Dynamics of the one-dimensional random transverse Ising model with next-nearest-neighbor interactions

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Abstract

The dynamics of the one-dimensional random transverse Ising model with both nearest-neighbor (NN) and next-nearest-neighbor (NNN) interactions is studied in the high-temperature limit by the method of recurrence relations. Both the time-dependent transverse correlation function and the corresponding spectral density are calculated for two typical disordered states. We find that for the bimodal disorder the dynamics of the system undergoes a crossover from a collective-mode behavior to a central-peak one and for the Gaussian disorder the dynamics is complex. For both cases, it is found that the central-peak behavior becomes more obvious and the collective-mode behavior becomes weaker as $K_i$ increase, especially when $K_i > J_i/2$ ($J_i$ and $K_i$ are exchange couplings of the NN and NNN interactions, respectively). However, the effects are small when the NNN interactions are weak ($K_i < J_i/2$).

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I. INTRODUCTION

There has been a considerable interest in the study of the dynamics of quantum spin systems in the past few decades [1, 2, 3], and the calculation of dynamic correlation functions remains a highly nontrivial and real challenging task until now. Some exact results have been obtained for the one-dimensional (1-D) pure quantum spin models, e.g., the 1-D transverse Ising model and the 1-D XY model [4, 5, 6]. Recently, more attention has been paid to the investigation of the dynamical behavior of disordered systems [7, 8, 9, 10, 11, 12], which can be applied to describe the properties of many materials such as window glass, magnets with frozen-in disorder, etc.. One simple but important example of such systems is the 1-D random transverse Ising model (RTIM).

The dynamical behavior of the 1-D RTIM with the bimodal distribution is studied by Florencio and Barroto [8], and it is found that the dynamics undergoes a crossover from a central peak behavior onto a collective mode one. Recently, we have investigated the effects of Gaussian disorder on the dynamics of the 1-D RTIM [12], and have found that there are two crossovers when the standard deviation of random variables is small and there is no crossover if the value of the standard deviation is large enough. Besides, the dynamical behavior of the random-bond transverse Ising model with four-spin interactions [13] and the disordered XY chain [9, 10, 11] have been studied.

In the work mentioned above only nearest-neighbor (NN) interactions are considered. To our knowledge, no related results of disordered quantum spin systems with next-nearest-neighbor (NNN) interactions have been reported so far. However, the work of Sen has shown the role of second neighbor interactions on the relaxation in $s = 1/2$ pure quantum spin chains [14]. The results show that the dynamical correlation in the NNN transverse Ising chain is noticeably different with that of the exactly solvable NN transverse Ising chain. Therefore, it is expected that considering additional spin-spin interactions in disordered systems will make some differences in the dynamical process.

Our main interest is to investigate the effects of NNN interactions on the dynamics of the 1-D disordered quantum spin systems. It is well known that the interactions between spins may be complex in real materials. For studying the properties of real systems theoretically and experimentally, the easy way is to consider a model with only the dominant NN interactions. In this paper, we consider the 1-D RTIM with both NN and NNN interactions.
The 1-D RTIM can be used to describe the dynamical property of many condensed-matter systems like the quasi-one-dimensional ferroelectric crystals (e.g., PbH$_{1-x}$D$_x$Po$_4$)\cite{19, 20}, and the Ising spin glass LiHo$_{0.167}$Y$_{0.833}$F$_4$\cite{21}. We investigate the cases that the exchange couplings between spins or transverse fields independently satisfy the bimodal distribution and the Gaussian distribution, respectively. Our calculations are based on the method of recurrence relations\cite{22, 23}, which is very powerful in the study of classical and quantum many-body dynamics\cite{3, 6, 17}. Meanwhile, we also used some reliable approximation schemes such as the so-called Gaussian terminator\cite{3, 24, 25} and the Padé approximants.

It is found in both disorder that the central-peak behavior becomes more obvious and the collective-mode behavior becomes weaker when $K_i > J_i/2$. We also find that the dynamics of the system is not sensitive to the property of the NNN interaction whether it is ferromagnetic or antiferromagnetic.

