Effects of disorder on the dynamics of the *XY* chain

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We investigate the effects of disorder on the dynamics of the $s=1/2$ XY model in one dimension. The energy couplings are randomly drawn independently from a bimodal distribution. We use an extension of the method of recurrence relations, in which an averaging over realizations of disorder is incorporated into the definition of the scalar product of the dynamical Hilbert space of $\sigma_j^z(t)$, to determine analytically the first six basis vectors as well as the corresponding recurrants. We then use an ansatz for the higher-order recurrants, based on the behavior of the first ones exactly determined, to obtain the time-dependent correlation functions and spectral densities for several degrees of disorder. We find that the dynamics at long times is governed by the stronger couplings present in the system even if only a very small amount of disorder is present. In the long-time limit, the correlation functions oscillate at the cutoff frequency of the disorderless stronger-coupling case, with the spectral densities displaying tails that end at the stronger-coupling cutoff frequency.

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I. INTRODUCTION

The behavior of disordered quantum spin chains has been of considerable theoretical interest in the the past two decades.[1–3] Most of the work, though, deals with phase diagrams, ground-state properties, thermodynamic functions, etc. Not much attention has been paid to the study of Hamiltonian dynamics in such systems. Only recently, calculations of dynamic correlation functions have been reported for some disordered quantum spin chains.[4–6] In this work, we investigate the effects of disorder on the dynamics of the XY model[7,8] in the high-temperature limit. We are interested in both the time-dependent spin-correlation functions and the spectral functions in the presence of disorder.

There exist studies in the literature which deal with dynamic correlation functions of disorderless spin chains. There are only a few exact solutions in the infinite temperature limit. For the XY model, the time-dependent longitudinal spin autocorrelation function is known since the work of Niemeijer[9] to behave as the squared Bessel function, $J_0(2Jt)^2$, where J is the nearest-neighbor energy coupling. On the other hand, the transverse autocorrelation function has an exact solution as a Gaussian.[10–13] Some exact results were also reported for finite temperatures.[14] The dynamics of the surface x-component spin in a semi-infinite XY chain was exactly determined by Sen.[15] There is also an exact solution by Stolze *et al.*[16] for the spin-autocorrelation functions of the first few spins of the semi-infinite XY model in one dimension at infinite temperature. Although some works have appeared in the literature for the XY chain with a single impurity,[17,18] the dynamics of the model with arbitrary concentration of disorder is still not understood.

The XY model is defined by the Hamiltonian

$$H=-\frac{1}{2}\sum_{i=1}^{N} J_i(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y), \tag{1}$$

where σ_i^α are Pauli matrices at sites i, $\alpha=x,y,z$. J_i are nearest-neighbor coupling constants and N is the number of spins. We assume periodic boundary conditions, that is, $\sigma_{i+N}^\alpha=\sigma_i^\alpha$. In this work, we consider the coupling energies between neighboring sites as random variables that can take the values J_A or J_B. The couplings are drawn independently from the bimodal distribution

$$\rho(\{J_i\})=\prod_i^N [(1-p)\,\delta(J_i-J_A)+p\,\delta(J_i-J_B)], \tag{2}$$

where $0\leqslant p\leqslant 1$, p representing the fraction of J_B bonds. Since Eq. (2) is normalized to unity, the average over disorder realizations of a given quantity $f(\{J_i\})$ is given by

$$\overline{f(\{J_i\})}=\int_{-\infty}^{\infty}\rho(\{J_i\})f(\{J_i\})\prod_i^N dJ_i. \tag{3}$$

Our main quantity of interest, the time-dependent correlation function, is defined by

$$C(t)=\overline{\langle\sigma_i^z(0)\sigma_i^z(t)\rangle}, \tag{4}$$

where $\overline{\langle\cdots\rangle}$ denotes an ensemble average followed by an average over the disorder variables. We use the method of recurrence relations[19–26] to obtain the short-time expansion of $C(t)$ and a continued-fraction analysis to extend the results to the long-time region. The results are then used in the calculation of the spectral densities.

