sum_{k=1}^{N/4}\left[\frac{\partial E_{k,0}}{\partial h}(\delta,\gamma,h)+\frac{\partial E_{k,1}}{\partial h}(\delta,\gamma,h)\right], \quad (5)$$

where GS denotes the ground state, which is the vacuum of the Bogoliubov particles' Fock space. (It should be noticed that the external field does not act as a chemical potential for these particles.)

From Eqs. (3) and (4), one easily obtains the critical field values where one of the modes becomes gapless, i.e., where the Ising transition occurs[8]

$$h_c=\pm\sqrt{\delta^2-\gamma^2}, \quad (6)$$

which shows that the Ising transition can only occur for $\delta>\gamma$.

The exact magnetization curve shown in Fig. 1 displays all the features we want to discuss (we focus in the region of

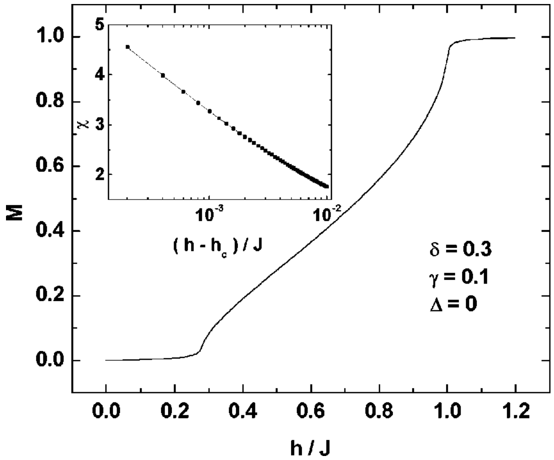

FIG. 1. Exact magnetization curve of the *XY* case. The inset displays the logarithmic singularity dominating the susceptibility at $h_c = \sqrt{\delta^2 - \gamma^2}$.

$h > 0$). First of all, one notices that there is no actual plateau since the magnetization starts to increase as soon as h is turned on, and this is due to the breaking of the U(1) symmetry for $\gamma \neq 0$. In the region of fields below h_c [Eq. (6)], we are in what we call the ''pseudoplateau region,'' where the slope of the magnetization curve is small and we have dominant density wave correlations. At the critical field, one observes the Ising transition, where the magnetization should behave as $M - M_c \propto (h - h_c)(\ln|h - h_c| - 1)$. This behavior can be understood from the analogy with the Ising model:[7,8] since the transition is driven by the magnetic field, it plays the role of temperature in the Ising model and, hence, the magnetization is the analog of the specific heat. For $h > h_c$, the system is in the *XY* phase, where the magnetization increases more rapidly and which should be characterized by a nonvanishing order parameter that is the x (or y) component of the staggered magnetization. However, the analysis of the latter becomes rather subtle—even for the simple nondimerized ($\delta = 0$) case.[17] These phases are illustrated schematically in Fig. 2. Finally, a second Ising transition is observed before saturation, which occurs at $h = 1$ independent of the values of δ and γ. For $\delta < \gamma$, the first transition does not occur.

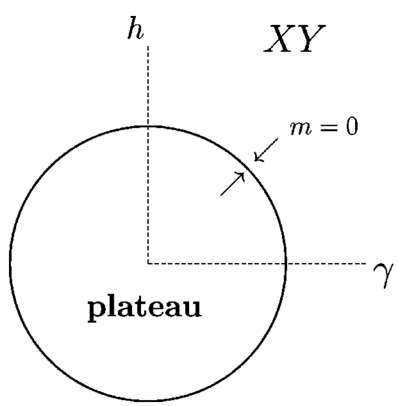

FIG. 2. Schematic ground-state diagram for $\Delta = 0$. On approaching the massless transition line (6), the magnetic susceptibility diverges as $\chi(h) \propto \ln|h - h_c|$.

