Comparison between disordered quantum spin 1/2 chains

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We study the magnetic properties of two types of one dimensional XX spin 1/2 chains. The first type has only nearest neighbor interactions which can be either antiferromagnetic or ferromagnetic and the second type which has both nearest neighbor and next nearest neighbor interactions, but only antiferromagnetic in character. We study these systems in the presence of low transverse magnetic fields both analytically and numerically. Comparison of results show a close relation between the two systems, which is in agreement with results previously found in Heisenberg chains by means of a numerical real space renormalization group procedure.

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I. INTRODUCTION

One-dimensional quantum spin systems have been extensively studied over the last years. In particular, randomness has a profound effect on their physical properties and is always present in real systems through impurities or structural disorder. This can even produce singular behaviors in the magnetic properties, not observed in pure systems. One of the main motivations to study disordered quantum spin chains is the possibility of classifying their behavior in universality classes associated to different regions in their phase diagrams.

In the last few years, numerical works have shown that the thermodynamic properties of disordered Heisenberg chains with nearest neighbors (NN) and next nearest neighbors (NNN) couplings, both antiferromagnetic, are very similar to those found in disordered chains with only NN couplings which can be either antiferromagnetic or ferromagnetic. In fact, it was shown that under Real Space Renormalization Group (RSRG) the former systems flow to a fixed point characterized as a chain with only NN couplings in a given distribution, taking both antiferromagnetic and ferromagnetic values.

More specifically, let us consider a Heisenberg chain with Hamiltonian

$$H = \sum_i \left( J_i \vec{S}_i \cdot \vec{S}_{i+1} + J'_i \vec{S}_i \cdot \vec{S}_{i+2} \right),$$

where $\vec{S}_i$ are spin-1/2 operators and the couplings $J_i > 0$ and $J'_i > 0$, both antiferromagnetic, follow probability distributions $P(J_i)$, $P(J'_i)$. Let us review the arguments of Ref. 22. If we consider the adjacent spins that are coupled by the strongest bond (say the spins 3 and 4 in the figure), and its neighbors, we have a problem whose Hamiltonian can be written as

$$H = H_0 + H_1 + H_{\text{rest}},$$

where

$$H_0 = J_{34} \vec{S}_3 \cdot \vec{S}_4,$$

$$H_1 = J_{23} \vec{S}_2 \cdot \vec{S}_3 + J_{45} \vec{S}_4 \cdot \vec{S}_5 + J'_{35} \vec{S}_3 \cdot \vec{S}_5 + J'_{24} \vec{S}_2 \cdot \vec{S}_4,$$

and $H_{\text{rest}}$ corresponds to all the other spins that are not coupled to spins 3 and 4.

The sole consideration of $H_0 + H_1$ is enough to determine the effective interaction between the spins 2 and 5, as follows. The ground state for the Hamiltonian $H_0$ is a singlet with energy $E_0 = -\frac{3}{4} J_{34}$ while excited triplet states have energy $E_1 = \frac{1}{2} J_{34}$. Since $J_{34}$ is the largest bond, one can take $H_1$ as a perturbation. Regarding $\vec{S}_3$ and $\vec{S}_5$ as external operators, a second-order perturbation calculation gives an effective Hamiltonian describing the low energy sector (we consider only the coupling generated between 2 and 5)

$$E = -\frac{3}{4} J_{34} - \frac{3}{16 J_{34}} [(J_{23} - J'_{24})^3 + (J_{35} - J_{45})^3]$$

$$+ \frac{(J_{23} - J'_{24})(J_{45} - J_{35})}{2 J_{34}} \vec{S}_2 \cdot \vec{S}_5.$$
From this result one can remove the spins $\vec{S}_3$, $\vec{S}_4$ from
the original Hamiltonian, replacing them by an effective NN coupling
$J_{25}$
\[
J_{25} = \frac{(J_{23} - J_{24})(J_{45} - J_{53})}{2J_{44}},
\]
between $\vec{S}_2$ and $\vec{S}_5$.

Following this RSRG decimation procedure one ends up with a NN spin 1/2 chain in which effective interactions like $J_{25}$ can be ferromagnetic. Notice that when the NNN couplings are very weak compared to the NN couplings the ferromagnetic effective interaction is unlikely to appear. On the contrary, for strong NNN couplings, RSRG does generate effective ferromagnetic couplings and the system flows to a phase controlled by large effective spins at low energies.