We find that disorder induces an unexpected feature: the long-time behavior is dominated by the presence of stronger couplings, even when their concentration is extremely small. We could not detect numerically any low-concentration threshold for the onset of the asymptotic stronger-coupling behavior. Hence, we are led to conclude that any concentration of stronger couplings, however small it may be, will

make the correlation function to behave like its analog in a given pure stronger-coupling chain at the long-time limit.

This paper is arranged as follows. In Sec. II, we review the method of recurrence relations employed here to include disorder, and in Sec. III the method is used to obtain the dynamic longitudinal correlation functions of the XY model for different amounts of disorder. Finally, in Sec. IV we summarize our results.

II. METHOD OF RECURRENCE RELATIONS

The time evolution of a Hermitian operator A in a system described by a Hamiltonian H is governed by the equation of motion

$$\frac{dA(t)}{dt} = iLA(t), \tag{5}$$

where L is the Liouville operator, $LA=[H,A]\equiv HA-AH$. The solution to Eq. (5) is cast in the form of the orthogonal expansion,

$$A(t) = \sum_{n=0}^{d-1} a_n(t) f_n, \tag{6}$$

where f_n are orthogonal basis vectors spanning a d-dimensional Hilbert space S.

In order to account for disorder, the scalar product is defined as the Kubo product averaged over the realizations of the disorder.[5] Accordingly, it reads

$$(X,Y) = \frac{1}{\beta}\int_0^\beta d\lambda \overline{\langle X(\lambda) Y^\dagger\rangle} - \overline{\langle X\rangle\langle Y^\dagger\rangle}, \tag{7}$$

where X and Y are vectors defined in S, $\beta = 1/k_B T$ is the inverse temperature, and $X(\lambda)=\exp(\lambda H)X\exp(-\lambda H)$. In the high-temperature limit, $T\to\infty$, the scalar product becomes

$$(X,Y) = \overline{\mathrm{Tr}\, XY^\dagger}/Z, \tag{8}$$

where the partition function Z now yields the number of quantum states of the system $Z=\mathrm{Tr}\,1$. In the case of spin-1/2 models, $Z=2^N$, where N is the number of spins in the system.

By choosing $f_0=A(0)$, it follows from Eq. (6) that $a_0(0)=1$ and $a_n(0)=0$ for $n\geqslant 1$. Furthermore, the remaining basis vectors are generated by the recurrence relation (RRI)

$$f_{n+1} = iLf_n + \Delta_n f_{n-1}, \quad 0\leqslant n\leqslant d-1, \tag{9}$$

where

$$\Delta_n = \frac{(f_n, f_n)}{(f_{n-1}, f_{n-1})}, \quad n\leqslant 1 \tag{10}$$

are the relative norms of basis vectors, also known as recurrants.[19] By definition, $f_{-1}\equiv 0$ and $\Delta_0\equiv 1$. The coefficients $a_n(t)$, which are the relaxation functions, satisfy a second recurrence relation (RRII)

$$\Delta_{n+1} a_{n+1}(t) = -\frac{da_n(t)}{dt} + a_{n-1}(t), \quad 0\leqslant n\leqslant d-1, \tag{11}$$

where $a_{-1}(t)\equiv 0$. Hence, $a_0(t)$ represents the relaxation function of linear-response theory. In the limit $T\to\infty$, $a_0(t)$ is simply the time-dependent autocorrelation function $\langle A(0)A(t)\rangle$.

Thus, the complete time evolution of $A(t)$ can be determined from RRI and RRII. By taking the Laplace transform of the recurrence relation RRII, one obtains

$$\Delta_1\alpha_1(z) = 1 - z\alpha_0(z), \quad n=0, \tag{12}$$

$$\Delta_{n+1}\alpha_{n+1}(z) = -z\alpha_n(z) + \alpha_{n-1}(z), \quad n\geqslant 1, \tag{13}$$

where

$$\alpha_n(z) = \int_0^\infty \exp(-zt) a_\nu(t) dt \quad \mathrm{Re}\, z\rangle 0. \tag{14}$$

