Effects of double-Gaussian disorder on the dynamics of the quantum XY chain

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We investigate the dynamics of the random one-dimensional spin-1/2 quantum isotropic XY model in high-temperature limit by the recurrence relations method. Both the time-dependent transverse autocorrelation function and the corresponding spectral density are calculated for the cases that the exchange couplings between spins or transverse fields satisfy the double-Gaussian distribution. It is found that when the value of σ_J (standard deviation of random exchange coupling) or σ_B (standard deviation of random external magnetic field) is small, the dynamics of the system undergoes a crossover between a central-peak behavior and a collective-mode one. However, when σ_J or σ_B is large enough, the crossover vanishes, and the system shows the most disordered behavior or a central-peak behavior. We also investigate the cases that the couplings or fields satisfy the bimodal distribution and Gaussian distribution, which are the two special cases of double-Gaussian distribution, and find that the dynamics of the system is similar to that of the one-dimensional transverse Ising system.

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I. INTRODUCTION

The dynamical properties of the quantum spin systems have been paid considerable attention in the past few decades.[1,2] One of the typical examples of such systems is the spin-1/2 XY model, which has been successfully related to some quasi-one-dimensional compounds, such as Cs_2CoCl_4 and $PrCl_3$.[3,4] Regarding the dynamics of this system, Niemeijer[5] found that the time-dependant longitudinal spin autocorrelation function for any temperature can be expressed as the square of the Bessel function.

On the other hand, for the transverse spin correlation function of the XY chain, some results indicate that it shows a Gaussian form at infinite temperature[6,7] and a power-law behavior at zero temperature.[1,8] For finite open XY chain, at $0<T<\infty$ (where T is the temperature of the system), the bulk regime of the long-time asymptotic decay of the autocorrelation function is exponential. However, it was proved by Lee[9] that for a Hermitian system, its autocorrelation may not exponentially decay.

Recently, more attention has been given to random quantum spin systems,[10–13] and there are some valuable results for the time-dependent correlation functions of the Ising and XY models in one-dimensional (1D) lattice. The dynamical properties of the 1D random transverse Ising model with the bimodal distribution have been found to undergo a crossover from a central-peak behavior to a collective mode behavior as a function of disorder.[10] Besides these, the 1D random-bond transverse Ising model with four-spin interactions has also been studied.[11] For the random isotropic XY chain, there exist some studies in literature, which deal with the longitudinal correlation function. The dynamics of this system in which the exchange couplings satisfy a bimodal distribution has been found to be governed by the stronger couplings at long time even if their concentration (the fraction that the exchange couplings take the larger value) is very small.[14] Both the properties of the quantum XY chain and two-leg XY ladder in a random field have been found sensitive to the percentage of disorder but not to the intensity of the field.[15]

Although some results have been reported for the longitudinal correlation function of random XY system, as we know, only a few results for the transverse correlation function of this system with arbitrary probability of disorder have been reported. In this paper, we investigate the effects of double-Gaussian disorder on the dynamics of the transverse autocorrelation function in the XY chain. We find that the system exhibits some interesting behavior, e.g., the system shows a crossover between a collective-mode behavior and a central-peak one when the standard deviation of the exchange couplings or magnetic fields is small, but the crossover vanishes when the standard deviation is large enough.

This paper is arranged as follows. In Sec. II, we introduce the model and method used in the present work. The results and discussion are given in Sec. III, and Sec. IV is the conclusions.

