

Effects of Gaussian disorder on the dynamics of the random transverse Ising model

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The effects of Gaussian disorder on the dynamics of the one-dimensional spin-1/2 random transverse Ising model are studied in the high-temperature limit by the recursion method. Both spin autocorrelation functions and the corresponding spectral densities are calculated for three types of disordered cases. It is found that when the standard deviation σ_J of the exchange coupling (or the standard deviation σ_B of the random transverse field) is small, the dynamics of the system undergoes two crossovers in sequence as the mean value of the exchange coupling (or the random transverse field) varies: from a central-peak behavior to a collective-mode one, and then to the precession of free spins in an external transverse magnetic field. However, when σ_J or σ_B are large enough, there is no crossover, i.e., the dynamics of the system shows a central-peak behavior and a disordered behavior, respectively.

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I. INTRODUCTION

It has been proved that the study of the properties of quantum spin systems was a real challenge. After more than 30 years research, the properties of quantum spin systems, especially dynamical properties, are still far from being completely understood. For pure quantum spin systems, only the Ising chain in a transverse field and the one-dimensional (1-D) spin-1/2 *XY* model are exactly studied until now.^{1,2} Both above systems can be mapped onto a solvable non-interacting fermions system. On the other hand, for disordered quantum spin systems, McKenzie has obtained the exact results for quantum phase transitions in random *XY* spin chains.³ Besides, it is worth noting that the dynamical properties of several quantum spin systems has been the subject of much research activity in the past decades.⁴⁻⁷ Recently, some results for the dynamics of the 1-D disordered quantum spin models are reported.⁸⁻¹²

One simple yet important example of the disordered quantum spin chains is the 1-D random transverse Ising model (RTIM), where both the exchange couplings J_i and the transverse fields B_i are considered as random variables. This model has a well-known physical interpretation in connection not only with some quasi-one-dimensional hydrogen-bonded ferroelectric crystals like $\text{Cs}(\text{H}_{1-x}\text{D}_x)_2\text{PO}_4$, $\text{PbH}_{1-x}\text{D}_x\text{PO}_4$, etc.,^{13,14} but also with Ising spin glass such as $\text{LiHo}_{0.167}\text{Y}_{0.833}\text{F}_4$.¹⁵ For the case of ferroelectric crystals, one may take B_i as the site-dependent random transverse magnetic fields, whereas the intra-chain interactions J_i remain unaltered; for spin glasses, J_i are site-dependent random variables while $B_i=B$.

As is well known, the spin autocorrelation function plays an important role in the study of the dynamics of quantum spin systems. There are several results of the time-dependent correlation functions for the pure as well as the disordered transverse Ising model, *XY* model, and *XXZ* model. Some results indicate that the transverse time-dependent correlation functions show a Gaussian behavior at $T=\infty$,^{16,17} an exponential behavior at $0 < T < \infty$,¹⁸ and a power-law behavior

at $T=0$,¹⁹ respectively. In addition, the longitudinal correlation functions of the *XY* model were exactly obtained by Niemeijer²⁰ and also Katsura, Horiguchi, and Suzuki²¹ for any temperature, in which the results show that it can be expressed by the square of the Bessel function in the high-temperature limit; but it has a more complicated expression for other temperature.

Recently, the dynamical properties of the 1-D random transverse Ising model with the bimodal distributions is investigated by Florencio and Barreto.⁸ However, to our knowledge, no related results of this model with continuous distributions have been reported so far. In this paper, we shall study the Gaussian disorder effects of the couplings and the random fields on the dynamics of the 1-D RTIM. We find that this model exhibits many new interesting phenomena, e.g., the crossover from a central-peak behavior to a collective-mode behavior vanishes gradually as the standard deviation increases. These interesting phenomena result from the competition between the spin interactions and the random transverse fields.

The remainder of this paper is organized as follows. We introduce the model and the recursion method in Sec. II. In Sec. III the spectral density of the spin autocorrelation function is calculated. Section IV gives the results and discussion for three types of disordered cases, and Sec. V provides conclusions.

II. MODEL AND METHOD

The 1-D RTIM considered in this paper is defined by the Hamiltonian

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

where σ_i^α ($\alpha=x, y, z$) are Pauli matrices, J_i and B_i are the exchange couplings and the transverse fields, respectively, which independently satisfy the Gaussian distribution²²

$$P(\beta_i) = \frac{1}{\sqrt{2\pi}\sigma_\beta} \exp[-(\beta_i - \beta)^2/2\sigma_\beta^2], \quad (2)$$

where β is the mean value of the random variables β_i , and σ_β is the standard deviation which denotes the degree of the disorder of the random variables β_i in the system. However, it is not always a fact that the larger σ_β is, the more disordered the system is. A physical reason for this phenomenon will be presented in Sec. IV.

