

Dynamics of the random one-dimensional transverse Ising model

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We study the dynamics of the spin-1/2 random transverse Ising model in the high-temperature limit by means of the method of recurrence relations. We analyze two types of disorder: a disorder on the transverse field, and a disorder on the exchange coupling. We find that the dynamics undergoes a crossover from a central peak behavior onto a collective mode behavior as a function of the disorder. [S0163-1829(99)04937-1]

One class of problems of great interest in statistical physics is the time evolution of disordered systems. One of the simplest yet nontrivial examples of such systems is the $s = 1/2$ random transverse Ising model (RTIM), where the exchange couplings J_i or the transverse fields B_i are random variables. The model is relevant to the dynamic properties of hydrogen (deuteron)-bond order-disorder ferroelectrics, such as the quasi-one-dimensional ferroelectrics $\text{Cs}(\text{H}_{1-x}\text{D}_x)_2\text{PO}_4$, $\text{PbH}_{1-x}\text{D}_x\text{PO}_4$, etc. It is well-known that hydrogen and deuteron have different tunneling frequencies within the bonds of those ferroelectrics crystals. The nonuniform deuteration of the hydrogen bonds is then modeled by a random site-dependent transverse field B_i , whereas the intra-chain interactions J_i remain unaltered, that is, $J_i = J$.¹⁻³ On the other hand, in the case of spin glasses one takes the exchange couplings as the random variables. A systematic study of the effects of a transverse magnetic field on the three-dimensional spin glass $\text{LiHo}_{0.167}\text{Y}_{0.833}\text{F}_4$ was carried out by means of neutron diffraction⁴ and has triggered a renewed interest in the RTIM.⁵⁻⁷ The system seems to exhibit a *quantum* phase transition at zero temperature, which is driven by the relative strength between the transverse field and the average exchange parameter. Such a transition had been predicted some time ago independently by Griffiths⁸ and McCoy.⁹ Near the critical point, the time-dependent correlation functions decay as a power law, whereas the static susceptibilities present unusual singularities even in the paramagnetic phase.^{7,9-13}

In general, the dynamic properties of *pure* quantum spin models, such as the transverse Ising model, the XY model, the Heisenberg model, etc., have proven much harder to obtain than the thermodynamic quantities. For instance, there is a rather long history on the attempts to obtain the time-dependent spin correlation functions of the $s = 1/2$ Heisenberg model in one dimension. To the best of our knowledge, this problem remains unsolved, albeit there exist a few rigorous results for the short time behavior of the spin autocorrelation functions.¹⁴⁻¹⁶ There are, however, some exact results for the dynamics of the transverse Ising and XY models in one dimension. The longitudinal time-dependent correlation functions were obtained by Niemeijer¹⁷ for any temperature, by using a mapping of the spin variables onto a collection of noninteracting fermions.¹⁸ The transverse correlation functions show a Gaussian behavior at infinite temperatures¹⁹⁻²² and a power-law behavior at zero temperature.²³⁻²⁶ There are also numerical results for the

time-dependent correlation functions for the pure²⁷⁻²⁹ as well as for the disordered^{13,30} transverse Ising and XY models.

Calculations based on Mori's continued fraction method using only three moments¹ have been used to describe the dynamics of the quasi-one-dimensional hydrogen-bonded ferroelectric crystals CsH_2PO_4 and PbHPO_4 , which are modeled by the transverse Ising model. Another three-moment based calculation was carried out by Tonegawa³¹ for the *classical* Heisenberg chain with impurities to obtain the neutron inelastic magnetic scattering cross section for the random one-dimensional antiferromagnet $(\text{CD}_3)_4\text{NMn}_{1-x}\text{Cu}_x\text{Cl}_3$ (TMMC: Cu), and reproduced well the qualitative features of the experimental data.^{32,33}