III. BOSONIZATION ANALYSIS

We discuss the results obtained so far within the bosonization approach given below, where we argue that the same picture is valid for arbitrary Δ, provided δ and γ are suitably renormalized. For small γ and δ, one can study the effects of such perturbations using bosonization, which allows one to include Δ and h exactly through the Bethe ansatz solution for the Luttinger parameter K.

The large-scale behavior of the *XXZ* chain can be described by a U(1) free boson theory with Hamiltonian

$$H_0 = \frac{1}{2} \int dx \left(vK(\partial_x \tilde{\phi})^2 + \frac{v}{K}(\partial_x \phi)^2 \right), \tag{7}$$

which corresponds to the Tomonaga-Luttinger Hamiltonian. The field ϕ and its dual $\tilde{\phi}$ are given by the sum and difference of the light-cone components, respectively. The constant K 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. 12 for a detailed summary, and references therein). We have $K = 1$ for the SU(2) symmetric case ($\Delta = 1$) which is related to the radius R of Ref. 12 by $K^{-1} = 2\pi R^2$. In Eq. (7), v corresponds to the Fermi velocity of the fundamental excitations of the system. In terms of these fields, the spin operators read

$$S_x^z \sim \frac{1}{\sqrt{2\pi}} \partial_x \phi + a{:}\cos(2k_F x + \sqrt{2\pi}\phi){:} + \frac{\langle M \rangle}{2}, \tag{8}$$

$$S_x^{\pm} \sim (-1)^x {:} e^{\pm i\sqrt{2\pi}\tilde{\phi}}[b\cos(2k_F x + \sqrt{2\pi}\phi) + c]{:}, \tag{9}$$

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 $k_F = (1 - \langle M \rangle)\pi/2$. The effect of an *XYZ* anisotropy and/or the external magnetic field is then to modify the scaling dimensions of the physical fields through K and the commensurability properties of the spin operators, as can be seen from Eqs. (8) and (9). The constants a, b, and c were numerically computed in the case of zero magnetic field[13] (see also Ref. 14).

The bosonized Hamiltonian including the perturbations then reads

$$H_{bos} = H_0 + \lambda_1 \int dx \cos(\sqrt{2\pi}\phi) + \lambda_2 \int dx \cos(\sqrt{8\pi}\tilde{\phi}), \tag{10}$$

where $\lambda_1 \propto \delta$ and $\lambda_2 \propto \gamma$.

The scaling dimensions of the perturbations in Eq. (10) are $K/2$ and $2/K$, respectively, which in the *XX* case ($K = 2$) are both equal to unity. This allows one to understand, within this approach, the appearance of the Ising transition[6] since in this self-dual case and for $h = 0$ one can map the bosonic system into two Majorana fields, and the critical line is given by $\lambda_1 = \pm \lambda_2$, where one of the masses of the two Majorana fields vanishes rendering criticality. As soon as the external field is turned on, the masses of these Majorana fermions change and we then need a bigger value of λ_1 (i.e., δ) to find the transition[8] [see Eq. (6)].

This can be extended for $\Delta > 0$, since its only effect is to modify the scaling dimensions of the two perturbations through $K(\Delta,h)$. It is interesting to note, however, that for $\Delta > 0$, the cosine of the dual field is less relevant, becoming barely marginal for $\Delta=1$ and $h=0$ $[K(1,0)=1]$; opening the question if one should still expect the Ising transition to occur. One can argue that this is so by analyzing the one-loop renormalization group equations given by

$$\frac{d\lambda_1(l)}{dl} = \left(2-\frac{K}{2}\right)\lambda_1(l),$$

$$\frac{d\lambda_2(l)}{dl} = \left(2-\frac{2}{K}\right)\lambda_2(l),$$

$$\frac{dK(l)}{dl} = -\frac{K^2}{2}\lambda_1^2(l) + 2\lambda_2^2(l). \tag{11}$$

The large-scale behavior of the parameters obtained from these equations shows that the competition between the two cosines can still occur, giving rise to the Ising criticality even in this limiting situation. From this qualitative analysis one expects, using power counting, a critical line for $h=0$ given by

$$\delta \propto \gamma^{\nu} \tag{12}$$

with $\nu = K_{eff}(1-K_{eff}/4)/(K_{eff}-1)$, where K_{eff} is the large-scale value of K.

