Random Bond XXZ Chains with Modulated Couplings

D. C. Cabra,[1,2] A. De Martino,[3] M. D. Grynberg,[1] S. Peysson,[3] and P. Pujol[3]

[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*
[3]*Laboratoire de Physique, Groupe de Physique Théorique ENS Lyon, 46 Allée d'Italie, 69364 Lyon Cédex 07, France*

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The magnetization behavior of q-periodic antiferromagnetic spin-$1/2$ Heisenberg chains under uniform magnetic fields is investigated in a background of disorder exchange distributions. By means of both real space decimation procedures and numerical diagonalizations in XX chains, it is found that for binary disorder the magnetization exhibits wide plateaus at values of $1 + 2(p - 1)/q$, where p is the disorder strength. In contrast, no spin gaps are observed in the presence of continuous exchange distributions. We also study the magnetic susceptibility at low magnetic fields.

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The study of low dimensional antiferromagnets has received much renewed attention largely owing to the synthesis of ladder materials [1]. One particular issue that captured both experimental and theoretical efforts in the past few years is the appearance of magnetization plateaus, i.e., massive spin excitations in the magnetization curve. In general, the latter are quite robust and for pure spin systems appear at rational magnetization values [2–4]. More recently, some experiments have indeed confirmed these theoretical predictions in a few particular cases [5] but some issues yet remain unresolved [6].

In order to make closer contact with experiments, one has to take into account the disorder that is almost inevitably present due to lattice imperfections and magnetic doping. A relevant question related to the appearance of magnetization plateaus is whether they are robust in the presence of quenched disorder. As a first step in this direction, in this paper we analyze the effect of a disordered distribution of exchange couplings with a periodically modulated mean on the magnetic behavior of an XXZ antiferromagnetic chain. Both even [7] and odd [8] modulations are known to exist and are ultimately responsible for the structure of the magnetization curve [2,3,9]. q-merized XX chains have also been studied in [10] using a Jordan-Wigner transformation.

By means of a decimation procedure similar to that used in [11,12] we argue that plateaus in the magnetization curve appear at specific magnetization values m which depend both on the couplings periodicity q and the strength of the disorder p. Hence disorder, instead of removing completely the plateau structure, shifts the position of certain plateaus in a precise way which depends on the disorder strength. Surprisingly, as we shall see from our numerical evidence, the plateaus predicted via this simple argument are indeed present. Moreover, they are rather wide and therefore could be eventually observable in low temperature experiments which in turn would allow for a precise determination of the disorder degree.

By extending the methods of [13], we also investigate the characteristics of the magnetic susceptibility at low fields. Its behavior shows an interesting even-odd effect, similar to that found in the study of disordered XX N-leg ladders [14]. In fact, for q odd we find the same kind of divergence as for the homogeneously disordered case ($q = 1$) [13], namely,

$$\chi_z \propto \frac{1}{H[\ln(H^2)]^3}, \tag{1}$$

whereas the even q modulations yield a generic nonuniversal power law behavior as in [15,16] for $q = 2$,

$$\chi_z \propto H^{\alpha - 1}, \tag{2}$$

where we give an analytic expression for α for arbitrary q. In principle, these results should emerge from experimental susceptibility measurements in disordered low dimensional compounds.

In what follows we focus attention on the occurrence conditions of zero temperature plateaus in a random q-merized XXZ spin-$1/2$ chain whose Hamiltonian is

$$H = \sum_i J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \tag{3}$$

where J_i are randomly distributed bonds. Specifically, let us consider a binary distribution of strength p ($p = 0$ corresponds to the pure q-merized case, while $p = 1$ corresponds to the uniform chain),

$$P(J_i) = p\,\delta(J_i - J') + (1 - p)\,\delta(J_i - J_0 - \gamma_i J), \tag{4}$$

where $\gamma_i \equiv \gamma$ $(-\gamma)$ if $i = qn$ $(i \neq qn)$, along with a Gaussian disorder $P(J_i) \propto \exp(-\frac{(J_i - \overline{J}_i)^2}{2\sigma_i^2})$ and a log-normal distribution given in terms of $W_i = \ln(J_i)$ and $P(W_i) \propto \exp(-\frac{(W_i - \overline{W}_i)^2}{2\lambda_i^2})$. All of these distributions, taken with same mean and variance, are built to enforce

q-merization, whose value is measured on average by γJ. In what follows we assume that J' is the smallest coupling and consider $0 < \gamma < J_0/J$.