In the present work, we investigate the dynamic properties of the $s = 1/2$ RTIM,

$$H = -\frac{1}{2} \sum_i J_i \sigma_i^x \sigma_{i+1}^x - \frac{1}{2} \sum_i B_i \sigma_i^z, \quad (1)$$

at the high temperature limit, where σ_i^α ($\alpha = x, y, z$) are Pauli matrices, and J_i and B_i are the exchange couplings and transverse fields, respectively. The couplings and fields may be regarded as random variables. The model is equivalent to the two-dimensional *classical* transverse Ising model with correlated disorder along one spatial direction.^{9,34} We are mainly interested in the average spin correlation function

$$C(t) = \overline{\langle \sigma_j^x(t) \sigma_j^x \rangle}, \quad (2)$$

where an average over the random variables is performed after the statistical average. We use the method of recurrence relations³⁵ to calculate exactly up to the eighteenth moment of $C(t)$,

$$C(t) = \sum_{k=0}^{\infty} \mu_{2k} t^{2k}, \quad (3)$$

$$\mu_{2k} = \frac{1}{(2k)!} \overline{\text{Tr} \sigma_i^x [H, [H, \dots [H, \sigma_i^x] \dots]]}. \quad (4)$$

We also calculate the spectral density by using the so-called Gaussian terminator^{36,37} for the continued fraction representation of the Laplace transform of $C(t)$.

The method of recurrence relations has proved to be very useful in the determination of the dynamic correlation func-

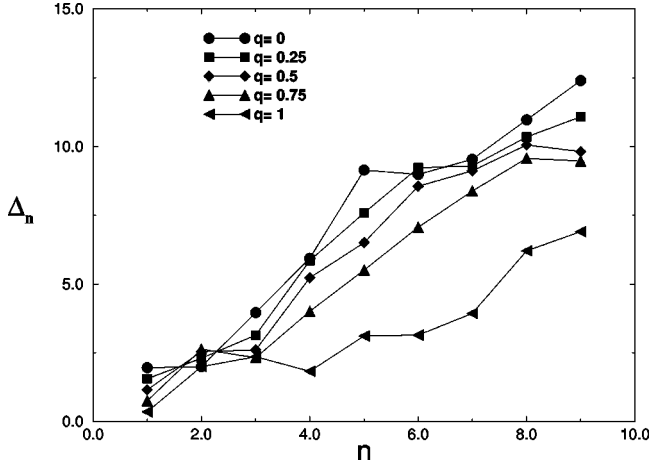


FIG. 1. Recurrants for the Ising model in a random transverse field B_j which can take the values 0.6 and 1.4 with probabilities q and $1-q$, respectively. The fields are given in units of the exchange coupling J .

tions of systems such as the electron gas,³⁵ the classical harmonic chain,³⁸ spin chains,^{16,22,37,39} etc. In order to apply the method to disordered systems, we need to modify it to account for the averages over the random variables J_i and B_i . Notice that the time-dependent correlation function of interest involves two averages: (1) the statistical mechanics average for a given set of values of the random variables and (2) the average over the random variables. The method must be modified so that, among other things, it will yield the averaged correlation functions of interest.

Let us consider the operator for a tagged spin σ_j^x whose dynamics is governed by the Hamiltonian (1). The time evolution of σ_j^x is given in the Heisenberg representation as

$$\sigma_j^x(t) = e^{iHt} \sigma_j^x e^{-iHt}, \quad (5)$$

in a system of units where $\hbar = 1$. In the method of recurrence relations $\sigma_j^x(t)$ is expressed as an expansion in a Hilbert space S ,

$$\sigma_j^x(t) = \sum_{\nu=0}^{d-1} a_\nu(t) F_\nu, \quad (6)$$

where d is the dimension of S , F_ν are orthogonal basis vectors spanning S , and $a_\nu(t)$ are time-dependent coefficients. We define the inner product in S at the high-temperature limit ($T = \infty$) in such way that it includes *both* the statistical and the random averages

$$(A, B) = \overline{\langle AB^\dagger \rangle} - \overline{\langle A \rangle} \overline{\langle B^\dagger \rangle}. \quad (7)$$

The above definition of the inner product keeps the original form of the recurrence relations.