II. MODEL AND METHOD

As a nontrivial solvable many-body spin system, the 1D quantum spin-1/2 XY model has attracted considerable attention. The Hamiltonian of this model is described by

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

where $\sigma_i^\alpha(\alpha=x,y,z)$ are the Pauli operators on a site i, B_i is the external magnetic field at site i, J_i and K_i are the x-component and y-component nearest-neighbor couplings of the spins, respectively. In this work, we consider the exchange couplings and the magnetic fields as random variables, which independently satisfy the double-Gaussian distribution,

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$$P(\mu_i) = p\ P_1(\mu_i) + (1-p)P_2(\mu_i), \tag{2}$$

where

$$P_1(\mu_i) = \frac{1}{\sqrt{2\pi}\sigma_\mu}\exp\left[-\frac{(\mu_i-\mu_1)^2}{2\sigma_\mu^2}\right]$$

and

$$P_2(\mu_i) = \frac{1}{\sqrt{2\pi}\sigma_\mu}\exp\left[-\frac{(\mu_i-\mu_2)^2}{2\sigma_\mu^2}\right] \tag{3}$$

are the Gaussian distributions,[16] μ_1 and μ_2 are the corresponding mean values of the random variables, σ_μ is the standard deviation that denotes the deviation of the random variables μ_i from the mean values μ_1 or μ_2, and p represents the probability of the variable that satisfies the Gaussian distribution $P_1(\mu_i)$, where $0 \leq p \leq 1$. $P(\mu_i)$ means that μ_i satisfy the Gaussian distribution $P_1(\mu_i)$ or $P_2(\mu_i)$ in the fraction of p and $(1-p)$, respectively.

The double-Gaussian distribution can be used to describe not only the case that the random variables satisfy a discrete distribution but also that the variables satisfy a continuous distribution. Typically, when the standard deviation $\sigma_\mu \to 0$, the Gaussian parts in Eq. (2) becomes δ functions so the double-Gaussian distribution becomes a bimodal distribution,

$$P(\mu_i) = p\ \delta(\mu_i-\mu_1) + (1-p)\delta(\mu_i-\mu_2). \tag{4}$$

When $p=0$ or $p=1$, Eq. (2) becomes the standard Gaussian distribution.

What we are mainly interested in this work is the transverse autocorrelation function of the XY system. It is defined by

$$C(t) = \overline{\langle \sigma_j^x(t)\sigma_j^x(0)\rangle}, \tag{5}$$

where $\overline{\langle \cdots \rangle}$ presents an average over the random variables following the statistical average. The corresponding spectral density $\Phi(\omega)$ is defined as the Fourier transformation of the spin autocorrelation function,

$$\Phi(\omega) = \int_{-\infty}^{+\infty} C(t)e^{i\omega t}dt. \tag{6}$$

The method of recurrence relations is a powerful tool for the calculation of dynamic correlation function and has been successfully applied to a lot of spin systems.[10,14,15,17–21] Next, we will use the recurrence relations method to obtain the short-time expansion of $C(t)$ and the spectral density $\Phi(\omega)$.

We consider the operator $\sigma_j^x(t)$ as a dynamical variable and expanded it as[17]

$$\sigma_j^x(t) = \sum_{\nu=0}^{\infty} a_\nu(t) f_\nu, \tag{7}$$

where $a_\nu(t)$ are the time-dependent coefficients and f_ν are the orthogonal basis vectors spanning a Hilbert space S. By choosing $f_0=\sigma_j^x(0)$, the remaining f_ν can be obtained by the following recurrence relation:[17,22]

$$f_{\nu+1} = iLf_\nu + \Delta_\nu f_{\nu-1}, \quad \nu \geq 0, \tag{8}$$

where L is the quantum Liouville operator, and the recurrants Δ_ν are defined as

$$\Delta_\nu = \frac{(f_\nu, f_\nu)}{(f_{\nu-1}, f_{\nu-1})}, \quad \nu \geq 1, \tag{9}$$

with $\Delta_0=1$ and $f_{-1}=0$. (f_ν, f_ν) is the inner product of the basis vectors in S, which include both the statistical and random averages.[7]