(a) *Decimation procedure.*—Here we follow the arguments used by Fisher in [12]. The procedure is roughly to decimate the strongest bonds up to an energy scale given by the temperature. The remaining spins can be considered as free, and each of them will then give rise to a Curie behavior in the magnetic susceptibility.

In our problem (which is at $T = 0$) the energy scale is provided by the magnetic field, and, in order to compute the magnetization, decimation has to be stopped at an energy scale of the order of the magnetic field. We assume that all spins coupled by bonds stronger than the magnetic field form singlets and do not contribute to the magnetization, whereas spins coupled by weaker bonds are completely polarized. The magnetization is thus proportional to the fraction of remaining spins at the step where we stop decimation. Our argument happens to apply well to the binary distribution, provided the energy scales of the involved exchanges are well separated.

(b) *Plateaus in q-merized chains.*—Let us first consider the case $q = 2$ and assume we start at high enough magnetic field, such that all spins are polarized (saturation, $m = 1$) and begin decreasing 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 $m = p$. This can be easily understood: at $h \sim J_0 + \gamma J$ we can decimate all of the strongest bonds $J_0 + \gamma J$ (the corresponding spin pairs form singlets and do not contribute), and the number of remaining (completely polarized) spins is $N - 2 \times (1 - p)N/2 = pN$. Here, the factor of 2 comes from the removal of two spins each time we decimate a bond. Hence, the first plateau occurs at $m = p$. The appearance of this spin gap is due to the fact that the remaining strongest bonds have values $J_0 - \gamma J$ [17], and all spins left from the first step of decimation remain polarized (and the magnetization constant) until the magnetic field decreases to $h \sim J_0 - \gamma J$. At this point the magnetization again decreases abruptly and a second plateau occurs. The abrupt change corresponds to the decimation of bonds $J_0 - \gamma J$ which leaves us with $N - 2 \times (1 - p)\frac{N}{2} - 2 \times (1 - p)\frac{N}{2}p^2$ completely polarized bonds. The plateau occurs then at magnetization $m = p - p^2 + p^3$. The term $(1 - p)\frac{N}{2}p^2$ comes from the bonds $J_0 - \gamma J$ which, having a J' bond at each side, were not decimated in the first step and thus is the number of bonds actually decimated at the second step. Evidently, for $q > 2$ we can follow the same reasoning. Thus, the number of spins which yield finite contributions to the total magnetization at $h \sim J_0 + \gamma J$ is simply $N - 2 \times (1 - p)N/q$. Hence, we find the first plateau at

$$m = 1 + \frac{2}{q}(p - 1). \quad (5)$$

Notice that this result locates correctly the spin gaps appearing in a pure q-merized chain ($p = 0$). In this sense, Eq. (5) provides an extension of this latter case [9] in the presence of binary disorder. Since the decimation procedure applies for generic XXZ chains [12], we conclude that the emergence of the plateaus predicted in (5) is a generic feature, at least with the anisotropy parameter $|\Delta| < 1$. It is straightforward to generalize this analysis to the case of an arbitrary but *discrete* probability distribution. Given a finite difference between the highest values of the couplings in the nonequivalent sites, one can predict the presence and position of the plateaus.