The zeroth basis vector is chosen as the dynamic variable of interest $F_0 = \sigma_j^x$, without loss of generality. It follows that the coefficient $a_0(t)$ can be identified as the time-dependent correlation function $C(t)$

$$a_0(t) = \overline{\langle \sigma_j^x(t) \sigma_j^x \rangle} \equiv C(t). \quad (8)$$

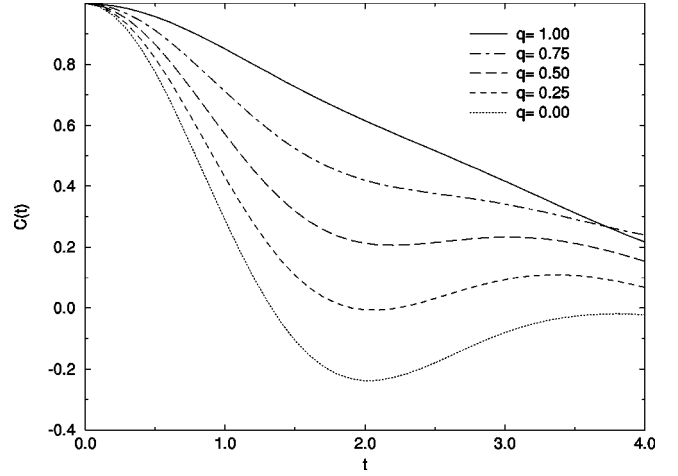


FIG. 2. Time-dependent correlation functions for the Ising model in a random transverse field, with the same parameters as in Fig. 1.

The remaining F_ν are obtained by using the recurrence relation

$$F_{\nu+1} = iLF_\nu + \Delta_\nu F_{\nu-1}, \quad \nu \geq 0, \quad (9)$$

where L is the Liouville operator

$$LA = [H, A] = HA - AH. \quad (10)$$

The recurrants Δ_ν are defined by

$$\Delta_\nu = \frac{(F_\nu, F_\nu)}{(F_{\nu-1}, F_{\nu-1})}, \quad (11)$$

with $\Delta_0 = 1$, and $F_{-1} \equiv 0$.

By taking $\nu=0$ in Eq. (9) we obtain the first basis vector $F_1 = B_j \sigma_j^y$. Its norm is then obtained, that is, $(F_1, F_1) = \overline{B_j^2}$. Since $(F_0, F_0) = 1$, the first recurrent is readily obtained, $\Delta_1 = \overline{B_j^2}$. By proceeding in a similar fashion we obtain

$$\begin{aligned} F_2 &= (\Delta_1 - B_j^2) \sigma_j^x + B_j J_{j-1} \sigma_{j-1}^x \sigma_j^z + B_j J_j \sigma_j^z \sigma_{j+1}^x, \\ F_3 &= -B_j (J_{j-1}^2 + J_j^2 + B_j^2 - \Delta_1 - \Delta_2) \sigma_j^y \\ &\quad - 2B_j J_{j-1} J_j \sigma_{j-1}^x \sigma_j^y \sigma_{j+1}^x + B_{j-1} B_j J_{j-1} \sigma_{j-1}^y \sigma_j^z \\ &\quad + B_j B_{j+1} J_j \sigma_j^z \sigma_{j+1}^y, \end{aligned} \quad (12)$$

etc. We have calculated the basis vectors up to F_9 .⁴⁰ The first three recurrants are then obtained

$$\Delta_1 = \overline{B_j^2},$$

$$\Delta_2 = 2\overline{J_j^2} - \overline{B_j^2} + \frac{\overline{B_j^4}}{\overline{B_j^2}},$$

$$\Delta_3 = \frac{\overline{B_j^6} + 2\overline{J_j^2} \overline{B_j^2} + 2\overline{J_j^4} \overline{B_j^2} + 2\overline{J_j^2} \overline{B_j^2} - \overline{B_j^4} \overline{B_j^2}}{2\overline{J_j^2} \overline{B_j^2} - \overline{B_j^2} + \overline{B_j^4}}. \quad (13)$$

TABLE I. First nontrivial moments of $C(t)$ case of a disordered transverse field. Here, the field can take two values $B_1=0.6$ ($q=1$), and $B_2=1.4$ ($q=0$). The coupling energy is $J_i=1$.