We have exactly obtained the first seven basis vectors.[17] Because most vectors are too lengthy, we just give the first two of them,

$$f_1 = B_j\sigma_j^y - K_{j-1}\sigma_{j-1}^y\sigma_j^z - K_j\sigma_{j+1}^y\sigma_j^z,$$

and

$$\begin{aligned} f_2 = {} & (\Delta_1 - B_j^2 - K_{j-1}^2 - K_j^2)\sigma_j^x + J_jK_{j-1}\sigma_{j+1}^x\sigma_{j-1}^y\sigma_j^y \\ & - 2K_{j-1}K_j\sigma_j^x\sigma_{j-1}^y\sigma_{j+1}^y + J_{j-1}K_j\sigma_{j-1}^x\sigma_j^y\sigma_{j+1}^y + (B_jJ_{j-1} \\ & + B_{j-1}K_{j-1})\sigma_{j-1}^x\sigma_j^z + (B_jJ_j + B_{j+1}K_j)\sigma_{j+1}^x\sigma_j^z \\ & - J_{j-2}K_{j-1}\sigma_{j-2}^x\sigma_{j-1}^z\sigma_j^z - J_{j+1}K_j\sigma_{j+2}^x\sigma_j^z\sigma_{j+1}^z. \end{aligned}$$

The squared norms of the vectors[7] are obtained as follows:

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

$$(f_1, f_1) = \overline{B_j^2} + \overline{K_{j-1}^2} + \overline{K_j^2},$$

and

$$\begin{aligned} (f_2, f_2) = {} & \overline{\Delta_1^2} - 2\overline{\Delta_1 B_j^2} + \overline{B_j^4} + \overline{B_j^2J_{j-1}^2} + \overline{B_j^2J_j^2} + 2\overline{B_{j-1}B_jJ_{j-1}K_{j-1}} \\ & - 2\overline{\Delta_1 K_{j-1}^2} + \overline{B_{j-1}^2K_{j-1}^2} + 2\overline{B_j^2K_{j-1}^2} + \overline{J_{j-2}^2K_{j-1}^2} + \overline{J_j^2K_{j-1}^2} \\ & + \overline{K_{j-1}^4} + 2\overline{B_jB_{j+1}J_jK_j} - 2\overline{\Delta_1K_j^2} + 2\overline{B_j^2K_j^2} + \overline{B_{j+1}^2K_j^2} \\ & + \overline{J_{j-1}^2K_j^2} + \overline{J_{j+1}^2K_j^2} + 6\overline{K_{j-1}^2K_j^2} + \overline{K_j^4}. \end{aligned}$$

Then, the first seven continued fraction coefficients are exactly calculated by Eq. (9). Because the Δ_ν sequence has a linear growth rate, Δ_8 and Δ_9 are also accepted by the assumption $\Delta_\nu = (\Delta_N/N)\nu$ for $\nu > N$.[10]

The coefficients $a_\nu(t)$ in Eq. (7) satisfy the second recurrence relation,

$$\Delta_{\nu+1}a_{\nu+1}(t) = -\frac{da_\nu(t)}{dt} + a_{\nu-1}(t), \quad \nu \geq 0, \tag{10}$$

where $a_{-1}(t) \equiv 0$, and $a_0(t)$ is the autocorrelation function of the system. By Laplace transformation $a_\nu(z) = \int_0^\infty e^{-zt}a_\nu(t)dt$, where $z=\varepsilon+i\omega$, $\varepsilon>0$, the continued-fraction form of $a_0(z)$ can be obtained as

$$a_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots}}}, \tag{11}$$

which denotes that the recurrants are the only factor that determines the dynamic correlation functions. If only a finite number of recurrants can be determined, it is necessary to