To enable an independent check of these assertions, we turn to a numerical diagonalization of the Hamiltonian (3), contenting ourselves with the analysis of the subcase $\Delta = 0$. This allows us to explore rather long chains, using a fair number of disorder realizations. In Figs. 1(a)–1(c) we show, respectively, the whole magnetization curves obtained for $q = 2$, 3, and 4 after averaging over 100 samples of $L = 5 \times 10^4$ sites under the exchange disorder (4).

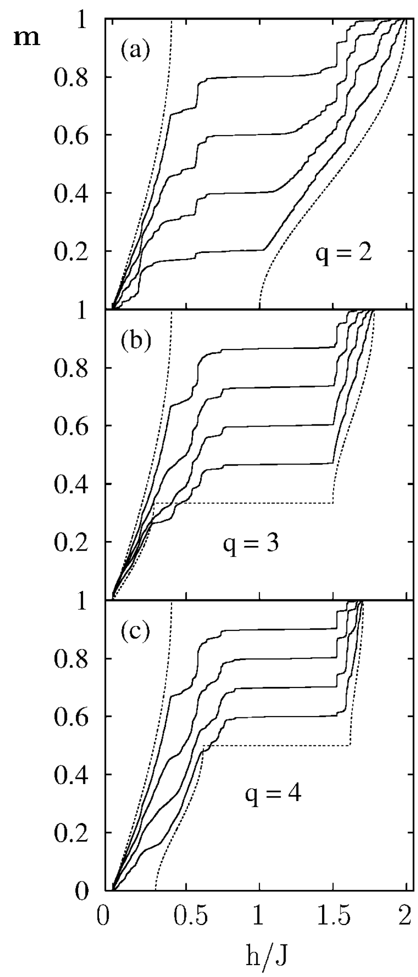

FIG. 1. Magnetization curves of modulated XX spin chains with $q = 2$ (a), 3 (b), and 4 (c), immersed in disordered binary backgrounds of strength p. The solid lines represent averages over 100 samples with 5×10^4 sites, $J'/J_0 = 0.2, \gamma J = 0.5$, and $p = 0.2$, 0.4, 0.6, and 0.8 in ascending order.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

It can be readily verified that this set of robust plateaus emerges quite precisely at the critical magnetizations given by Eq. (5). The secondary plateaus, though narrower, are still visible in Fig. 1.

It is important to stress that the derivation of our results for the quantization conditions derived above relies strongly on the discreteness of the probability distribution and would not be applicable to an arbitrary continuous exchange disorder. In fact, for the Gaussian case referred to above it turns out that no traces of plateaus can be observed. Furthermore, the magnetic susceptibility in the Gaussian case vanishes asymptotically only when approaching the saturation regime, as can be seen in Fig. 2, for a variety of coupling periodicities. Here, the sampling was improved up to 5×10^4 realizations though the length of the chain was reduced to $L = 1500$ sites, as the CPU time per spectrum grows as L^2.