Moment	$q=0$	$q=0.25$	$q=0.5$	$q=0.75$	$q=1$
μ_0	1.0	1.0	1.0	1.0	1.0
μ_2	-0.98	-0.78	-0.58	-0.38	-0.18
μ_4	0.3234	0.2514	0.1794	0.1074	0.0354
μ_6	-6.42488×10^{-2}	-4.81395×10^{-2}	-3.2919×10^{-2}	-1.85875×10^{-2}	-5.1448×10^{-3}
μ_8	9.8792×10^{-3}	6.93831×10^{-3}	4.39364×10^{-3}	2.24516×10^{-3}	4.92874×10^{-4}
μ_{10}	-1.35479×10^{-3}	-8.67367×10^{-4}	-4.89716×10^{-4}	-2.14222×10^{-4}	-3.32669×10^{-5}
μ_{12}	1.72512×10^{-4}	9.96185×10^{-5}	4.91530×10^{-5}	1.76628×10^{-5}	1.69563×10^{-6}
μ_{14}	-1.98858×10^{-5}	-1.04744×10^{-5}	-4.54290×10^{-6}	-1.32685×10^{-6}	-6.89941×10^{-8}
μ_{16}	2.01290×10^{-6}	9.86048×10^{-7}	3.83910×10^{-7}	9.26958×10^{-8}	2.35236×10^{-9}
μ_{18}	-1.76770×10^{-7}	-8.18414×10^{-8}	-2.92522×10^{-8}	-6.01823×10^{-9}	-7.05746×10^{-11}

We then use the remaining basis vectors to obtain the recurrants $\Delta_4, \Delta_5, \dots, \Delta_9$. The averages over the random variables can be calculated once their distribution functions are specified.

As can be seen in Eq. (6), the time dependence is contained entirely in the $a_\nu(t)$'s. These obey a second recurrence relation

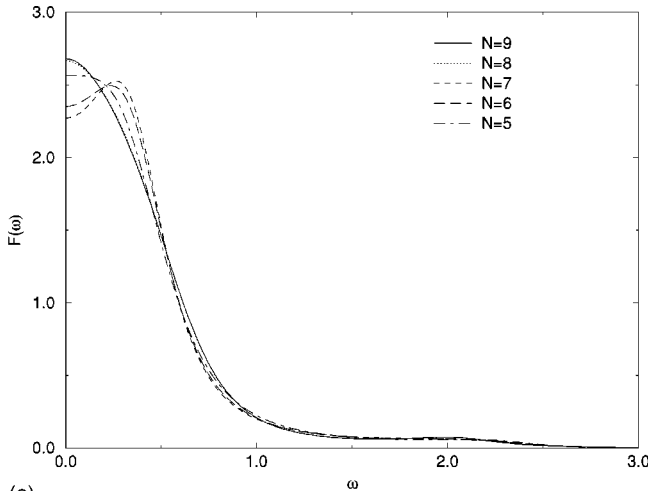
$$\Delta_{\nu+1} a_{\nu+1}(t) = -\frac{da_\nu(t)}{dt} + a_{\nu-1}(t), \quad \nu \geq 0, \quad (14)$$

with $a_{-1} \equiv 0$. Note that the only ingredients that enter the determination of $a_\nu(t)$ are the recurrants. Of particular interest is the Laplace transform of $a_0(t)$,