It has been proved that the recursion method is very powerful in the study of classical and quantum many-body dynamics. For example, it has been applied to a lot of many-body systems⁶ such as spin chains,^{8–10,17,23–25} the electron gas,²⁶ and the classical harmonic chain.²⁷ Next we will simply present this method for the systems above.

Let X, Y be the basis vectors defined in an abstract Hilbert space S . To account for disorder, the inner product is defined as the Kubo product averaged over the realizations of the disorder⁹

$$(X, Y) = k_B T \int_0^{1/k_B T} d\lambda \overline{\langle X(\lambda) Y^\dagger \rangle} - \overline{\langle X \rangle \langle Y^\dagger \rangle}, \quad (3)$$

where $X(\lambda) = e^{\lambda H} X e^{-\lambda H}$, $\langle X \rangle = \text{Tr}(e^{-H/k_B T} X) / \text{Tr}(e^{-H/k_B T})$ denotes the statistical average value of X , and $\overline{\langle \dots \rangle}$ an average over the disorder variables, k_B and T are the Boltzmann constant and the absolute temperature, respectively. In the high-temperature limit, $T \rightarrow \infty$, the inner product becomes

$$(X, Y) = \frac{1}{Z} \overline{\text{Tr} X Y}, \quad (4)$$

where the partition function Z now equals the number of quantum states of the system $Z = \text{Tr} 1$. In the present case, $Z = 2^N$, where N is the number of spins of this system.

Consider a dynamical variable A and assume that it is Hermitian. The time evolution of A is governed by the Liouville equation

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

where L is the Liouville operator defined by $LA = [H, A] \equiv HA - AH$. Then the solution of Eq. (5) can be formally given as

$$A(t) = \sum_{\nu=0}^{\infty} a_\nu(t) f_\nu, \quad (6)$$

where $\{a_\nu(t)\}$ is a set of time-dependent real functions, $\{f_\nu\}$ is a complete orthogonal sequence in the Hilbert space S which is defined by Eqs. (4)–(6). The basis vectors f_ν satisfy the recurrence relation²⁶

$$f_{\nu+1} = iL f_\nu + \Delta_\nu f_{\nu-1}, \quad \nu \geq 0, \quad (7)$$

where the coefficients are defined as

$$\Delta_\nu = \frac{(f_\nu, f_\nu)}{(f_{\nu-1}, f_{\nu-1})}, \quad \nu \geq 1 \quad (8)$$

with $f_{-1} \equiv 0$, and $\Delta_0 \equiv 1$. In the recurrence relation (7) f_0 can be arbitrary chosen. Given a choice, the others can be determined by this relation. It can be seen that the sequence of numbers Δ_ν contains all the information necessary for the construction of the spectral density of the spin autocorrelation function.

Noting that Eq. (6) must satisfy Eqs. (5) and (7), it yields a recurrence relation for $\{a_\nu(t)\}$:

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\frac{da_\nu(t)}{dt} + a_{\nu-1}(t), \quad \nu \geq 0, \quad (9)$$

where $a_{-1}(t) \equiv 0$.

Let $f_0 = A$, there are some relations between $\{a_\nu(t)\}$ and the dynamical response functions, i.e., $a_0(t)$ represents the relaxation function (the time-dependent autocorrelation function) $(A(t), A(0)) / (A, A)$ and the other $a_\nu(t)$'s are relative to the relaxation of the random force defined by the generalized Langevin equation.²⁶ Obviously, for the random transverse Ising chain, $f_0 = \sigma_j^x$, the average spin autocorrelation function is given by

$$C(t) = \overline{\langle \sigma_j^x(t) \sigma_j^x \rangle}. \quad (10)$$

$C(t)$ can be written as the form of moment expansion

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

with

$$\mu_{2k} = \frac{(-1)^k}{(2k)!} \overline{\text{Tr} \sigma_j^x [H, [H, \dots [H, \sigma_j^x] \dots]]}, \quad (11)$$

where μ_{2k} is the $2k$ th moment of the spin autocorrelation function. Supposing that the first Q moments have been obtained, then the autocorrelation functions $C(t)$ can be determined by constructing the Padé approximant. In this paper, to obtain more accurate approximation of the spin autocorrelation function $C(t)$, we have exactly calculated up to the 20th moment of $C(t)$ by Eq. (11), and have constructed the highest-order Padé approximants for the spin autocorrelation functions.