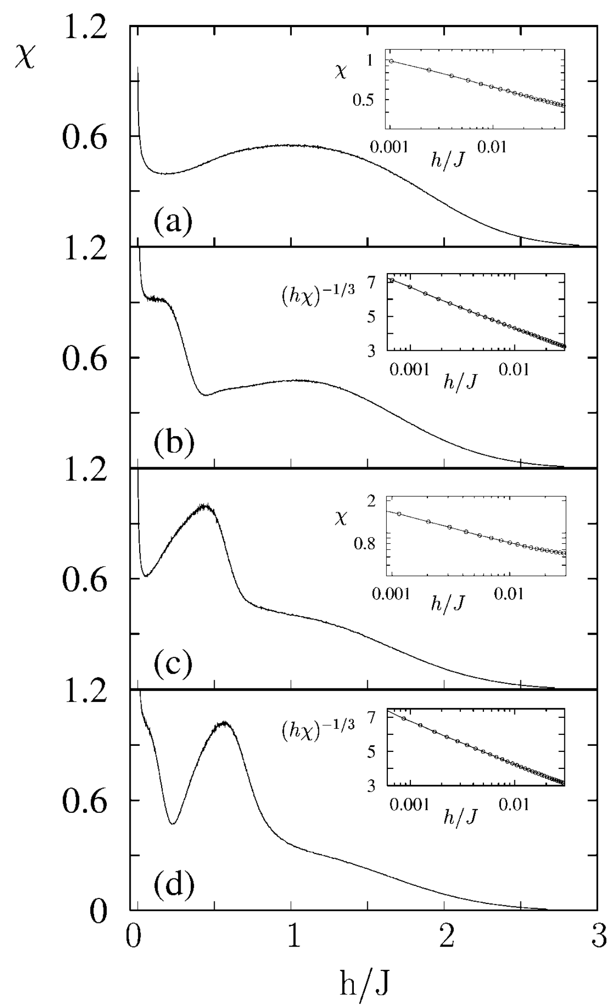

FIG. 2. Magnetic susceptibility of q-merized XX chains after averaging over 5×10^4 samples with 1500 sites, using q-periodic Gaussian exchange distributions for $q = 2$ (a), 3 (b), 4 (c), 5 (d), and strength $p = 0.4$. The insets show the susceptibility behavior at low magnetic fields which follows closely the regimes predicted by Eqs. (1) (q odd), and (2) (q even) in the text.

From the numerical curves, it appears that the usual Dzhaparidze Nersesyan–Pokrovsky Talapov (DN-PT) [18] transition is smoothed in the presence of disorder, both in the cases of binary and Gaussian distributions. By using the exact results of [19] for a family of Poissonian distributions, one sees that the behavior of the magnetization close to saturation has a nonuniversal exponential decrease. On the other hand, this nonuniversality is reflected for the binary case, in the fact that saturation occurs with an upper bound given by $2J_{\max}$. Since the universal DN-PT transition is destroyed near saturation, we expect that the same will occur in the vicinity of a nontrivial plateau. In fact, this is noticeable in the numerical data.

(c) *Susceptibility at low magnetic fields.*—For homogeneously disordered chains (i.e., $q = 1$), one can use the decimation procedure of [12], along with the universality of the fixed point, to show that either for discrete or continuous distributions the low field magnetic susceptibility behaves according to Eq. (1). Following a simple argument based on random walk motion used in [13], it can be readily shown that, for $\Delta = 0$ (or XX chains), these arguments can be extended to the case of *q odd* giving the same singularities. In fact, these expectations can be compared to the numerical results obtained for q odd with both Gaussian and binary disorders, as shown in Figs. 2 and 3, respectively. In particular, we direct the reader to the semilog insets of Figs. 2(b), 2(d), 3(b), and 3(d) which evidently follow the universal singularity referred to in Eq. (1). The numerical results for the log-normal distribution lead to the same qualitative behavior obtained for the Gaussian case.

For *q even*, for which there is a plateau at $m = 0$ in the pure case, the situation is more subtle. By using the notation of [13], for XX chains we can again define a random walk of the variable $u_i = \ln(\Delta_i)$ between the boundaries $\ln(\tilde{V}^2/E)$ and $\ln(E)$, now with a driving force F and diffusion coefficient D given by

$$F = \frac{2}{q}\langle \ln J_{i=qn}^2 - \ln J_{i\neq qn}^2 \rangle, \tag{6}$$

$$D = \frac{1}{q}[\mathrm{var}^2(\ln J_{i=qn}^2) + (q - 1)\mathrm{var}^2(\ln J_{i\neq qn}^2)]. \tag{7}$$

By means of the method given in [13] for the undriven random walk, one can approximate the problem to a discrete time diffusion problem with an absorbing and reflecting wall. One can then show that the average number of bonds for a cycle to be completed now goes like $\bar{n} \sim e^{\alpha \Delta u/2}$, which gives the asymptotic behavior for the magnetic susceptibility as in (2). The non-universal exponent α turns out to depend on the distribution parameters (6) and (7), namely, $\alpha = 2F/D$. Also, this exponent coincides with the results obtained in [16], using decimation and other methods for the $q = 2$, XXZ chain.