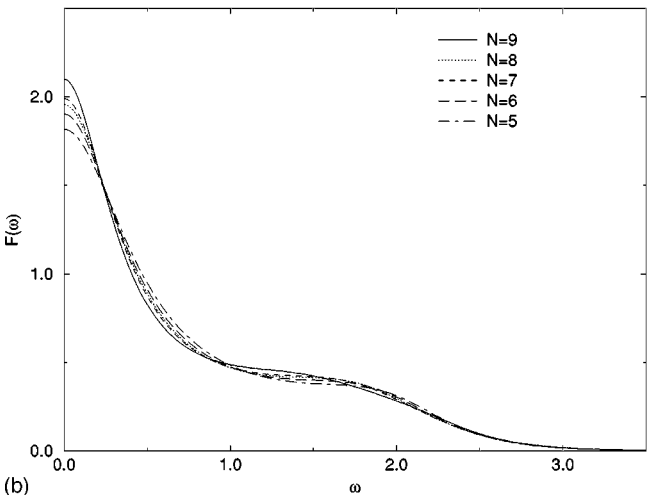
$$a_0(z) = \int_0^\infty e^{-zt} a_0(t) dt, \quad \text{Re } z \geq 0, \quad (15)$$

which can be cast as a continued fraction

$$a_0(z) = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \dots}}}. \quad (16)$$



(a)



(b)

FIG. 3. Sequence of approximants for the spectral density according to the level N of the continued fraction of $a_0(z)$ (see text) where a Gaussian termination is employed. Notice the agreement between the approximants for $N=8$ and $N=9$. (a) Pure case, $J_i=1$ and $B_i=0.6$. (b) Disorder in the transverse field, $B_i=0.6$ or 1.4 with same probability, and uniform exchange coupling $J_i=1$.

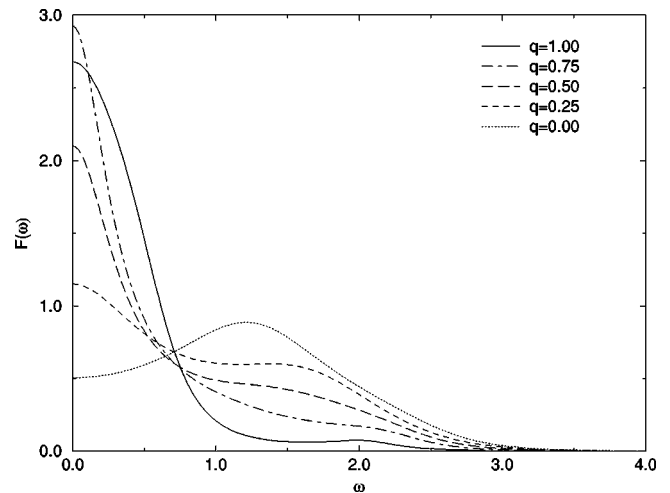


FIG. 4. Spectral density for the case $J_i=1, B_i=0.6$ (1.4) with probability q ($1-q$). Notice that the system moves from a collective mode dynamics to a central peak type of dynamics as the disorder parameter q varies from 0 ($B>J$) to 1 ($B<J$).

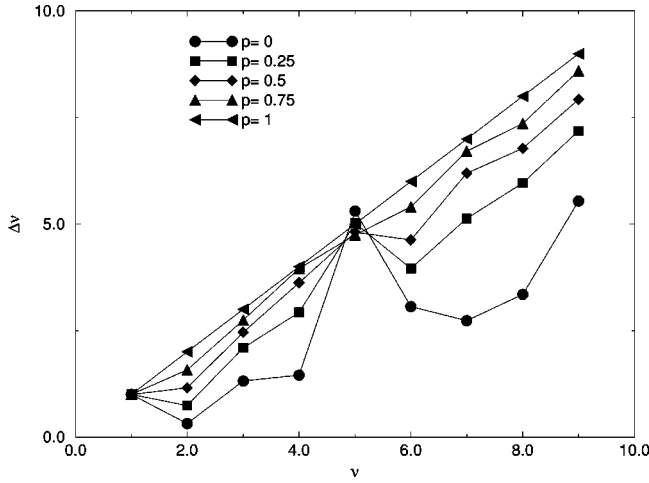


FIG. 5. Recurrants for the spin glass case of $J_i=1(0.4)$ with probability $p(1-p)$ and $B_i=1$. The pure case $p=1$ reproduces the known Gaussian behavior.