Applying the Laplace transformation $a_\nu(z) = \int_0^{+\infty} e^{-zt} a_\nu(t) dt$ ($z = \varepsilon + i\omega$ is a complex number, $\varepsilon > 0$) to the recurrence relation (9), we have

$$\Delta_{\nu+1} a_{\nu+1}(z) - \delta_{\nu,0} = -z a_\nu(z) + a_{\nu-1}(z), \quad \nu = 0, 1, 2, \dots \quad (12)$$

Using the above Eq. (12), one can get the continued fraction

$$a_0(z) = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \dots}}}. \quad (13)$$

Generally, we are only able to determine a finite number of continued-fraction coefficients $\Delta_1, \dots, \Delta_M$. So it is neces-

sary to use a scheme to terminate the continued fraction. The one that serves best our problem is the so-called Gaussian terminator.^{6,25,28} In this approximation, based on the continued-fraction coefficients $\Delta_1, \dots, \Delta_M$, the others are assumed to be $\Delta_\nu = \nu(\Delta_M/M)$ for $\nu > M$. The accuracy of this approximate method has been discussed by Florencio and Barreto.⁸

III. SPECTRAL DENSITY

The spectral density $\Phi(\omega)$ that may be measured directly in experiments is defined as the Fourier transformation of the spin autocorrelation function

$$\Phi(\omega) = \int_0^{+\infty} C(t) e^{-i\omega t} dt. \quad (14)$$

It can be proved that $\Phi(\omega)$ is able to be determined directly by Eq. (13),

$$\Phi(\omega) = \lim_{\varepsilon \rightarrow 0} \text{Re } a_0(z)|_{z=\varepsilon+i\omega}. \quad (15)$$

Next we will apply the recursion method to the 1-D RTIM to obtain the spectral density of the spin autocorrelation function in the high-temperature limit. First of all, we choose the zeroth basis vector $f_0 = \sigma_j^x$, and then determine the others f_1, f_2, \dots by relation (7). The basis vectors up to f_9 have been exactly calculated. Because some of them are too lengthy to be illustrated here, we just give the first four of them

$$f_1 = B_j \sigma_j^y,$$

$$f_2 = (\Delta_1 - B_j^2) \sigma_j^x + B_j J_{j-1} \sigma_{j-1}^x \sigma_j^z + B_j J_j \sigma_{j+1}^x \sigma_j^z,$$

$$f_3 = -B_j(-\Delta_1 - \Delta_2 + B_j^2 + J_{j-1}^2 + J_j^2) \sigma_j^y - 2B_j J_{j-1} J_j \sigma_{j-1}^x \sigma_j^y \sigma_{j+1}^x + B_{j-1} B_j J_{j-1} \sigma_{j-1}^y \sigma_j^z + B_j B_{j+1} J_j \sigma_{j+1}^y \sigma_j^z,$$

and

$$f_4 = (\Delta_1 \Delta_3 + B_j^4 - B_j^2(\Delta_1 + \Delta_2 + \Delta_3 - J_{j-1}^2 - J_j^2)) \sigma_j^x + B_j J_{j-1} (\Delta_1 + \Delta_2 + \Delta_3 - B_{j-1}^2 - B_j^2 - J_{j-1}^2 - 3J_j^2) \sigma_{j-1}^x \sigma_j^z + B_j J_j (\Delta_1 + \Delta_2 + \Delta_3 - B_j^2 - B_{j+1}^2 - 3J_{j-1}^2 - J_j^2) \sigma_{j+1}^x \sigma_j^z + 2B_j^2 J_{j-1} J_j \sigma_{j-1}^x \sigma_j^x \sigma_{j+1}^x - 3B_{j-1} B_j J_{j-1} \sigma_{j-1}^y \sigma_j^y \sigma_{j+1}^x - 3B_j B_{j+1} J_j \sigma_{j-1}^y \sigma_j^y \sigma_{j+1}^x + B_{j-1} B_j J_{j-2} J_{j-1} \sigma_{j-2}^x \sigma_{j-1}^z + B_j B_{j+1} J_j J_{j+1} \sigma_{j+1}^z \sigma_{j+2}^x.$$