This paper is arranged as follows. In Sec. II we introduce the model used in this paper and the method of recurrence relations. Secs. III and IV give the dynamical results for the bimodal disorder and the Gaussian disorder, respectively. Sec. V provides conclusions.

II. MODEL AND METHOD

The Hamiltonian of the 1-D RTIM with both NN and NNN interactions can be written as

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

(1)

where $\sigma_i^\alpha$ ($\alpha = x, y, z$) are Pauli matrices at site $i$, $B_i$ denote the external fields, while $J_i$ and $K_i$ are exchange couplings between NN spins and NNN spins, respectively. The periodic boundary conditions $\sigma_{i+N}^\alpha = \sigma_i^\alpha$ are assumed in next calculation, where $N$ is the number of spins. For simplicity, we assume that $K_i = \alpha J_i$ ($0 \leq \alpha < 1$) and consider $J_i$ and $B_i$ are uncorrelated random variables which satisfy the probability distributions $\rho(J_i)$ and $\rho(B_i)$, respectively. It is obvious that, in the limit $K_i \to 0$ in Eq. (1), this model can be reduced to the 1-D RTIM\cite{8, 12}.

The dynamical behavior of classical or quantum many-body systems is conveniently expressed in terms of dynamic correlation functions. In this paper, we are interested in the
time-dependent transverse correlation function defined by
\[ C(t) = \langle \sigma^z_j(t) \sigma^z_j(0) \rangle, \] (2)
where \( \langle \cdots \rangle \) denotes an ensemble average followed by an average over the disorder variables.

The spectral density \( \Phi(\omega) \) (\( \omega \) is the frequency) which is able to be determined directly from experiments is defined as the Fourier transformation of the correlation function,
\[ \Phi(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} C(t) \, dt. \] (3)

The method of recurrence relations has already been applied to solve a variety of many-body systems, such as the classical harmonic chain[17], the electron gas[22, 23], spin systems[15, 16, 24] and ergodic theory[18] etc., successfully. In the following we will summarize this method.

Consider a many-body system defined by a Hamiltonian \( H \). The time evolution of a dynamical operator \( A \) is described by the Liouville (or Heisenberg) equation of motion
\[ \frac{dA(t)}{dt} = iLA(t), \] (4)
where \( L \) is the Liouville operator, \( LA = [H, A] \equiv HA - AH \). The solution of Eq. (4) can be given as the form of the orthogonal expansion[22]
\[ A(t) = \sum_{\nu=0}^{\infty} a_\nu(t) f_\nu, \] (5)
where \( \{f_\nu\} \) are an orthogonal set of basis vectors spanning a Hilbert space \( S \), the coefficients \( a_\nu(t) \) are time dependent functions representing the projection of \( A(t) \) onto \( f_\nu \) at \( t \).

In the high-temperature limit \( T = \infty \), the inner product which includes both the statistical and random averages in our system is described as[8, 9, 10]
\[ (X, Y) = \langle XY \rangle, \] (6)
where \( X \) and \( Y \) are basis vectors defined in \( S \).