The above expression shall be useful in the calculation of the spectral density.

Consider now the case where the transverse fields B_i are randomly distributed on the lattice sites whereas the exchange couplings are uniform, $J_i=J$. Let us assume the transverse fields are independent variables drawn from the bimodal distribution

$$\rho(B) = \prod_i [q\delta(B_i - B_1) + (1-q)\delta(B_i - B_2)], \quad (17)$$

where q takes values from 0 to 1. We can now use the above distribution to obtain the configuration averages of the norms of the basis vectors. The first nine recurrants are shown in Fig. 1 for several values of q . We have set $J_i=1$, which fixes the energy scale, and varied the transverse field from the value $B_1=0.6$ ($q=1$) to $B_2=1.4$ ($q=0$). This allows the system to move from a situation in which the transverse field has a lower value than the exchange coupling to the situation where the strength of the transverse field is higher than the exchange coupling. Notice the irregular pattern of the recurrants in the figure, what makes it difficult to infer the behavior of the higher order recurrants. The first nine nontrivial moments of Eq. (4) are given in Table I, for the same pa-

rameters used in Fig. 1. Next we use the moments to construct Padé approximants for the time-dependent correlation functions $C(t)$. The highest-order Padé approximants are depicted in Fig. 2. We distinguish two different behaviors: for transverse field weaker than the exchange coupling ($q=1, B_1=0.6$), $C(t)$ shows an oscillatory behavior; for transverse field stronger than the exchange coupling ($q=0, B_2=1.4$), the correlation function behaves monotonically.

These different dynamic behaviors will become more evident if we look at the spectral function $F(\omega)$, given by

$$F(\omega) = \text{Re} \int_0^\infty C(t) e^{-zt} dt = \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi} \text{Re} a_0(\epsilon + i\omega). \quad (18)$$

We shall use the continued fraction representation of $a_0(z)$, Eq. (16), to calculate $F(\omega)$. Generally, the continued fraction has an infinite number of levels which, incidentally, is the case with the present problem. That means that its calculation involves the knowledge of the infinite number of Δ 's. Since it is usually impossible to obtain *all* the Δ 's, it becomes necessary to use a scheme to terminate the continued fraction, yet preserving the moments sum rules. Several truncation schemes have been used in the literature. The one that serves best our problem is the so-called Gaussian terminator.³⁶ Suppose one knows only the first N recurrants. In that approximation, the unknown coefficients of the continued fraction are assumed to be of the form $\Delta_n = (\Delta_N/N)n$ for $n > N$. Such a scheme provides a smooth approximation to the spectral function. As long as the true spectral function does not have any singularities, as it seems to be the case with the present model, the Gaussian termination works reasonably well. In order to check convergence of the Gaussian terminators, we calculate a sequence of approximants corresponding to $N=1, 2, \dots, 9$, for a given set of parameters. The results are shown in Figs. 3(a) and 3(b). In Fig. 3(a) we have the pure case ($q=1$), whereas in Fig. 3(b) we have maximum disorder ($q=0.5$). In both figures we have used $J_i=1, B_1=0.6, B_2=1.4$. Notice that the sequences of approximants have already attained reasonably good convergence at $N=9$ for both the pure and disordered cases. The highest order approximants for the spectral function are plotted in Fig. 4, for several values of q . From that figure, one can infer that the system shows a central-peak type of behavior at $q=1$ ($B < J$) and moves onto a collective-mode type of

TABLE II. Moments of $C(t)$ for the spin glass in a homogeneous transverse field $B_i=1.0$. The coupling energies take up the values $J_1=1.0$ ($p=1$) and $J_2=0.4$ ($p=0$).