It follows from Eqs. (12) and (13) that $\alpha_0(z)$ can be cast in the continued-fraction form

$$\alpha_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z+\cdots}}}. \tag{15}$$

Note that the recurrants Δ_n are the sole ingredients that enter the determination of the dynamic correlation functions. In addition, the knowledge of Δ_n enables one to obtain the moments of the spectral density,

$$\mu_{2k} = \frac{1}{Z}\overline{\mathrm{Tr}\,\sigma_i^z[H,[H,\ldots[H,\sigma_i^z]\ldots]]}, \tag{16}$$

in which there are $2k$ nested commutators. The moments can be used to obtain the Taylor time series expansion for the correlation function in the infinite temperature limit as follows:

$$C(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!}\mu_{2k} t^{2k}. \tag{17}$$

Usually, only a few Δ_n can be determined analytically, since the calculation of higher-order recurrants can be too lengthy or time consuming. Even though the moments enter in a simple manner in the correlation functions, it is preferable to inspect the behavior of the recurrants in order to devise any extrapolation scheme.

There are several types of approximations found in the literature to estimate the time-dependent correlation functions based on the limited information contained in just a few moments (or recurrants). One can truncate the continued fraction for $\alpha_0(z)$ by introducing a terminating function. Examples are the n-pole approximations[27] and the Gaussian terminator.[28]

In the same spirit is the direct summation method[29] in which an ansatz is set for the unknown higher-order recur-

rants, and the truncation uses as many recurrants as is computationally feasible. In this way, one can manage to obtain results which are valid at longer times. In any event, once the ansatz of recurrants is chosen, one is able to obtain readily the corresponding moments, since there are as many nontrivial moments as there are recurrants. In this way, one obtains the first coefficients of the short-time expansion for $C(t)$ from the knowledge of the moments. In general, one could extend the region of validity in time by constructing Padé approximants to the full time series or by using other extrapolation schemes.[30] We do not find it necessary to employ any of those methods, since we already use as many short-time coefficients from the ansatz as we can to obtain sensible results numerically. In the present work, we shall adopt the following strategy. First, after examining the structure of the recurrants, we will put forward a model for the remaining Δ_n. From these we will get the first short-time coefficients of $C(t)$. Finally, the spectral density $\Phi(\omega)$, defined as the Fourier transform of the time-dependent correlation function,

$$\Phi(\omega)=\int_{-\infty}^{\infty} e^{i\omega t}C(t)dt, \tag{18}$$

will be obtained numerically. That quantity could, in principle, be compared with experimental results from nuclear-magnetic resonance, electron-spin resonance, and inelastic neutron scattering, on appropriate magnetic systems that represent one-dimensional XY behavior with disorder.[31]

III. DYNAMICS OF THE DISORDERED XY CHAIN

Since we are interested in the longitudinal correlation function, let us consider $\sigma_j^z(t)$ as the dynamic variable in the XY linear chain, Eq. (1). According to Eq. (6), its time evolution is given by

$$\sigma_j^z(t)=\sum_{\nu=0}^{d-1} a_\nu(t) f_\nu, \tag{19}$$

with the choice $f_0=\sigma_j^z(0)=\sigma_j^z$. The other basis vectors f_1, f_2, etc., are determined by using the recurrence relation RRI. We have obtained the basis vectors up to f_6. Their norms in the limit $T\to\infty$ are obtained with the use of the scalar product, Eq. (8). For example, f_1 is found to be

$$f_1=-J_j\sigma_j^y\sigma_{j+1}^x-J_{j-1}\sigma_{j-1}^x\sigma_j^y+J_j\sigma_j^x\sigma_{j+1}^y+J_{j-1}\sigma_{j-1}^y\sigma_j^x, \tag{20}$$

while its squared norm is given by

$$(f_1,f_1)=4[(1-p)J_A^2+pJ_B^2]. \tag{21}$$

Note that the first recurrant Δ_1 coincides with the squared norm of f_1, since $(f_0,f_0)=(\sigma_j^z,\sigma_j^z)=1$. The expressions for the remaining basis vectors are increasingly lengthier and, thus, shall not be reported here.[32]