Set \( f_0 = A(0) \), which gives \( a_0(0) = 1 \) and \( a_\nu(0) = 0 \) for \( \nu > 0 \) by Eq. (5). The basis vectors \( f_\nu \) satisfy the recurrence relation (RRI)
\[ f_{\nu+1} = iL f_\nu + \Delta_\nu f_{\nu-1}, \quad \nu \geq 0, \] (7)
where the coefficients, also known as recurrants, are defined as
\[
\Delta_\nu = \frac{(f_\nu, f_\nu)}{(f_{\nu-1}, f_{\nu-1})} \quad (\nu \geq 1)
\] (8)
with \( f_{-1} \equiv 0 \) and \( \Delta_0 \equiv 1 \). Meanwhile, the coefficients \( a_\nu(t) \) satisfy a second recurrence relation (RRII)
\[
\Delta_{\nu+1} a_{\nu+1}(t) = -\frac{da_\nu(t)}{dt} + a_{\nu-1}(t), \quad \nu \geq 0,
\] (9)
where \( a_{-1}(t) \equiv 0 \), and \( a_0(t) \) is the time-dependent correlation function \( \langle A(t)A(0) \rangle \). Obviously, by choosing \( f_0 = \sigma_j^x \) the average spin correlation function is just given by \( C(t) = \langle \sigma_j^x(t) \sigma_j^x(0) \rangle \) (Eq. (2)), which can be written as the form of moment expansion
\[
C(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \mu_{2k} t^{2k}
\] with
\[
\mu_{2k} = \frac{1}{Z} \text{Tr} \sigma_j^x \left[ H, \left[ H, \cdots \left[ H, \sigma_j^x \right] \cdots \right] \right],
\] (10)
where \( \mu_{2k} \) is the \( 2k \)th moment of \( C(t) \). The partition function \( Z = \text{Tr} 1 = 2^N \) equals the number of quantum states of the system. Using the first \( 2\nu \) moments, we can calculate the correlation function \( C(t) \) by constructing Padé approximants.

By taking the Laplace transformation of the recurrence relation (RRII), one obtains
\[
\Delta_{\nu+1} a_{\nu+1}(z) - \delta_{\nu,0} = -za_\nu(z) + a_{\nu-1}(z), \quad \nu = 0, 1, 2 \cdots,
\] (11)
where \( z = \varepsilon + i\omega \) (\( \varepsilon > 0 \)) is a variable of the complex plane. Then one can get the continued-fraction form
\[
a_0(z) = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \cdots}}},
\] (12)
Furthermore, it is proved that the spectral density \( \Phi(\omega) \) (Eq. (3)) is able to be determined directly by Eq. (12),
\[
\Phi(\omega) = \lim_{\varepsilon \to 0} \text{Re} a_0(z).
\] (13)
Note that \( \Delta_\nu \) are the key quantities for calculating the dynamic correlation functions.

Generally, only a finite number of continued-fraction coefficients can be determined. So it is necessary to use a scheme to terminate the continued fraction. The one that serves our
model best is the so-called Gaussian terminator. Suppose the first \( M \) recurrants are determined, in this approximation, the others are assumed to be of the form \( \Delta_\nu = \nu (\Delta_M/M) \), for \( \nu > M \).

### III. DYNAMICS FOR BIMODAL DISORDER

After a lengthy calculation, the first eight basis vectors are exactly obtained by Eq. (7). In the following, we just give the first two of them:

\[
\begin{align*}
f_1 &= B_j \sigma_j^y , \\
f_2 &= (\Delta_1 - B_j^2) \sigma_j^y + B_j K_{j-2} \sigma_j^z + B_j J_{j-1} \sigma_j^x + B_j J_{j} \sigma_j^x + B_j K_{j} \sigma_j^x + B_j J_{j+1} \sigma_j^z ,
\end{align*}
\]

The squared norms of the basis vectors are given by Eq. (6) as follows:

\[
\begin{align*}(f_0, f_0) &= 1 , \\
(f_1, f_1) &= B_j^2 , \\
(f_2, f_2) &= \Delta_1^2 - 2 \Delta_1 \Delta_2 ^2 - \Delta_3 - \Delta_2 J_2 + B_j^2 J_2 + B_j^2 K_2 + B_j^2 K_2 ^2 + B_j^2 K_2 ^2 .
\end{align*}
\]

Using the above results, we have calculated the first eight coefficients \( \Delta_1, \Delta_2, \cdots, \Delta_8 \) exactly, and the \( \Delta_9 \) through the assumption \( \Delta_\nu = \nu (\Delta_M/M) \) approximately. Meanwhile, the first 18 moments are obtained and the correlation function \( C(t) \) can be determined by constructing the Padé approximants.