The norms of the above vectors can be obtained by Eq. (4) as follows:

$$(f_0, f_0) = 1,$$

$$(f_1, f_1) = \overline{B_j^2},$$

$$(f_2, f_2) = 2\overline{J_j^2} \overline{B_j^2} - \overline{B_j^2} + \overline{B_j^4},$$

$$(f_3, f_3) = \overline{B_j^6} + 2\overline{J_j^2} \overline{B_j^2} + 2\overline{J_j^4} \overline{B_j^2} + 2\overline{J_j^2} \overline{B_j^2} - \overline{B_j^4} / \overline{B_j^2},$$

and

$$(f_4, f_4) = W/V,$$

where

$$W = \overline{B_j^4}^3 - 2\overline{B_j^2} \overline{B_j^4} \overline{B_j^6} + \overline{B_j^6}^2 + \overline{B_j^2} \overline{B_j^8} - \overline{B_j^4} \overline{B_j^8} + 2\overline{B_j^2}^3 \overline{B_j^4} \overline{J_j^2} - 8\overline{B_j^2} \overline{B_j^4} \overline{J_j^2} + 6\overline{B_j^2}^2 \overline{B_j^6} \overline{J_j^2} + 2\overline{B_j^4} \overline{B_j^6} \overline{J_j^2} - 2\overline{B_j^2} \overline{B_j^8} \overline{J_j^2} + 28\overline{B_j^4} \overline{J_j^2}^2 - 26\overline{B_j^2}^2 \overline{B_j^4} \overline{J_j^2}^2 - 2\overline{B_j^4}^2 \overline{J_j^2}^2 - 56\overline{B_j^2}^3 \overline{J_j^2}^3 + 12\overline{B_j^2} \overline{B_j^4} \overline{J_j^2}^3 + 36\overline{B_j^2}^2 \overline{J_j^2}^4 + 4\overline{B_j^4} \overline{J_j^2}^4 - 2\overline{B_j^2}^2 \overline{B_j^4} \overline{J_j^2}^4 - 6\overline{B_j^2}^2 \overline{J_j^2}^4 + 4\overline{B_j^2} \overline{B_j^6} \overline{J_j^2}^4 + 22\overline{B_j^2}^3 \overline{J_j^2}^4 \overline{J_j^2} - 26\overline{B_j^2} \overline{B_j^4} \overline{J_j^2}^4 \overline{J_j^2} - 36\overline{B_j^2}^2 \overline{J_j^2}^4 \overline{J_j^2}^4 + 4\overline{B_j^2}^3 \overline{J_j^2}^4 \overline{J_j^2}^6 - 2\overline{B_j^2} \overline{B_j^4} \overline{J_j^2}^6 - 4\overline{B_j^2}^2 \overline{J_j^2}^4 \overline{J_j^2}^6,$$

and

$$V = \overline{B_j^2}^2 - \overline{B_j^4} - 2\overline{B_j^2} \overline{J_j^2}.$$

Using the above results, one is able to obtain the continued-fraction coefficients $\Delta_1, \Delta_2, \Delta_3$, and Δ_4 , etc. by Eq. (8). We have calculated the continued-fraction coefficients up to Δ_9 . By means of the Gaussian terminator to Eq. (13), we can further obtain the spectral density $\Phi(\omega)$ of the spin autocorrelation function.

IV. RESULTS AND DISCUSSION

In the following, we will give some results of the spin autocorrelation functions $C(t)$ and the corresponding spectral densities $\Phi(\omega)$. In order to investigate the effects of Gaussian disorder on the dynamics of the present system, we next study three cases as follows.

A. The random-bond model

For this model, the exchange couplings J_i independently satisfy the Gaussian distribution which is defined by Eq. (2), while the transverse fields B_i remain unaltered. Without loss of generality, take $B_i = B = 1$ which fixes the energy scale, and that J (the mean value of exchange couplings) varies from 0 to 4, and σ_j from 0 to 3. The numerical results of the time-dependent correlation functions $C(t)$ and the corresponding spectral densities $\Phi(\omega)$ are shown in Figs. 1 and 2, respectively. The insets to Fig. 2 present the continued-fraction coefficients Δ_ν ($\nu = 1, \dots, 9$).