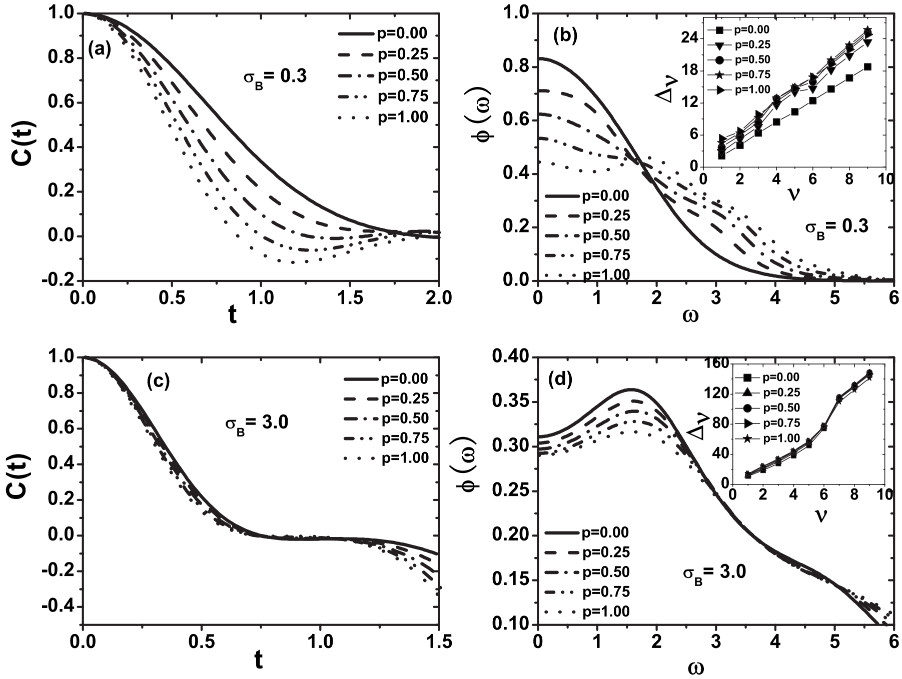

FIG. 1. Time-dependent correlation functions and the corresponding spectral densities for the two typical cases. The system undergoes a crossover from a central-peak behavior to a collective-mode behavior when $\sigma_J=0.3$; however, when $\sigma_J=3.0$, the crossover vanishes and the system only shows a behavior between a central-peak behavior and a collective-mode one. The insets of (b) and (d) present the recurrant $\Delta_\nu(\nu=1,\ldots,9)$.

use a scheme to terminate the continued fraction. Of the several truncation schemes that have been used in literature, the Gaussian terminator[17,23] is the one that best serves our problem. After calculating $a_0(z)$ by using the Gaussian terminator, we approximately obtain the spectral density by

$$\Phi(\omega)=\lim_{\varepsilon\to 0}\mathrm{Re}\,a_0(z),\quad z=\varepsilon+i\omega. \tag{12}$$

Meanwhile, by using the first nine recurrants, we obtain the corresponding 18 moments and then calculate the $C(t)$ by means of the Padé approximate.

III. RESULTS AND DISCUSSIONS

In the following, we give some results of $C(t)$ and $\Phi(\omega)$ to study the effects of the double-Gaussian disorder on the isotropic (i.e., $J_i=K_i$ for every i) XY system. Besides, we also investigate the two limiting cases of the double-Gaussian distribution, i.e., bimodal distribution and Gaussian distribution.

A. Double-Gaussian distribution

Assume that the transverse fields B_i or exchange couplings J_i satisfy the double-Gaussian distribution, which is defined by Eq. (2), we consider two cases.

1. Case of random field and uniform bond

In this case, the transverse fields B_i satisfy the double-Gaussian distribution, while exchange couplings $J_i=J=1$, which fixes the energy scale. When the mean values of the fields in the distribution take $B_1=1.8$ and $B_2=0.2$, the transverse autocorrelation function $C(t)$ and corresponding spectral density $\Phi(\omega)$ are as shown in Fig. 1 for the two typical cases that $\sigma_B=0.3$ and 3.0. The insets of Figs. 1(b) and 1(d) present the recurrants.