We provide numerical evidence for the validity of Eq. (12) with $\nu=1$ below.

c. Numerical Results. In what follows, we examine this latter conjecture by studying numerically the extreme SU(2) case ($\Delta=1$). On the other hand, this enables an independent test of the bosonization scenario within nonperturbative regimes.

First, we computed the gap of Hamiltonian (1) at $\langle M \rangle = 0$ by means of Lanczos diagonalizations[15] of finite chain lengths L with periodic boundary conditions. If $L/4$ is an integer, it turns out that the ground state is even, i.e., $\exp(i\pi\Sigma_n \sigma_n^+ \sigma_n^-) \equiv 1$, otherwise the gap spectrum has to be computed within the odd subspace of H.[16] In Fig. 3, we display the results so obtained for $14 \leqslant L \leqslant 22$ (see Ref. 18). As expected, finite-size effects become noticeable on approaching the critical regime encompassed within the pronounced gap minima, whereas convergence towards the thermodynamic limit becomes typically logarithmic.[19] Interestingly, the locations of these minima result, however, fairly independent of the system size, thus, facilitating the estimation of the critical line. For $L \leqslant 12$, however, the spectrum gap increases monotonically with $|\gamma|$. Therefore, to avoid misleading results, we dismiss the data of these small sizes. In turn, this impedes the usage of most of the recursive extrapolation algorithms encountered in the literature,[19] which show their full strength only if they can be iterated several times on a large sequence of sizes. Thus, we content ourselves with a standard (logarithmic) gap extrapolation of

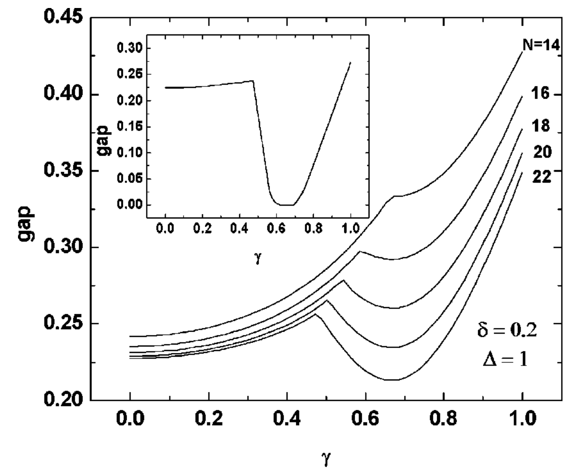

FIG. 3. Gap spectrum for different sizes of Hamiltonian (1) with $\Delta=1$. The inset exhibits the (estimative) gap extrapolations to the thermodynamic limit.

the form $g \simeq \mathrm{gap}(L) + A/L^B$. Though semiquantitative [i.e., $A=A(\gamma,\delta)$ and $B=B(\gamma,\delta)$], the results shown in the inset of Fig. 3, nevertheless, indicate a gap closing at the minima of the finite-size data.

In studying numerically the massless regime, obtained from such minima, however, it should be borne in mind that finite-size corrections to the gap of the homogeneous Heisenberg chain ($\gamma=\delta=0$) vary slowly as $\ln(\ln L)/\ln^2 L$, thus affecting the results over a wide range of sizes.[20] Therefore, we are confronted to restricting considerations to regimes where either $|\gamma|$ or $|\delta|$ is not too small. Figure 4 exhibits our estimation of the critical line down to $\delta=0.15$, above which, however, a wide linear regime shows up, in agreement with the bosonization approach. Indeed, our numerical estimations suggest $\nu \approx 1$. Similar results were observed for $0 < \Delta < 1$ as well.