In Fig. 1, we present numerical results for the first six recurrants for several concentrations p of couplings of type J_B. We use $J_A=1$ and $J_B=1.5$ in that figure and in all the others. In the disorderless cases, the recurrants start at the value $\Delta_1=(2J)^2$, $J=J_A$ or J_B, and then oscillate about their starting value, but with decreasing amplitude. On the other hand, in the cases with disorder the recurrants tend to oscillate away from their starting value Δ_1 toward the stronger-coupling recurrants. Even a small amount of disorder drives the higher-order recurrants to oscillate toward that region. We did consider concentrations as low as $p=0.01$, but obtained qualitatively similar results. Such feature guided us in the construction of the extrapolation scheme for the higher-order recurrants.

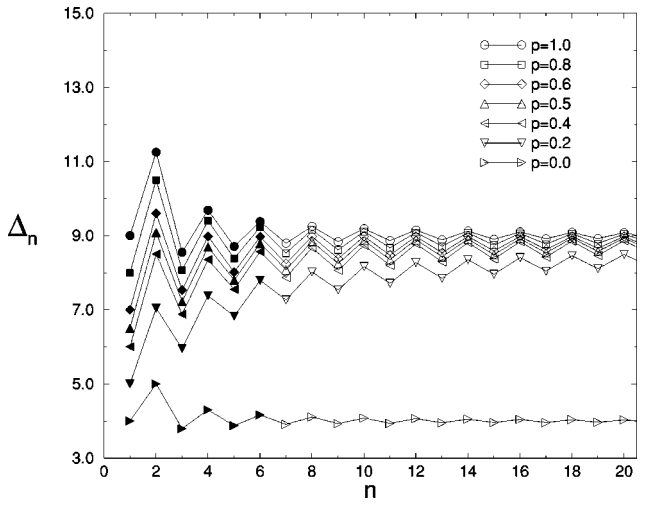

FIG. 1. Recurrants for the longitudinal dynamic correlation functions of the XY disordered chain in the high-temperature limit. The first six recurrants (full symbols) are exact, while the remaining ones (open symbols) are extrapolations, following the ansatz, Eqs. (22)–(24). In this figure as well as in the other figures of this work, we have set $J_A=1$ and $J_B=1.5$, which are the parameters of the bimodal distribution, Eq. (2). Here, $p=0$ and $p=1$ correspond to the pure cases where all couplings are of type J_A and J_B, respectively. The lines are guides to the eye.

We then used the following ansatz for the remaining recurrants:

$$\Delta_n=\frac{A}{n^\eta}+\Delta_\infty, \quad n=1,3,5,\ldots,$$

$$A=(\Delta_3-\Delta_\infty)3^\eta,$$

$$\eta=-\ln\left(\frac{\Delta_\infty-\Delta_5}{\Delta_\infty-\Delta_3}\right)/\ln\left(\frac{5}{3}\right), \tag{22}$$

and

$$\Delta_n=\frac{B}{n^\xi}+\Delta_\infty, \quad n=2,4,6,\ldots,$$

$$B=(\Delta_4-\Delta_\infty)4^\xi,$$

$$\xi=-\ln\left(\frac{\Delta_\infty-\Delta_4}{\Delta_\infty-\Delta_6}\right)/\ln\left(\frac{3}{2}\right). \tag{23}$$