Moment	$p=0$	$p=0.25$	$p=0.5$	$p=0.75$	$p=1$
μ_0	1.0	1.0	1.0	1.0	1.0
μ_2	-0.5	-0.5	-0.5	-0.5	-0.5
μ_4	5.5×10^{-2}	7.25×10^{-2}	0.09	0.1075	0.125
μ_6	-3.00667×10^{-3}	-6.36083×10^{-3}	-1.045×10^{-2}	-1.52742×10^{-2}	-2.08333×10^{-2}
μ_8	1.13767×10^{-4}	4.581167×10^{-4}	9.87967×10^{-4}	1.70332×10^{-3}	2.60417×10^{-3}
μ_{10}	-4.14123×10^{-6}	-3.165166×10^{-5}	-8.29627×10^{-5}	-1.58932×10^{-4}	-2.60417×10^{-4}
μ_{12}	1.82266×10^{-7}	2.09525×10^{-6}	6.17108×10^{-6}	1.26323×10^{-5}	2.17014×10^{-5}
μ_{14}	-8.55208×10^{-9}	-1.24706×10^{-7}	-3.99168×10^{-7}	-8.63568×10^{-7}	-1.55010×10^{-6}
μ_{16}	3.56256×10^{-10}	6.43698×10^{-9}	2.23825×10^{-8}	5.14016×10^{-8}	9.68812×10^{-8}
μ_{18}	-1.24069×10^{-11}	-2.87222×10^{-10}	-1.09846×10^{-9}	-2.70197×10^{-9}	-5.38229×10^{-9}

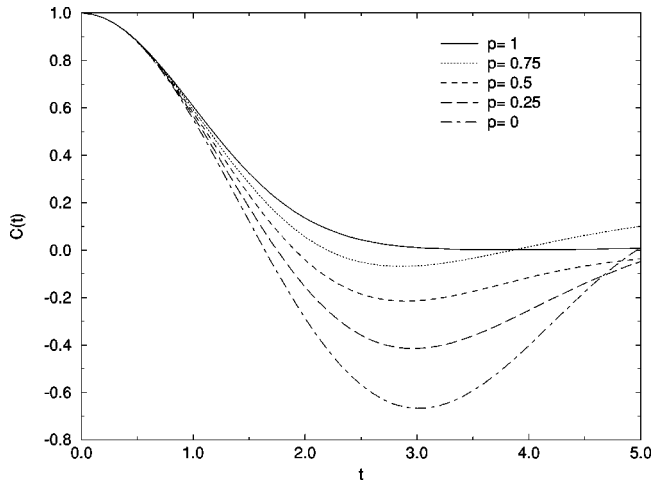


FIG. 6. Time-dependent correlation function for the same parameters as in Fig. 5.

behavior (resonant structure) at $q=0$ ($B>J$). For values of $q \neq 0, q \neq 1$, i.e., for the disordered case, both behaviors are present in the dynamics of the system (see, e.g., the cases $q=0.75$ or $q=0.25$).

Consider now the case of a spin glass in a homogeneous transverse field. Let us analyze the effects of the randomness of the exchange couplings on the dynamics. We keep the transverse field $B=1$, which sets the energy scale, and assume a bimodal distribution for the exchange couplings

$$\rho(J) = \prod_i [p \delta(J_i - J_1) + (1-p) \delta(J_i - J_2)], \quad (19)$$