It is the aim of the present note to further understand the connection between these and related systems, in more general situations. In particular we are interested in comparing magnetic properties of easy plane XX spin 1/2 chains in the presence of uniform magnetic fields.

We first study analytically the magnetic properties of quantum XX spin 1/2 chains with antiferromagnetic and ferromagnetic NN interactions, using an elegant argument relating magnetization with random walk problems. In a second step we implement a numerical self consistent method based in a mean field approximation, which allows for analyzing quantum XX spin 1/2 chains with NN and NNN interactions, to be applied in the antiferromagnetic case. Finally, common features found in these spin systems are discussed.

The structure of the paper is the following. Analytical results derived from the random walk argument are presented in section II for homogeneous and dimerized disorder in antiferromagnetic NN chains, as well as novel results for dimerized distributions of antiferromagnetic and ferromagnetic couplings in NN chains. The self consistent numerical method is presented in Section III, then tested on pure (ordered) NN antiferromagnetic chains in Section IV, and finally applied to the NN disordered case in Section V. Numerical results are compared with exact diagonalization for small chains, up to 24 spins, at each step. The comparison between both types of chains, summary and conclusions are presented in Section VI.

II. ANALYTICAL TREATMENT FOR NN SPIN 1/2 CHAINS

In this Section we study analytically the magnetization of one dimensional spin 1/2 systems with NN interactions whose Hamiltonian in the XX model is
\[
H = \sum_i J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - h \sum_i S_i^z,
\]
where $J_i$ are random nearest neighbor couplings (either antiferromagnetic (AF) or ferromagnetic (F)) and $h$ is a uniform magnetic field. By means of the Jordan-Wigner transformation
\[
S_i^{+} \equiv e^{\frac{t}{\sigma}} c_i^\dagger, \\
S_i^{-} \equiv e^{-\frac{t}{\sigma}} c_i, \\
S_i^z \equiv c_i^\dagger c_i - \frac{1}{2},
\]
where $\phi_i \equiv \sum_{i=1}^{i-1} c_i^\dagger c_i$, we can rewrite this Hamiltonian in terms of spinless fermionic operators
\[
H = \sum_i t_i (c_i^\dagger c_{i+1} + \text{H.c.}) - h \sum_i c_i^\dagger c_i,
\]
in (this Section we use $t = J/2$). Notice that the magnetic field acts as a chemical potential for the fermions.

We start with the study of the homogeneous disordered case where the couplings follow a homogeneous distribution ($P(t_i) = P(t_j) \forall i, j$). Following the argument presented in Ref. [6], one can introduce a random variable $u_i$ which, for a one particle eigenstate of the Hamiltonian in eq. (2), undergoes a random walk behavior between a reflecting barrier at $u_{\text{max}} = \log(t^2/E)$ and an absorbing barrier at $u_{\text{min}} = \log(E)$. In the energy of the eigenstate and $t$ the positive average value of AF couplings $t_i$. The relevant quantity to compute here is the number of eigenstates $N(E)$ with energies below $E$, which for low energies is related to the average number $\bar{n}$ of steps necessary to complete a diffusion cycle from the reflecting barrier to the absorbing one. The relation between them is
\[
N(E) = \frac{1}{2^n} + \frac{1}{2}.
\]
In the present case one gets $\bar{n} \sim (u_{\text{max}} - u_{\text{min}})^2/\sigma^2$, where $\sigma^2$ is the variance of the coupling distribution $P$.

This result indeed describes the magnetization of the spin system $\mathcal{S}$. We write the mean magnetization $m$ in terms of fermionic variables using the Jordan-Wigner transformation
\[
m = \langle \sum_i S_i^z \rangle = \sum_i \langle c_i^\dagger c_i \rangle - 1/2,
\]
in order to exhibit the relation between magnetization and fermion filling. Recalling that the magnetic field acts as a chemical potential and regulates the fermion filling, for low magnetic field we finally obtain a mean magnetization per site
\[
M(h) \sim \frac{1}{2} \left( \frac{\sigma^2}{[\text{ln}(t/h)^{\text{2}}]^{\text{2}}} \right).
\]
(Here $M = 2m/N$, with $N$ the number of spins in the chain, is normalized to 1 at saturation).
Now we turn to the case of dimerized inhomogeneous distributions \((P_{\text{odd}}(t_i)\text{ for odd sites }i \text{ different from }P_{\text{even}}(t_j) \text{ for even sites }j)\). The result above was suitably generalized in Ref. [10] for this case: the random variable \(u_i\) undergoes a random walk with diffusion coefficient \(D\) and a driving force \(F\) given by