Figure 1(a) shows that when σ_B is small ($\sigma_B=0.3$), the dynamics of the system is increasingly dominated by the transverse magnetic fields as p increases: When $p=0$, the system shows a central-peak behavior for the value of the exchange couplings are much larger than that of the transverse fields. When $p=0.25$, due to the transverse fields, it shows a weak oscillatory behavior, which is aggravated as p increases further. When $p=1$, the central-peak behavior is replaced by the collective-mode behavior. The peak of $\Phi(\omega)$ shown in Fig. 1(b) moved from $\omega=0$ to 2 as p increases. This also indicates that when σ_B is small, the effects of disordered magnetic fields are to change the central-mode behavior to the collective-mode behavior.

Figures 1(c) and 1(d) show that when σ_B is enough large ($\sigma_B=3.0$), the system exhibits a behavior between a central-peak behavior and a collective-mode one. By comparing Fig. 1(a) to Fig. 1(c), we can also see that as the standard deviation σ_B increases, the crossover from central-peak behavior to collective-mode behavior vanishes. The interpretation for this is that as σ_B increases, the transverse fields are dominant in the competition with the spin interactions and drive the system into a most disordered state.

2. Case of random bond and uniform field

In this case, the exchange couplings independently satisfy the double-Gaussian distribution, while the transverse fields are uniform. When the mean exchange couplings in the distribution take the value $J_1=1.0$ and $J_2=0.4$, the autocorrelation functions and the corresponding spectral densities for both cases of $\sigma_J=0.1$ and 2.0 are as shown in Fig. 2. We can see that when $\sigma_J=0.1$ [see Figs. 2(a) and 2(b)], there is a crossover from a collective-mode behavior to a central-peak one as the concentration p increases. However, when $\sigma_J=2.0$ [see Figs. 2(c) and 2(d)], the dynamics of the system is dominated by the spin interaction and shows a central-peak behavior.

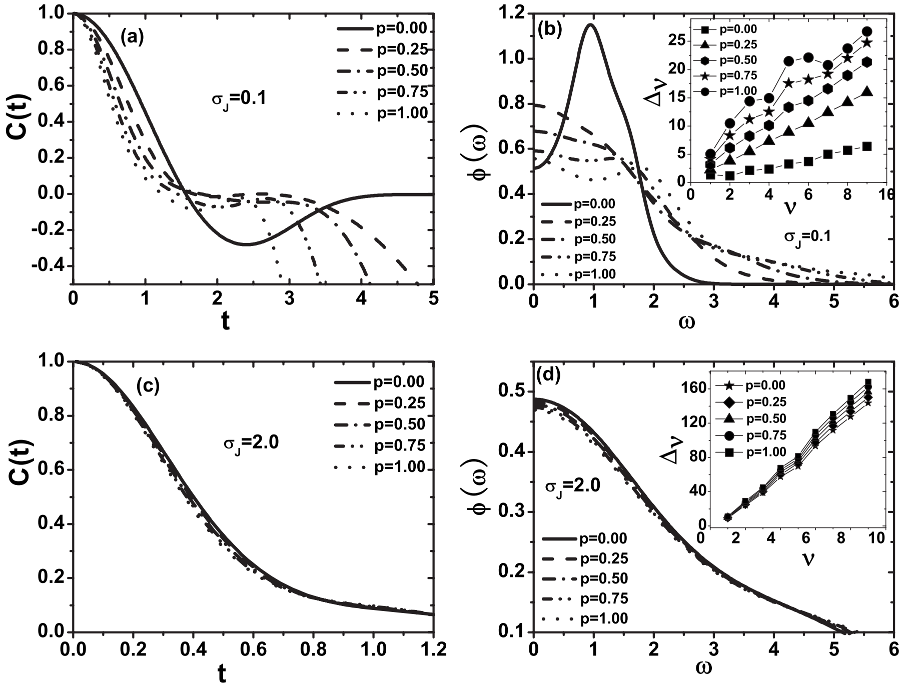

FIG. 2. Autocorrelation functions and spectral densities for the case that the bonds satisfy the double-Gaussian distribution, while $B=1$. The standard deviations take two typical values $\sigma_J=0.1$ and 2.0. By comparing the insets of (b) and (d), we can conclude that the recurrants fall on a straight line as σ_J increases.