Notice that the coefficients (see Eq. (8)) are even functions of \( K_i \) and the correlation functions are determined uniquely by the recurrants. Thus, the dynamical property of the system is independent of that the NNN interactions are ferromagnetic or antiferromagnetic. Actually, the system is in its paramagnetic phase in the high-temperature limit. Next, we only consider the case of ferromagnetic NNN interactions \( K_i > 0 \). We calculate two typical cases that the random variables satisfy the bimodal distribution and the Gaussian distribution, respectively.

In the following, we assume that the exchange couplings \( J_i \) or the transverse fields \( B_i \) satisfy the bimodal distribution

\[
\rho (\{ \beta_i \}) = \prod_1^N [p \delta (\beta_i - \beta_a) + (1 - p) \delta (\beta_i - \beta_b)] ,
\]
FIG. 1: Time-dependent correlation functions $C(t)$ and corresponding spectral densities $\Phi(\omega)$ for the case of random bond which satisfy the bimodal distribution in which $J_a = 1.0$ and $J_b = 0.4$. (a) and (b) plot of the pure cases that $p = 0$ and 1. The results in (c) and (d) are the disordered cases for $p = 0.25$ and 0.75. The central-peak behavior becomes more obvious and the collective-mode behavior becomes weaker as $K_i$ increase. The black solid line in (a) is monotonic for $t < 3$.

where $\beta_i = J_i$ or $B_i$, $p$ is the concentration of coupling $J_a$ or magnetic field $B_a$ and takes values from 0 to 1.

We first consider the random band and uniform field model. In this case, without loss of generality we set $B_i = B = 1$, and choose $J_a = 1.0$ and $J_b = 0.4$, which have been used in Ref. [8]. In this assumption, the exchange couplings $J_i$ change from $J_i < B$ ($p < 1$) to $J_i = B$ ($p = 1$). The transverse correlation functions $C(t)$ and the corresponding spectral densities $\Phi(\omega)$ are given in Fig. 1 for several values of bond concentration $p$. In order to show better the effects of the NNN interactions on the dynamics of the system, we have considered the cases that $K_i = 0$, $J_i/4$, $J_i/2$ and $3J_i/4$, respectively. Obviously, for the $K_i = 0$ case, the results are just of the 1-D RTIM studied by Florencio and Barreto[8].
From different cases of $K_i$ shown in Fig. 1, we can see that the system shows a collective-mode behavior for small values of $p$ (i.e. $p = 0$ or $0.25$), and exhibits a central-peak behavior when $p = 1$. In general, when the external field is small, the spin-spin interactions play an important role, thus the central-peak behavior dominates the dynamics of the system, while for large $B$ the dynamical behavior is collective-mode one, which is due to the precession of spins in the transverse field. This means that the dynamics of the present model with bimodal distributions is similar to that of Ref. [8].

By comparing the curves for the cases that $K_i = J_i/4$, $J_i/2$, and $3J_i/4$ with those of the $K_i = 0$ case (see Fig. 1), we can see that the dynamics has no evident change if the NNN interactions are weak (e.g. $K_i = J_i/4$). However, there are some obvious differences when $K_i > J_i/2$. The dot-dashed curve for the pure case $p = 1$ when $K_i = 0$ in Fig. 1(a) describes the dynamics for the exactly solvable limit in which $J_i = B_i = 1$, now the $C(t)$ is a Gaussian function [6]. Meanwhile, the other curves for the cases that $p = 1$ when $K_i = J_i/4$, $J_i/2$, and $3J_i/4$ in Fig. 1(a), respectively, all behave monotonically but exhibit slower decay than for the $K_i = 0$ case, and are not a Gaussian. On the other hand, the lines shown in Fig. 1(a) for the pure case $p = 0$ indicate that the collective-mode behavior becomes weaker as $K_i$ increase. The same results can be also obtained from the corresponding spectral densities. As shown in Fig. 1(b) the central peak increases, meanwhile, the collective-mode peak becomes lower and the width of the spectral line broaden as $K_i$ increase. For the disordered case that $p = 0.25$ (see Figs. 1(c) and (d)), we also find weaker collective-mode behavior if the NNN interactions become stronger. However, for the disordered case that $p = 0.75$ when $K_i = 3J_i/4$ (see the black solid line in Fig. 1(c)), the $C(t)$ decays monotonically to zero, and the dynamics of the system is a central-peak behavior which is not as the case that $p = 0.75$ when $K_i = 0$ (the lines for $p = 0.75$ when $K_i = 0$ or $J_i/4$ in Figs. 1(c) and (d) show a disordered behavior which is something between the collective-mode behavior and the central-peak one). All the above results indicate that the interactions between spins are stronger in our system, and that the effects of the NNN interactions on the dynamics of the system cannot be neglected.