From Figs. 1 and 2, we can see that for the case of the standard deviations σ_J are small (e.g., $\sigma_J = 0.1$), the system shows three types of dynamical behavior with different values of J : the precession of free spins in an external transverse magnetic field, the collective-mode behavior, and the central-

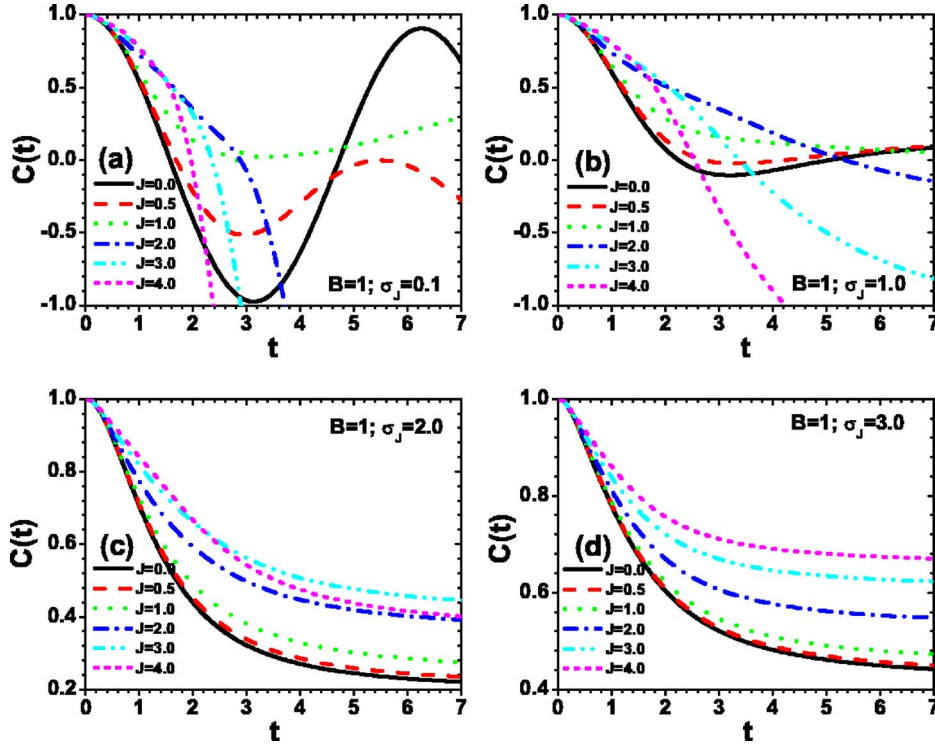


FIG. 1. (Color online) Spin autocorrelation functions for some cases. For small σ_J ($\sigma_J=0.1$), there are two crossovers from the precession of free spins in the transverse magnetic field ($J=0.0$) to a collective-mode one ($J=0.5$), and then to a central-peak behavior ($J \geq 1$) with the mean value of J_i varies from 0 to 4. Only the central-peak behavior is found when σ_J are large enough.

peak behavior. The black solid curve ($J=0$) is a very slightly damped cosine. In fact, without the faint disorder in J , it is a cosine, because it is nothing but the precession of independent free spins in an external transverse magnetic field. Besides, the black solid curve ($J=0$) in Fig. 2(a) shows that the center frequency of $\Phi(\omega)$ approaches 1. This result is consistent well with the Larmor frequency ω_L of the precession of the single spin in an external transverse field B , since $\omega_L = \gamma B$ (let γ be a unit of frequency).

When $J < B$ but not $J \ll B$ (e.g., $J=0.5$), the system exhibits a collective-mode behavior. One can easily verify that this curve differs from the damped cosine. In this case, the influence of the spin interactions on the dynamics of the system cannot be neglected. As the mean value J increases further, the collective-mode behavior becomes weaker, so that the dynamics is increasingly dominated by a central-peak behavior,^{8,25} i.e., the system undergoes a crossover from the collective-mode behavior to a central-peak one.