B. Bimodal distribution and Gaussian distribution

1. Bimodal distribution

For this case, we assume the following: (a) The exchange couplings are constants ($J_i=J=1.0$), whereas the transverse fields satisfy the bimodal distribution [Eq. (4)] and vary from the value $B_2=0.2$ ($q=0$) to $B_1=1.8$ ($q=1$), where $0\leq q\leq 1$. This allows the system to move from a situation, in which the value of the transverse field B smaller than the exchange coupling J to the situation that B is larger than J. (b) The exchange couplings J_i satisfy the bimodal distribution and change from $J_2=0.4$ ($p=0$) to $J_1=1.0$ ($p=1$), while the transverse fields are uniform ($B_i=B=1.0$). In this assumption, the exchange coupling J changes from $J<B$ to $J=B$ as p increases.

Figure 3 shows that the system has a crossover from a collective-mode behavior to a central-peak behavior as J/B increases in both of the above cases. Generally, when $J<B$, the system is dominated by a collective-mode behavior; however, for $J>B$, the main mode is the central-peak behavior. So, the dynamics of the system changes according to the concentration of B or J.

By comparing the results of the present transverse correlation function when the magnetic fields satisfy the bimodal distribution to the results of the longitudinal correlation function of the *XY* system obtained by Nunes *et al.*, we find some

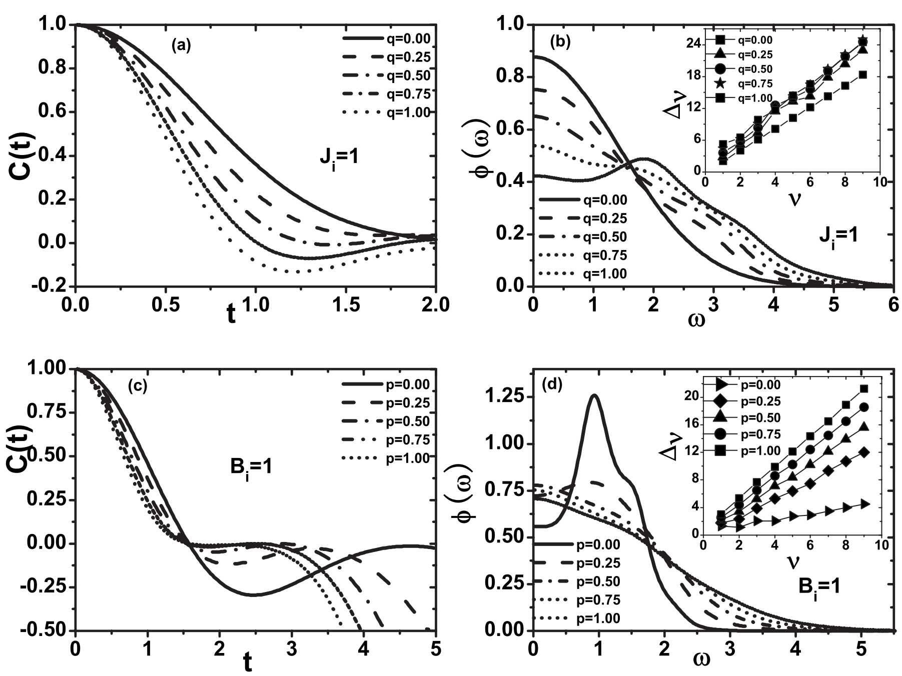

FIG. 3. Time-dependent correlation functions and spectral densities for two cases that exchange couplings and magnetic fields, respectively, satisfy bimodal distribution. (a) and (b) are the results that the system in a random transverse fields B_i, which can take the values of 0.2 and 1.0 with probabilities q and $1-q$, respectively. The case of the random exchange couplings J_i with uniform transverse fields B is shown in (c) and (d). The values of J_i are varied from $J_1=0.4$ ($p=0$) to $J_2=1.0$ ($p=0$). The inset in (d) shows that the larger the value of spin interactions the better the linear relation between the recurrants.