We now consider the random field and uniform band model, in which the transverse fields satisfy the bimodal distribution $\rho(B_i)$ and can take the values $B_a = 0.6$ ($p = 1$) and $B_b = 1.4$ ($p = 0$), while the exchange couplings are constants ($J_i = J = 1$, $K_i = 0$, 1/4, 1/2 or 3/4). This allows the external fields changing from $B_i > J$ to $B_i < J$ as $p$ increases.
FIG. 2: Correlation functions and corresponding spectral densities for the random field model, in which $B_a = 0.6$ and $B_b = 1.4$. The system undergoes a crossover from a collective-mode behavior to a central-peak one as $q$ increases. The central-peak behavior becomes more obvious and the collective-mode behavior becomes weaker as $K_i$ change from 0 to 3/4.

The results of $C(t)$ and $\Phi(\omega)$ for different values of $p$ are shown in Fig. 2. The curves for $p = 0$ are the pure cases dominated by the stronger field energy. In this case, the system is at the collective mode regime. When $p = 1$ and 0.75, the correlation functions decay monotonically, and thus the dynamics is dominated by the central-peak behavior. However, for the disordered case $p = 0.25$, the dynamics of the system is neither central-peak nor collective-mode type, but something between them. Hence, for this model, the system also undergoes a crossover from a collective-mode behavior to a central-peak one as $p$ increases from 0 to 1.

The same as the above random bond model, it is found that the central-peak behavior becomes more obvious and the collective-mode behavior becomes weaker as $K_i$ increase, especially when $K_i > J_i/2$. From the curves for $p = 1$ in Fig. 2(a) and $p = 0.75$ in Fig. 2(c),
we can find that the $C(t)$ decays more slowly as $K_i$ changing from 0 to $3/4$. Meanwhile, the magnitude for $\Phi(\omega)$ at $\omega = 0$ increases as $K_i \neq 0$ (see Figs. 2(b) and (d)). The results of $p = 0$ in Fig. 2(a) and (b) indicate that the collective-mode behavior becomes weaker if the NNN interactions are stronger, since the oscillatory curves are less damped.

IV. DYNAMICS FOR GAUSSIAN DISORDER

In the following, we assume that the exchange couplings $J_i$ or the transverse fields $B_i$ are uncorrelated random variables which satisfy the Gaussian distribution

$$\rho(\{\beta_i\}) = \prod_i^N \frac{1}{\sqrt{2\pi}\sigma_\beta} \exp \left[ -\frac{(\beta_i - \beta)^2}{2\sigma_\beta^2} \right],$$

where $\beta$ denotes the mean value of the random variables $\beta_i$, and $\sigma_\beta$ is the standard deviation. Next, we discuss two different cases that the random-bond and the random-field model, respectively. We find that the effects of $K_i$ on the dynamics are not obvious when $K_i < J_i/2$, which is similar as the above case of the bimodal disorder. In the following, we only give the results for $K_i = J_i/2$ and $3J_i/4$ in the random-bond model, and for $K_i = 3J_i/4$ in the random-field model.