\[
D = \frac{1}{2} \left[ \text{var}_{\text{odd}}(\log(t_i^2)) + 2 \text{var}_{\text{even}}(\log(t_j^2)) \right],
\]

\[
F = \langle \log(t_i^2) \rangle_{\text{odd}} - \langle \log(t_j^2) \rangle_{\text{even}},
\]

where var stands for the variance of the corresponding distribution. The average numbers of steps for a diffusion cycle to be completed behaves now as \(\bar{n} \sim e^{\alpha (u_{\max} - u_{\min})/2}\). Then the magnetization of the system is seen to follow a power law

\[
M(h) \sim h^\alpha,
\]

with \(\alpha = \frac{2F}{D}\).

In what follows we generalize this procedure to study the system of interest here, namely a disordered spin 1/2 chain with AF and F NN interactions. Let us consider the following binary coupling distribution

\[
P(t_i) = xP_F(t_i) + (1-x)P_{AF}(t_i),
\]

with weight \(x\) for F couplings and \(1-x\) for AF ones, combined with dimerization in the sense described above (both \(P_F\) and \(P_{AF}\) are different for even and odd sites). A similar pattern for disorder was proposed in recent numerical studies [11].

We can again map the system onto a random walk problem with driving force and appropriate barriers. In particular the driving force can be written in terms of the single distribution parameters as

\[
F = x \langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_F + (1-x) \langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_{AF},
\]

where subindexes odd and even indicate the distribution to be used for disorder average.

Notice that even under the strong hypothesis that both single distributions are dimerized (inhomogeneous)

\[
\langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_F \neq 0,
\]

and

\[
\langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_{AF} \neq 0,
\]

the competition between AF and F couplings can eventually cancel the driving force, under the condition

\[
\langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_{AF} = x \langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_F - \langle \log(t_i^2) \rangle_{\text{odd}} / \langle \log(t_j^2) \rangle_{\text{even}} \rangle_{AF}.
\]

This shows that there are two phases present in the system. For the coupling distribution in eq. (17) we have that, at least for low magnetic field \(h\), the magnetization follows a power law \(M \sim h^\alpha\) in most of the parameter space, while there exists a line, with \(x\) satisfying eq. (20), where the magnetization is logarithmic in \(h\), \(M \sim \frac{1}{\log(h^2)}\).

It is important to stress that in the power law regime the dynamical exponent \(\alpha\) can be larger or smaller than one. For the present case it is still given by \(2F/D\) where \(F\) and \(D\) are computed as in eqs. (13) and (14) but with the binary even and odd distributions in eq. (17). When the disorder parameter (in this case \(\text{var}[\log(t^2)]\)) is small and the dimerization is no longer considered, the dynamical exponent turns out to be larger than one. In contrast, when the disorder is stronger the dynamical exponents take values smaller than one and the magnetic susceptibility displays a singularity at the origin. It is worth to point out that this behavior was also reported by RSRG studies in dimerized NN chains [11].

### III. Numerical Self Consistent Treatment for Antiferromagnetic NN Spin 1/2 Chains

In this Section we consider a spin 1/2 XX Hamiltonian in \(d = 1\) with both NN and NNN AF position dependent interactions under a uniform magnetic field, namely

\[
H = \sum_{i=1}^{N} \left[ J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_i' (S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) - h \sum_{i=1}^{N} S_i^z, \right]
\]

where \(N\) is the number of spins in the chain and periodic boundary conditions are assumed. The inclusion of NNN couplings does not allow the analytical procedure used above. We then perform a numerical self consistent mean field (SCMF) study of this system.

We first review the procedure proposed in [7] and then apply it to our present case. In terms of the fermion operators in eq. (9) this Hamiltonian reads

\[
H = \sum_{i=1}^{N} J_i \left[ \frac{c_i^{+} c_{i+1} + \text{H.c.}}{2} \right] + \sum_{i=1}^{N} J_i' \left[ e^{-i\pi n_{i+1}} c_i^{+} c_{i+2} + \text{H.c.} \right] - h \sum_{i=1}^{N} \left( c_i^{+} c_i - \frac{1}{2} \right).
\]