Once more, our numerical results for the binary and Gaussian coupling distributions considered above lend further support to this nonuniversal picture of even modulations. Specifically, there are in fact situations for which

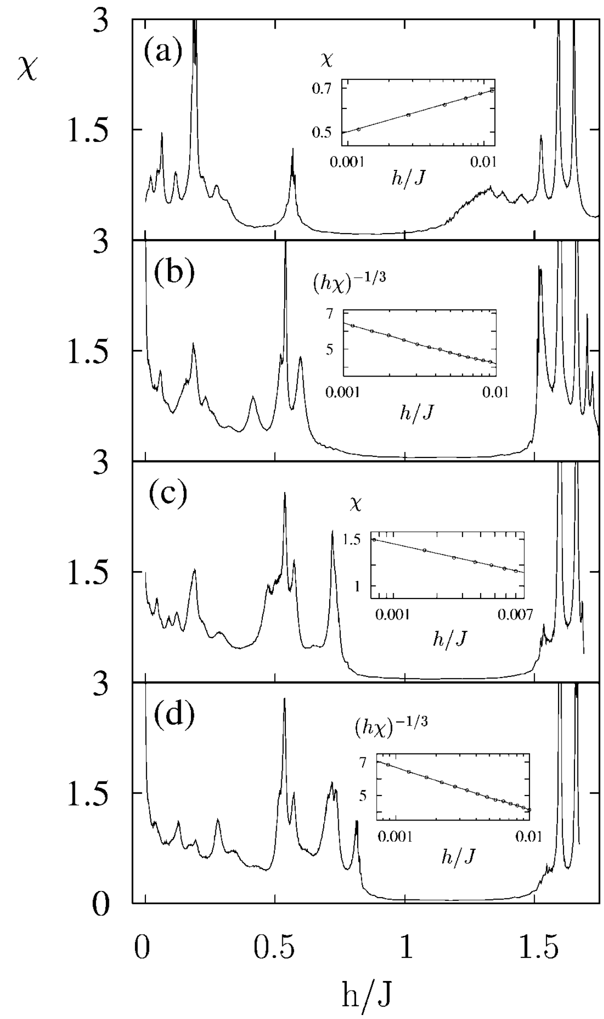

FIG. 3. Same as Fig. 2, but averaging over a binary exchange disorder of strength $p = 0.4$. The small field susceptibility behavior displayed in the insets reflects the typical singularity of odd periodicities [$q = 3$ (b) and 5 (d)], whereas even modulated distributions [$q = 2$ (a) and 4 (c)] are nonuniversal in this regime.

the low field susceptibility can either diverge ($\alpha < 1$) as displayed in Figs. 2(a), 2(c), and 3(c) or collapse ($\alpha > 1$) as shown in Fig. 3(a). Moreover, we checked that our α exponents can fit reasonably the numerical behavior obtained in this regime, as indicated by the log-log insets of Figs. 2(a) and 2(c).

To summarize, we have studied the effect of disorder on the plateaus structure in q-merized *XXZ* chains. By means of a simple real space decimation procedure we could account for a nontrivial phenomenon, namely, the shift in the magnetization values for which certain plateaus emerge, as compared to the pure system. This was tested by numerical diagonalizations of large *XX* chains finding a remarkable agreement with Eq. (5). We have also analyzed the behavior of the low magnetic field susceptibility which exhibits a clear q-odd (-even) logarithmic (power law) behavior. Our theoretical predictions could be experimentally checked on dimerized compounds such as $CuGeO_3$ doped with Si [20] under magnetic fields. Also trimerized compounds exist in nature [8] and it would be interesting to see if they can be doped. We trust this work will convey an interesting motivation for further experimental studies.

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