Second, we turn to the GS magnetization curves of Hamiltonian (1). These were calculated numerically as $(1/L)\Sigma_j \langle GS|\sigma_j^z|GS\rangle$, where in general the parity $\exp(i\pi\Sigma_n \sigma_n^+ \sigma_n^-)$ of $|GS\rangle$ comes out to be both field and size dependent. In spite of the existence of a whole massive re-

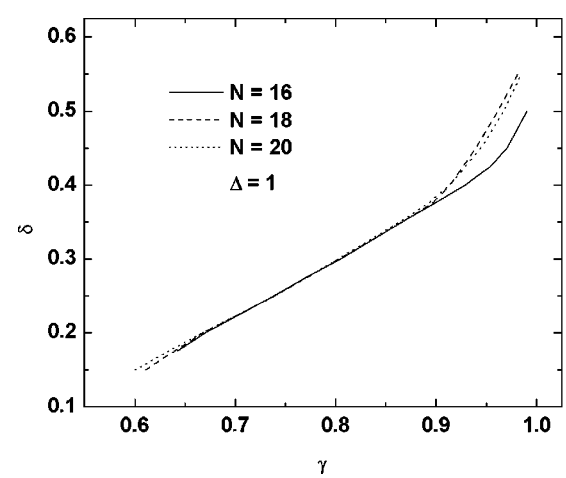

FIG. 4. Gapless line of Hamiltonian (1) in the (γ,δ) coupling parameter space arising from the positions of the gap minima of finite samples with $\Delta=1$ and $\langle M \rangle = 0$.

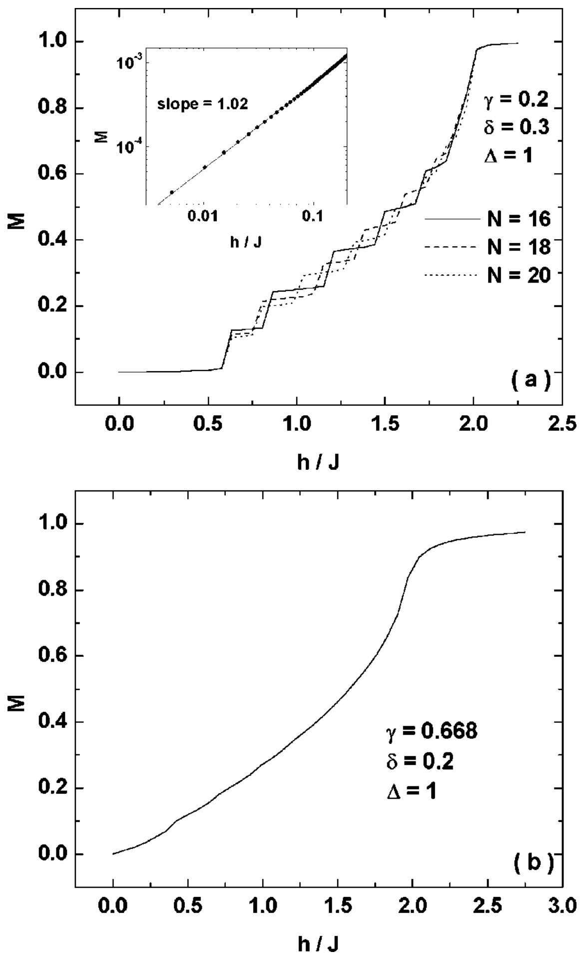

FIG. 5. Magnetization curves for $\Delta = 1$. (a) The piecewise continuous behavior is related to parity changes in the ground state. The inset exhibits the linear response at low-field regimes. (b) Results arising for a massless (γ, δ) point.

gime away the critical line, the magnetization grows linearly for small applied fields h (a feature that holds also for $\Delta = 0$), rather than displaying a plateau at $\langle M \rangle = 0$. This is shown by the inset of Fig. 5(a). Since this latter regime is dominated by a finite gap width (i.e., short-range correlations), finite-size effects become negligible there. This renders our low-field results most reliable, until the first parity change in $|GS\rangle$ occurs (signaled by an abrupt increase of the magnetization), probably associated to the emergence of gapless modes such as those referred to in the free fermion case. When selecting the Hamiltonian parameters in a massless (zero-field) point, an interesting effect—yet to be understood—occurs. As is shown in Fig. 5(b), this results in the removal of all the pseudoplateaux observed in Fig. 5(a) with a massive γ-δ point. Also, notice that near the brink of saturation, in either case the susceptibility tends to diverge, alike the XY situation.