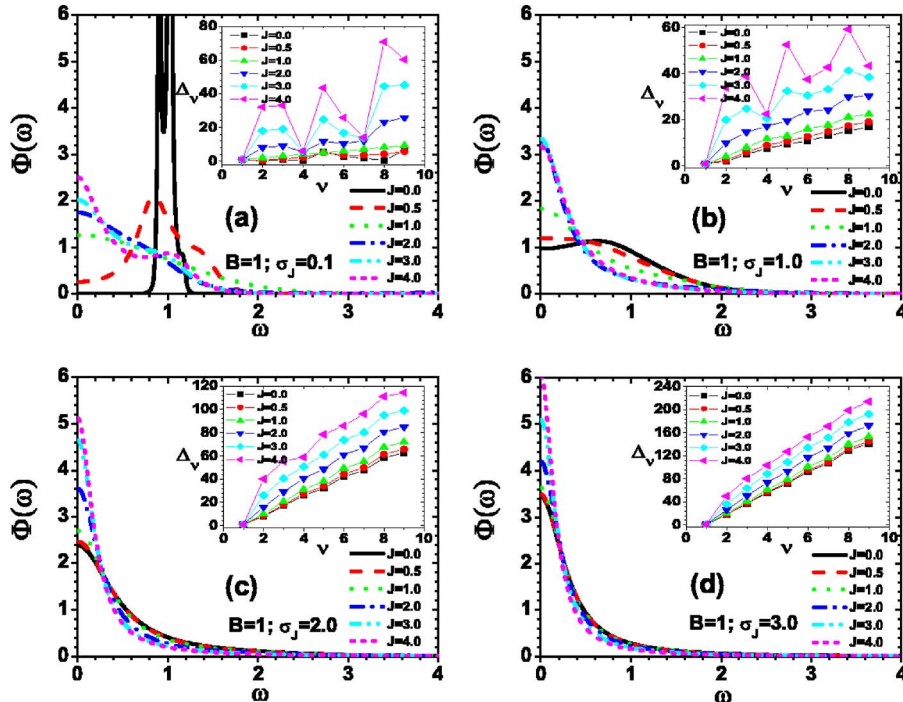


FIG. 2. (Color online) The corresponding spectral densities for the same parameters as in Fig. 1. The insets show the continued-fraction coefficients Δ_ν ($\nu = 1, \dots, 9$). The lines in the insets are just a guide to the eye. As σ_J increases, the continued-fraction coefficients for the same parameters lean to fall on a straight line.

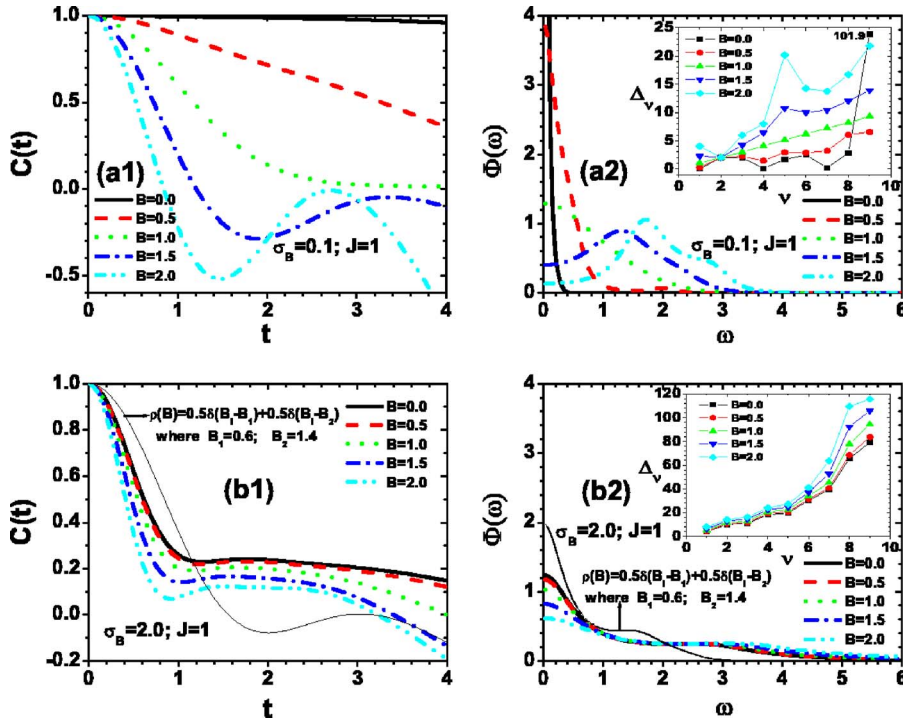


FIG. 3. (Color online) Time-dependent correlation functions and the corresponding spectral densities for two groups different parameters. The dynamics varies from a central-peak behavior to a collective-mode behavior as the mean value of B_i increases from 0 to 2. However, when σ_B are large enough, the system only exhibits a type of dynamical behavior between a central-peak behavior and a collective-mode one. The thin solid curves in both (b1) and (b2) represent the most disorder case in which B_i independently satisfy the bimodal distribution.