First, in order to enable a single particle treatment of \(H\), we approximate the local fermionic occupation numbers \(\hat{n}_i = c_i^{+} c_i\) by their expectation values in an arbitrarily chosen initial state to be varied and determined self consistently. The local parameters \(n_i\) satisfy the constraint
\[ \sum_{i=1}^{N}(n_i - 1/2) = m, \] with \( m \) the system magnetization. Then, in this mean field (MF) approximation the Hamiltonian can be written as a quadratic form
\[ H_{XX}^{(MF)}(\{n_i\}) = \sum_{i,j} c_i^\dagger J_{ij}(\{n_i\}) c_j, \] (22)

where
\[ J_{ij}(\{n_i\}) = \begin{cases} \frac{J}{2} & \text{if } i, j \text{ are NN}, \\ \frac{J'}{2} e^{i\pi n_{i+1}} & \text{if } i, j \text{ are NNN}, \\ 0 & \text{otherwise}. \end{cases} \]

We have omitted the Zeeman term \( h \sum_{i=1}^{N}(c_i^\dagger c_i - \frac{1}{2}) \) as, being diagonal, it can be added later on.

It is our aim to find an approximation to the actual ground state (GS) at a given magnetization \( m \). Thus, we estimate this state in the MF Hamiltonian \( H_{XX}^{(MF)} \) by solving the one particle spectrum and filling the lowest energy-levels to satisfy the constraint \( \sum_{i=1}^{N}(n_i - 1/2) = m \). Then, we compute a new set of local parameters \( n'_i = \langle GS | c_i^\dagger c_i | GS \rangle \) which we use again as input for Eq. (22). Iterating this procedure, we finally obtain a fixed point configuration of occupation numbers \( n'_i(\{n_p\}) = n_p \).

Specifically, the quadratic Hamiltonian can be written in diagonal form
\[ H = \sum_{k=1}^{N} \epsilon(k) d_k^\dagger d_k, \] (23)

where the operators \( c_i \) are related with \( d_k \) by the unitary transformation
\[ c_i = \sum_k d_k (Q^t)_{ki}, \] (24)

where \( Q_{ik} \) is the matrix of eigenvectors of \( J_{ij}(\{n_i\}) \). Using standard methods\(^{12}\) we can easily compute the eigenvalues \( \epsilon(k) \) of \( H_{XX}^{(MF)}(\{n_i\}) \) and eigenvectors \( Q_{ik} \) for fairly large spin systems. The set of \( d_k \) satisfy fermion anticommutation relations \( \{d_k, d_{k'}^\dagger\} = \delta_{k,k'} \) and the total fermion number is conserved
\[ N_f = \sum_{i=1}^{N} c_i^\dagger c_i = \sum_{k=1}^{N} d_k^\dagger d_k. \] (25)

So, the ground state with magnetization \( m \), in the diagonal basis is given by
\[ |GS\rangle = \prod_{k=1}^{m+N/2} d_k^\dagger |0\rangle. \] (26)

In this state the energy at zero temperature (for zero magnetic field) is simply given by

\[ E_{GS}(m,0) = \sum_{k=1}^{m+N/2} \epsilon(k), \] (27)

whereas for \( h \neq 0 \) the total energy is shifted as \( E_{GS}(m,h) = E_{GS}(m,0) - h m \). The magnetization curve \( m(h) \) can finally be obtained by minimizing the energy \( E_{GS}(m,h) \) for different given magnetizations.

IV. RESULTS FOR THE PURE CASE

We have tested the SCMF procedure in a pure (ordered) \( J - J' X X \) model using chain lengths of up to the order of 100 spins, and compared its results with those found by exact diagonalization in smaller chains. In Fig. 2 we show the magnetization behavior under a magnetic field for \( J'/J = 0.6 \) which clearly indicates the existence of a magnetization plateau at \( M = 0 \).

This initial plateau shows up only in a narrow region of \( J'/J \) which in the SCMF approximation was estimated within the bounds \( 0.55 \lesssim J'/J \lesssim 0.75 \). No subsequent plateaus were observed in the system. Notice that in other models (e.g the \( X X Z \) model\(^{12}\)) there is a plateau at \( M = 1/3 \), however this not the case in the \( XX \) situation.