Finally, we address to the predicted Ising behavior of the magnetization curves near the critical fields h_c discussed in the previous sections. Upon estimating the former with the fields $h_c(L)$ involving the first parity jump in the GS of a finite chain, we obtained a fair logarithmic regime actually applying over more than two decades in $(h-h_c)(\ln|h-h_c|$

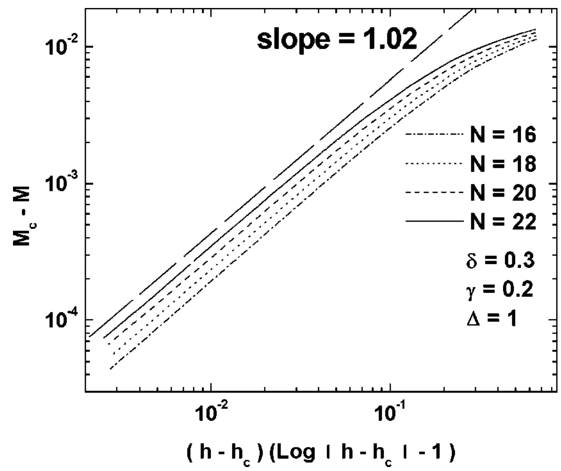

FIG. 6. Magnetization behavior for $\Delta = 1$ near critical fields referred to in the text. The slope value suggests the emergence of a logarithmic regime as that observed in Fig. 1.

$-1)$. This is displayed in Fig. 6. The value of the upper line slope results almost independent of the system size and is indicative of the logarithmic regimes entailed both by the free fermion and bosonization approaches.

IV. CONCLUSIONS

To summarize, we have studied how the tendencies towards the formation of massive spin excitations (through dimerized δ exchanges) and towards the XY ordering (via pairing of γ-interactions), compete with each other. In the bosonization picture, these tendencies manifest themselves in the existence of two (competing) relevant interactions and bring about the Ising transition, which in fact is connected to the same one driven by an external field. Due to the breaking of the U(1) symmetry, the latter does not couple to any conserved quantity and, therefore, the magnetization process gets essentially modified with respect to the $\gamma = 0$ case, i.e., it ever increases in spite of the presence of massive regimes.

Both the bosonization and the numerical analyses support the picture that the physical mechanism rendering the Ising transition is quite general, and valid both in the strong and weak coupling limits. Following the ideas given in Ref. 21, one can conjecture that a similar picture for each plateaux in the XYZ Fibonacci chain holds. The mechanism in that case is the same, where the relevant operator coming from dimerization is replaced for each plateaux by the operator *commensurate* at the corresponding frequency of the Fibonacci Fourier spectrum. From this, one concludes that a similar picture as that found in the XY case[10] is also valid for generic XYZ Fibonacci chains.

The numerical analysis lent further support to our theoretical results within several nonperturbative situations. We found evidence of a massless line along with the expected Ising like behavior near critical fields. In turn, this suggests that most basic features of the fully interacting system can be captured by the free fermion picture discussed above. How ever, the issue as to whether or not *all* of the GS parity changes induced by the field [Fig. 5(a)] correspond to Ising transitions in the thermodynamic limit, remains quite open. In this latter regard, it will be interesting to elucidate whether there is an intrinsic relation between the vanishing of these quasiplateaux [Fig. 5(b)] with the gap closing at $h\equiv 0$.

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