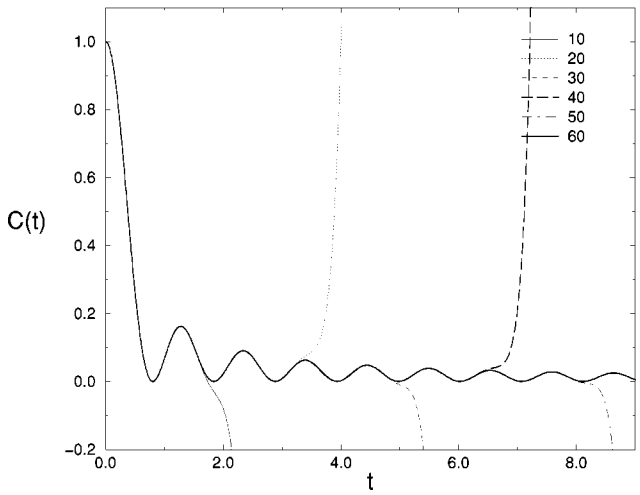

FIG. 2. Comparison between exact and approximate longitudinal spin time-dependent correlation functions of the XY chain at the high-temperature limit. Shown are the exact results for the pure case $p=1$, $J_0(3t)^2$, and those in which a given finite number of recurrants was used. Note the convergence as the number of recurrants increases.

Note that A, B, η, and ξ depend on p implicitly through the recurrants, as they were determined by imposing that the first six recurrants from the ansatz match the six known ones. As $n\to\infty$, each recurrant converges to the terminal value Δ_∞, given by

$$\Delta_\infty = 4J_B^2 \quad \text{for} \quad p>0$$

$$= 4J_A^2 \quad \text{for} \quad p=0. \tag{24}$$

The above ansatz is best visualized in Fig. 1, where we plot the first 20 recurrants for each concentration p. As can be seen, in all cases the recurrants start at a given value Δ_1 and then oscillate toward Δ_∞, with power-law decaying amplitude. The fact that the recurrants have an upper bound is a reflection of the fact that the time-dependent correlation function falls off to zero asymptotically by oscillating with a finite frequency. That feature is known in the disorderless case, where

$$C(t)=J_0(2Jt)^2 \sim \frac{1}{\pi Jt}\cos^2(2Jt-\pi/4) \tag{25}$$

as $t\to\infty$. Note that in the long-time regime, $C(t)$ oscillates with frequency $\omega=4J$, since the cosine function is squared.

Our calculations of $C(t)$ involve the determination of the moments from the knowledge of the recurrants. From a given number of recurrants, one finds an equal number of moments. Thus, from those moments we construct a polynomial approximation for $C(t)$, that is, a short-time expansion.

Our approximate scheme, as outlined above, including the use of the ansatz for the recurrants, was tested with the known correlation function $J_0(2Jt)^2$ for the disorderless case of $p=1$ ($J_i=J_B=1.5$). The results are shown in Fig. 2. Note that the power-law ansatz, Eqs. (22)–(24), produces accurate results in the scale of the figure. The time region in which the approximation is good is enlarged as more recurrants from the ansatz are used. We find that we need at least 60 recurrants to obtain reasonable results.

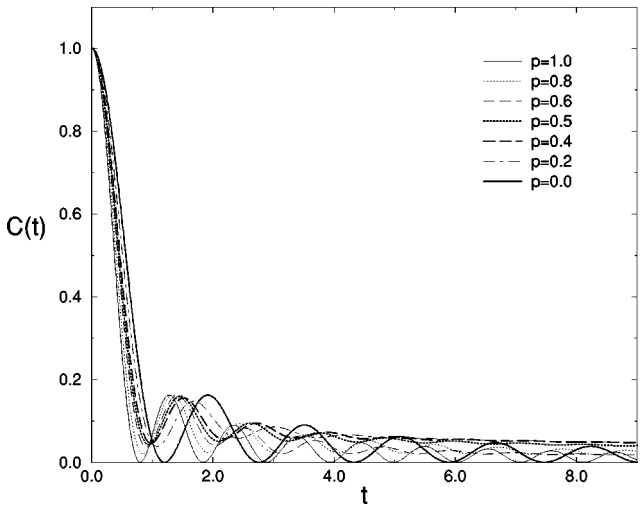

FIG. 3. Time-dependent spin-correlation function for the disordered XY chain at the high-temperature limit. The energy couplings are of type $J_B=1.5$ with probability p, otherwise the couplings are set to $J_A=1$.