Figures 1 and 2 also indicate that as the standard deviation σ_J increases, the precession of free spins in the transverse field and the collective-mode behavior vanish in turn. Finally, the system does not exhibit the disordered behavior but only the central-peak behavior when the standard deviations σ_J are large enough [see Figs. 1(d) and 2(d)]. In this case, the strong exchange couplings play an important role, i.e., the spin interactions are dominant in the competition between the spin interactions and the random transverse fields. So the crossover gradually vanishes as σ_J increases.

B. The random-field model

In this case, the random transverse fields B_i are independent and satisfy the Gaussian distributions, while the exchange couplings are uniform. In Fig. 3 we show the auto-correlation functions and the corresponding spectral densities for two typical cases of $\sigma_B=0.1$ and 2.0 . Figures 3(a1) and 3(a2) also show that there is a crossover from a central-peak behavior to a collective-mode behavior as the mean value B increases from 0 to 2 when the standard deviation σ_B is small.

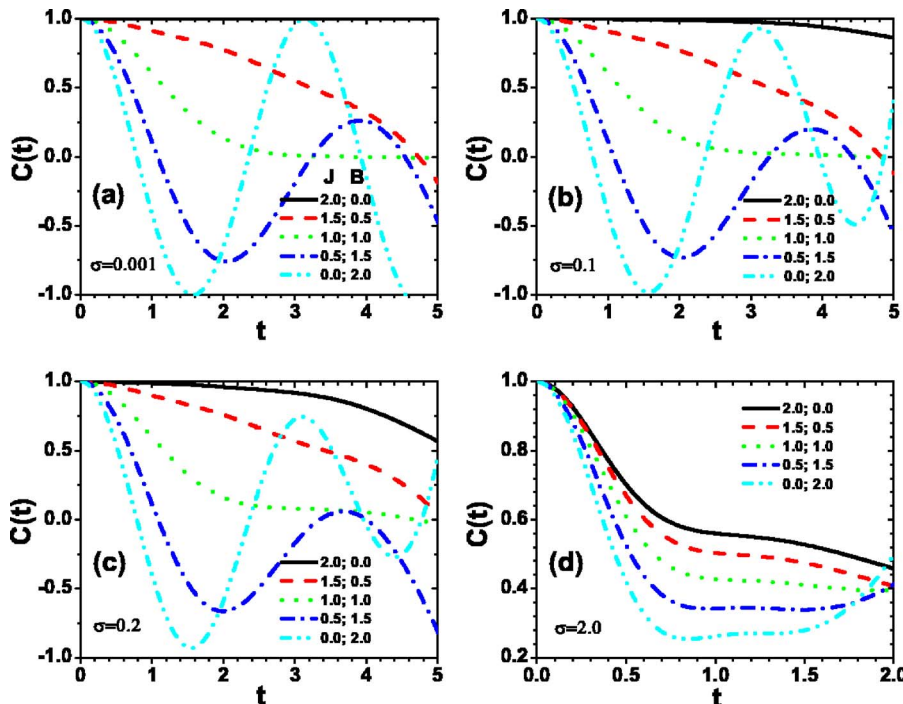


FIG. 4. (Color online) Auto-correlation functions $C(t)$ for the cases in which $\sigma_J = \sigma_B = \sigma$, $J = 2 - 0.5i$ ($i=0,1,2,3,4$), and $B = 2 - J$.