where the bond concentration p varies from 0 to 1. We elect to consider $J_1=1.0$ and $J_2=0.4$. Hence, when $p=1$ the exchange couplings $J_i=1=B$, a case with known exact solution. There, the recurrants have a linear behavior with its order, and the time-dependent correlation function is Gaussian. As p is lowered toward zero, bonds with coupling energies $J_1=B$ are replaced randomly by bonds with weaker coupling energies $J_2<B$. When $p=0$, all the bonds will have the same coupling energy J_2 . By using the above distribution to calculate the norms of the basis vectors, we obtain the first nine recurrants, which are shown in Fig. 5, for several values of the bond concentration p . Note that apart from the expected linear behavior of the pure case $p=1$, the structure of the recurrants has an irregular pattern. The moments of $C(t)$ are given in Table II and are used to construct the Padé approximants for $C(t)$. The highest-ordered approximants are displayed in Fig. 6, for several values of p . That figure indicates an oscillatory behavior for $C(t)$ for values of $p<1$. For case $p=1$, $C(t)$ is a Gaussian. The spectral function is shown in Fig. 7. Again, we see that the system shows a central-peak dynamics for the pure case $p=1$ ($J_i=B$) and moves into a collective-mode dynamics on the other extreme pure case, $p=0$ ($J_i<B$). In disordered configurations such as $p=0.5$ the dynamics cannot be singly characterized by either behavior.

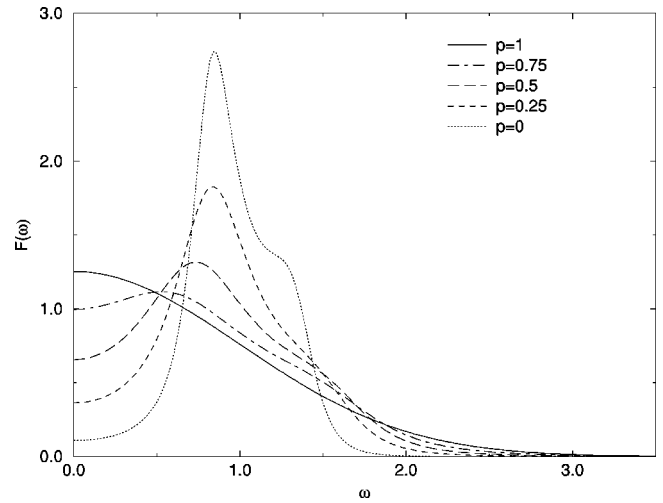


FIG. 7. Spectral densities for $J_i=1(0.4)$ with probability $p(1-p)$, and uniform transverse field $B_i=1$. Again, the system moves from a collective mode type of dynamics to a central peak type of dynamics as p is raised from 0 to 1.

To summarize, we have studied the time evolution of the spin variable $\sigma_i^x(t)$ in the one-dimensional disordered transverse Ising model at infinite temperature by the method of the recurrence relations. We obtained the autocorrelation function and the spectral function for different concentrations of either the transverse field or the exchange coupling. We found that the dynamics of the system changes according to the concentration of B or J . For the pure cases, two distinct behaviors appear, according to the concentrations of B or J . Basically, when $J>B$, a central-peak behavior dominates the dynamics, while for $J<B$ a collective-mode behavior is the main mode. The physical interpretation of these behaviors can be obtained by analyzing the root-mean square internal field associated with the exchange coupling and the transverse frequency. The field due to the exchange coupling in the infinite temperature limit is

$$G_{ij}^2 = \sum_{j,k} J_{ij} J_{ik} \langle \sigma_i^x \sigma_j^x \rangle = \sum_j J_{ij}^2 \langle (\sigma_i^x)^2 \rangle = J^2 (q=0). \quad (20)$$

So, the root-mean-square goes as J . Roughly speaking, for large B ($B>J$) the system behaves as independent spins precessing about the field B . The fluctuating internal field causes a damping of the precessing spins and gives to the spectral line its width. The resonant structure (collective-mode) disappears when the transverse field is less than the root-mean-square internal field ($B<J$). Now, for the disordered situations the general dynamic behavior of the system is neither central-peak- nor collective-mode-like, but something in between those behaviors.

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