For the random-bond model, the exchange couplings $J_i$ satisfy the Gaussian distribution while the transverse fields $B_i$ are constants. We keep $B_i = B = 1$ which sets the energy scale, and consider that the mean value $J$ varies from 0 to 2 and the standard deviation $\sigma_J$ changes from 0.3 to 3.0. Both the correlation functions $C(t)$ and the corresponding spectral densities $\Phi(\omega)$ are shown in Figs. 3 and 4, respectively. The insets to Fig. 4 present the first nine recurrants.

From Figs. 3 and 4 we can see that for the case of small values of $\sigma_J$ (e.g., 0.3), there are two typical dynamics: the collective-mode behavior and the central-peak behavior. It is obvious that the black solid curve for $J = 0$ in Fig. 3(a) is a damped cosine function, which is due to the precession of spins in an external transverse magnetic field [12]. As $J$ increases, the system first shows a weak collective-mode behavior for the case of $J < B$ (e.g., $J = 0.5$), then exhibits a central-peak behavior when $J > B$ (e.g., $J = 1.5$).

For the case of large $\sigma_J$ (e.g., 3.0), it is found that the system only shows a central-peak behavior, and there is no crossover. In this case, the strong exchange couplings play an important role in the dynamics of the system. That is, the spin-spin interactions are
FIG. 3: Correlation functions $C(t)$ for the case that the bonds satisfy the Gaussian distribution while the external fields are constants. Two typical cases that $\sigma_J = 0.3$ and 3.0 are considered. The mean value $J$ varies from 0 to 2.

dominant in the competition between the spin-spin interactions and the external fields. It is also found that, further increasing the NNN interactions will make the curves of $C(t)$ for the central-peak behavior decay more slower and the magnitude for $\Phi(\omega)$ at $\omega = 0$ become larger. This all indicate that the dynamical behavior of the system is sensitive to the inclusion of the NNN interactions.

We next discuss the results of the random-field model, in which the transverse fields $B_i$ satisfy the Gaussian distribution, while the exchange couplings remain unaltered ($J_i = J = 1$, $K_i = 3/4$). Let the mean value $B$ varies from 0 to 2. From Fig. 5 we can see that for $\sigma_B = 0.3$ the system undergoes a crossover from a central-peak behavior to a collective-mode one as $B$ increases. When $\sigma_B$ is large enough ($\sigma_B = 3.0$), the system only shows one type of dynamics and there is no crossover. That is a most-disordered state\[12\], which is something between the central-peak behavior and the collective-mode behavior. By comparing the
FIG. 4: Corresponding spectral densities $\Phi(\omega)$ for the same parameters as in Fig. 3. For $\sigma_J = 3.0$ the central-peak increases as $K_i$ change from $J_i/2$ to $3J_i/4$. For $\sigma_J = 0.3$ the collective-mode behavior becomes weaker as $K_i$ increase.

results with those of Ref. [12], we can find that the oscillatory behavior becomes weaker as $K_i$ increase. However, different from the effects of the NNN interactions on the dynamics of the random-bond model, increasing $K_i$ in this case will make no difference when $\sigma_B$ is large enough. That is, the dynamics of the system now is dominated by the disordered external field.

V. CONCLUSIONS

In this paper, we have studied the effects of the NNN interactions on the dynamics for the 1-D RTIM in the high-temperature limit. We have considered the cases that the random variables satisfy the bimodal distribution and the Gaussian distribution, respectively. It is found in both cases that the dynamical property of the present model is similar to that of
FIG. 5: Correlation functions and corresponding spectral densities for the random field model when $K_i = 3J_i/4$. The insets to (b) and (d) present the first nine recurrants. Let the mean value $B$ varies from 0 to 2. For $\sigma_B = 0.3$ there is a crossover from a central-peak behavior to a collective-mode one as $B$ increases. For $\sigma_B = 3.0$ the system exhibits a most disordered behavior.

the 1-D RTIM when $K_i < J_i/2$. However, the central-peak behavior becomes more obvious and the collective-mode behavior becomes weaker as the NNN interactions increase (i.e. $K_i > J_i/2$). It is expected that we can get similar results in other disordered quantum spin systems, e.g., the $XY$ and the $XYZ$ models.

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