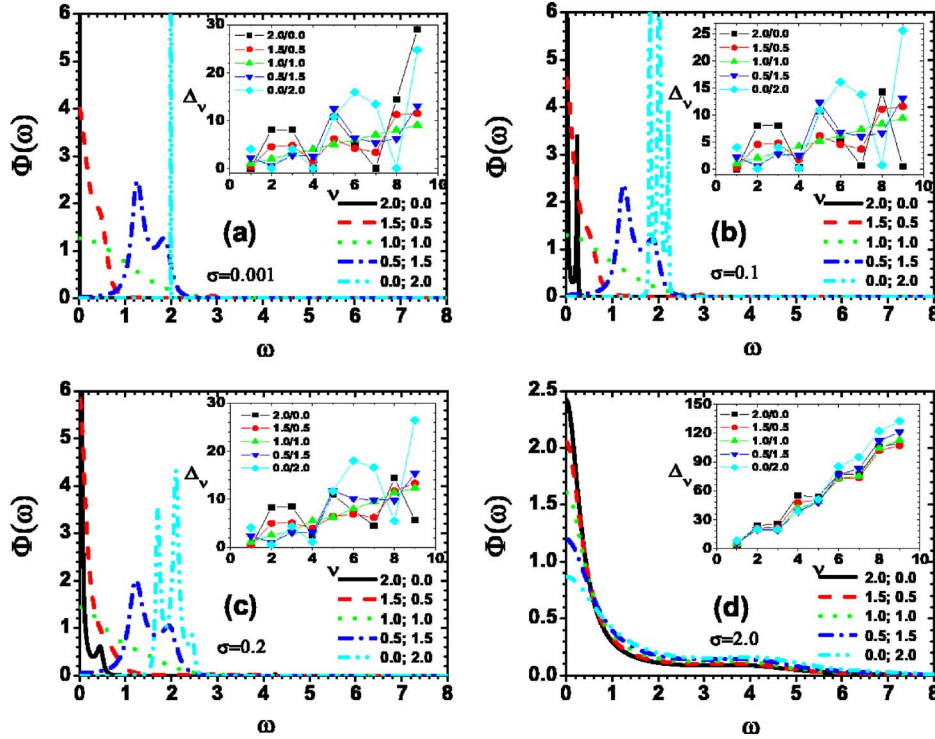


FIG. 5. (Color online) The corresponding spectral densities for the same parameters as in Fig. 4. The continued-fraction coefficients Δ_ν ($\nu=1, \dots, 9$) are shown in the insets. The lines in the insets are just a guide to the eye.

When σ_B is large enough [e.g., $\sigma_B=2$, see Figs. 3(b1) and 3(b2)], the system is in a most-disordered state, which exhibits a type of dynamical behavior between a central-peak behavior and a collective-mode one. We find these cases are very similar to the most-disordered case mentioned by Florencio.⁸ The physical interpretation of these behaviors is that the random transverse fields drive the system to be more disordered as σ_B increases.

C. The random-bond and random-field model

For this model, both the couplings J_i and the transverse magnetic fields B_i independently satisfy Gaussian distributions. Some numerical results are shown in Figs. 4 and 5. In the limit $\sigma \rightarrow 0$, the Gaussian function becomes a delta function, therefore, the disordered system degenerates into a pure one. Our results of $\sigma=0.001$ and $J=B=1$ as shown in Figs. 4(a) and 5(a) are in agreement with those of a pure system.^{16,29}

For the above case we find four types of dynamical behavior: for the case of $J=0, B=2.0$, $C(t)$ is a cosine function, $\Phi(\omega)$ is a delta function, it is nothing but the precession of free spins in an external transverse magnetic field; for $J=0.5, B=1.5$, $C(t)$ shows a damped oscillatory behavior which is typical of the collective mode behavior; for $J=1.0, B=1.0$, it is a Gaussian behavior;^{16,29} for $J=1.5, B=0.5$, $C(t)$ decreases monotonically, $\Phi(\omega)$ is now peaked at zero frequency, it is the central-peak behavior. The same is true for the cases of $\sigma=0.1$ and $\sigma=0.2$. These numerical results indicate that when σ are small, the system sequentially undergoes two crossovers as J/B increases.

On the other hand, the damped oscillations weaken and the width of the spectral functions broaden as σ increases. Finally, similar to some cases as we mentioned above, the

system only shows one type of dynamical behavior when the standard deviations of the random variables are large enough [see Figs. 4(d) and 5(d)]. Obviously, this type of behavior is intervenient between the behaviors as shown in Figs. 2(d) and 3(b2).

V. CONCLUSIONS

In this paper, we have studied the effects of Gaussian disorder on the dynamics of the 1-D RTIM in the high-temperature limit by the recursion method. We find that the dynamics of the RTIM with Gaussian disorder is affected by the competition between the spin interactions and the random transverse fields, and the competitive result depends on many factors, such as the standard deviations σ_J and σ_B and the mean values J and B . Generally speaking, when σ_J (or σ_B) is small, the dynamics of the system undergoes two crossovers in sequence as J/B decreases: from a central-peak behavior to a collective-mode one, and then to the precession of free spins in an external transverse magnetic field. On the other hand, for the case of large σ_J the system presents a central-peak behavior; but it shows a disordered behavior not a collective-mode one for large σ_B .

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