To lend further support to our SCFM approach, we compared the above results with those obtained in smaller systems using exact diagonalization\(^{12}\). In Fig. 3 we exhibit the magnetization curve obtained by Lanczos technique using chains of 12, 18 and 24 spins, where an \( M = 0 \) plateau also emerges at \( J'/J = 0.6 \). The regime where this plateau appears turns out to be slightly higher than that found with SCMF. This can be observed in Fig. 4 where we show the magnetic phase diagram obtained in a wide region of coupling parameters. Here, each line stands for a critical field above which the magnetization is increased by flipping one spin. In agreement with our
we show a schematic diagram of our SCMF expectations, we can see that the first critical field $h/J \approx 0$ is higher in the region $J' > 0$ and size effects become substantially reduced. We now apply the SCMF procedure to our main interest, namely disordered antiferromagnetic $XX$ chains with a Hamiltonian given by eq. (20). In this case $J_i$ and $J'_i$ are random NN and NNN coupling exchanges respectively. For concreteness, let us consider Gaussian distributions of exchanges $P(J_i) \propto e^{-|J_i|^2}$ with mean value $J = J > 0$ for NN couplings, $J = J' > 0$ for NNN couplings and the same disorder strength $\sigma$ in both cases (we explicitly forbid negative couplings in the Gaussian tail). We compute numerically the chain magnetization by averaging over many disorder realizations. Typically we considered over 200 samples with periodic boundary conditions and random sets of initial fermionic distributions.

V. RESULTS FOR THE DISORDERED CASE

We now apply the SCMF procedure to our main interest, namely disordered antiferromagnetic $XX$ chains with a Hamiltonian given by eq. (20). In this case $J_i$ and $J'_i$ are random NN and NNN coupling exchanges respectively. For concreteness, let us consider Gaussian distributions of exchanges $P(J_i) \propto e^{-|J_i|^2}$ with mean value $J = J > 0$ for NN couplings, $J = J' > 0$ for NNN couplings and the same disorder strength $\sigma$ in both cases (we explicitly forbid negative couplings in the Gaussian tail). We compute numerically the chain magnetization by averaging over many disorder realizations. Typically we considered over 200 samples with periodic boundary conditions and random sets of initial fermionic distributions.

We focused particular attention on low magnetic fields, so as to detect possible singularities near $h = 0$ as those observed in disordered NN chains. In Fig. 5 we display the magnetization curve for 102 spins with $J'/J = 0.6$ and $\sigma/J = 0.5$. Notice that the magnetization plateau observed in the pure case ($\sigma = 0$) is now totally suppressed. In fact, all studied values of $\sigma$ suggest that the plateau of the pure system is unstable under disorder. This observation was also corroborated in smaller systems after diagonalizing them exactly over 100 disorder realizations. In Fig. 6 we show for comparison the magnetization curves obtained for the same values of $J$, $J'$ and $\sigma$. On the contrary, the magnetization remains finite and drops quickly to zero at zero field. Actually, the magnetic susceptibility $\chi = \frac{\partial M}{\partial h}$ exhibits a divergence at $h = 0$, as shown in the inset of Fig. 5.

A thorough exploration of mean values of NN and NNN couplings and disorder strength shows that the low field magnetization curve shows a behavior compatible with a power law $M(h) \sim h^\alpha$ in most of the parameter space, except on a small region $J'/J \lesssim 10^{-4}$ where $M$ decreases in a logarithmic form $M \sim \frac{1}{(\log(h/J))^\alpha}$. In the power law region an exponent $\alpha < 1$ is obtained for disorder strength $\sigma/J \gtrsim 0.3$, corresponding to a singularity in the zero field magnetic susceptibility. For $\sigma/J \lesssim 0.3$ the magnetization decreases with an exponent $\alpha$ generally larger than one.

In Fig. 7 we show a schematic diagram of our SCMF numerical results. The dashed zone denotes a logarithmic behavior, the light gray region represents a power law behavior decrease of $M$ with exponent $\alpha < 1$, whereas in...
we have found three phases in these systems, the dominant one being a power law dependence of the magnetization with the low external field in most of the parameter space. Also, a logarithmic dependence of the magnetization was found just within a small region of parameters. Our results show that the two systems have similar low energy properties. A similar analogy has been found in the study of the same two systems for the Heisenberg ($SU(2)$) version. In both of them there are three phases and most of the parameter space is dominated by a power law dependence of $M(h)$. Both systems also show a small region where the magnetization displays the same kind of logarithmic singularity. In both systems the power law region follows a dynamical exponent $\alpha > 1$ for weak disorder, thus yielding a well behaved magnetic susceptibility. On the contrary, strong disorder yields exponents smaller than one and consequently the susceptibility becomes singular at $h = 0$. This later behavior has been also found in dimerized spin-1/2 chains with disordered NN interactions.

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