IV. DISCUSSION AND CONCLUSIONS

The time-dependent correlation functions for several cases with disorder are displayed in Fig. 3, while the corresponding spectral densities are shown in Fig. 4. For $p=0.0$, we have the disorderless XY model with $J_i=J_A=1.0$, while $p=1.0$ corresponds to $J_i=J_B=1.5$. Thus, the curves corresponding to the pure cases are the same, aside

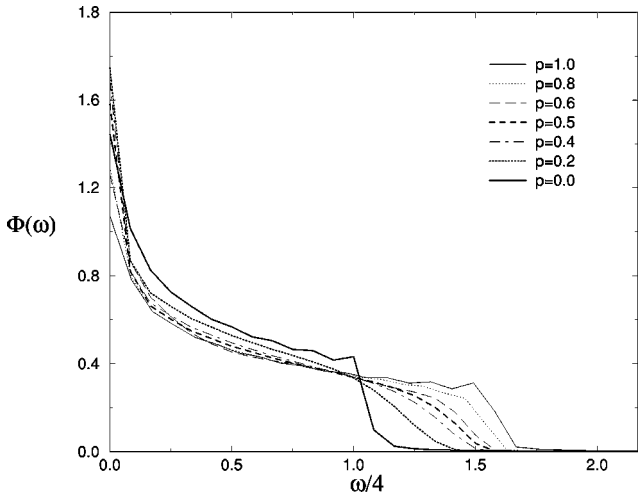

FIG. 4. Spectral density of the XY model for several values of p. The energies are in units of J_A, which serves to fix the horizontal scale. The vertical scale is such that the area under each curve for $\omega\geqslant 0$ equals π. Notice the large drops of the spectral density at $\omega=4.0$ and 6.0, which correspond to the pure cases $p=0.0$ ($J_i=J_A=1.0$) and $p=1.0$ ($J_i=J_B=1.5$), respectively. Those drops are at the cutoff frequencies ($\omega=4J$) of the exact results for each realization of the coupling energy (Ref. 10).

from a time scale as one would expect. Thus, the correlation function for the stronger-coupling case oscillates with higher frequencies. In the limit $t\to\infty$, it oscillates with a single frequency, $\omega=4J_B$, which is the cutoff frequency for the exact spectral density. In our calculations, where we truncated the continued fractions at the 60th level, where some information on the long-time dynamics was lost, the result is that the spectral densities for the cases $p=0.0$ and $p=1.0$ do not have the sharp edges as the exact functions do at their cutoff frequencies. In addition, the logarithmic divergence of the spectral density at $\omega=0$ caused by the t^{-1} behavior of $C(t)$ at large times is only hinted in our numerical results. There are also some minor spurious structures in $\Phi(\omega)$ that should be ignored. These pitfalls are all due to computational constraints that limited us to use only 60 recurrants for each case. Yet, our approximation still provides a reasonably good account on the effects of disorder in the model.

As p takes on small values, the effect of disorder is to lift up the curves $C(t)$ above the $J_0(2t)^2$ result of the pure case $J_i=J_A=1$, as can be seen in Fig. 3. The lifting reaches a maximum when $p=0.5$, that is, when the chain is most disordered. Upon further increase of p, the reverse takes place, that is, the curves for $C(t)$ start to drop toward the pure case with stronger energy couplings $J_B=1.5$. The plot of the spectral density, Fig. 4, shows smooth curves for the cases with disorder, $0<p<1$. Instead of having a sharp drop, the curves are smooth and show a tail that ends at the cutoff frequency of the stronger-coupling pure case $p=1.0$. Thus, according to our results, there is also a cutoff frequency for the disordered cases, which is the same as the cutoff frequency of the pure stronger-coupling case, which is valid for all p, down to $p=0.01$. That is, the long-time dynamics of the disordered chain is dominated by the stronger couplings even if their concentration is very small. Based on our numerical evidence, we conjecture that such feature holds for all $0<p<1$. It would be interesting to see how much of that asymptotic behavior could also appear in the cases where the coupling energies were drawn from a continuous distribution. A similar behavior can be found in the density of states of one-electron systems in a binary alloy, where there appears a low-energy tail, the so-called Lifshits tail, which is dominated by the rare large fluctuations of the potential.[33]

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