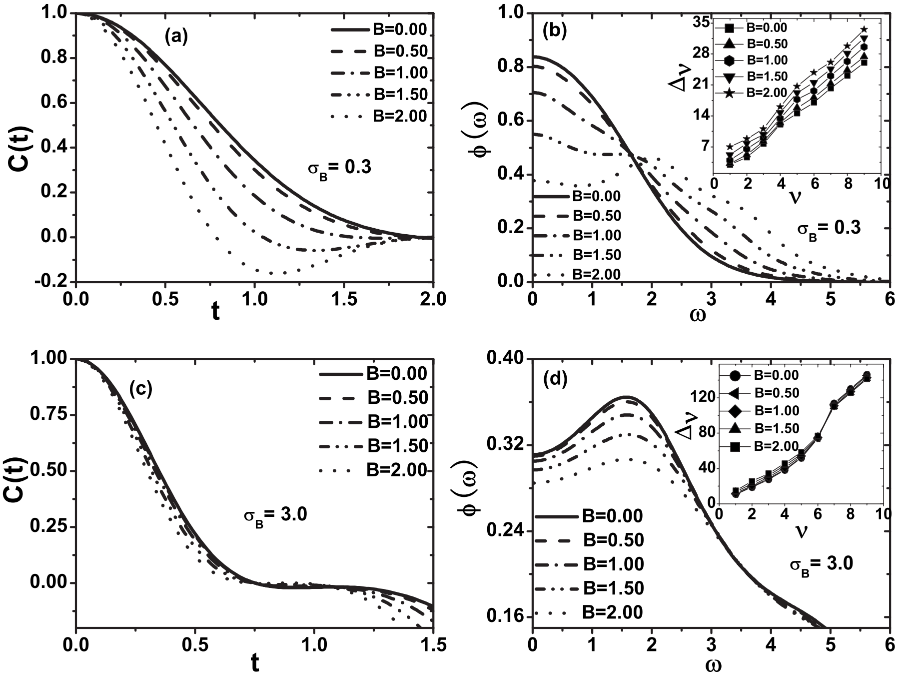

FIG. 4. Autocorrelation functions and the corresponding spectral densities for two groups different parameters when the random fields satisfy Gaussian distribution. When the standard deviation is small (σ_B=0.3), (a) and (b) show that the dynamics of the system changes from a central-peak behavior to a collective-mode one as the mean value of B_i increases from 0 to 2; however, when σ_B=3.0, the system is only in a most disordered state.

differences: For the transverse correlation function, it is found that the dynamics of the system is decided by the competition between the magnetic fields and the exchange couplings. When $B<J$, the dynamics of the system is dominated by the exchange couplings and shows a central-peak behavior. When $B>J$, the magnetic fields are dominant in the competition with the exchange couplings, so the system exhibits a collective-mode behavior. For the longitudinal correlation function that was calculated by Nunes *et al.*,[15] the results show that the presence or absence of a uniform field does not alter the autocorrelation function, and for several distributions of fields, disorder lifts $C(t)$ and makes it decay slower at large t.

2. Gaussian distribution

Now, we consider the case wherein the random variables satisfy the Gaussian distribution. We give two suppositions to investigate the effect of Gaussian disorder on the dynamics of the system. The results that the magnetic fields and exchange couplings, respectively, satisfy the Gaussian distribution are shown in Figs. 4 and 5. We let the standard deviation (σ_B or σ_J) take the two values: a small one (0.3) and a larger one (3.0). It is shown that when the standard deviation is small (σ_B=0.3 or σ_J=0.3), the system undergoes a crossover between a central-peak behavior and a collective-mode one. However, the crossover vanishes when the standard deviation is large enough, i.e., the system shows only a

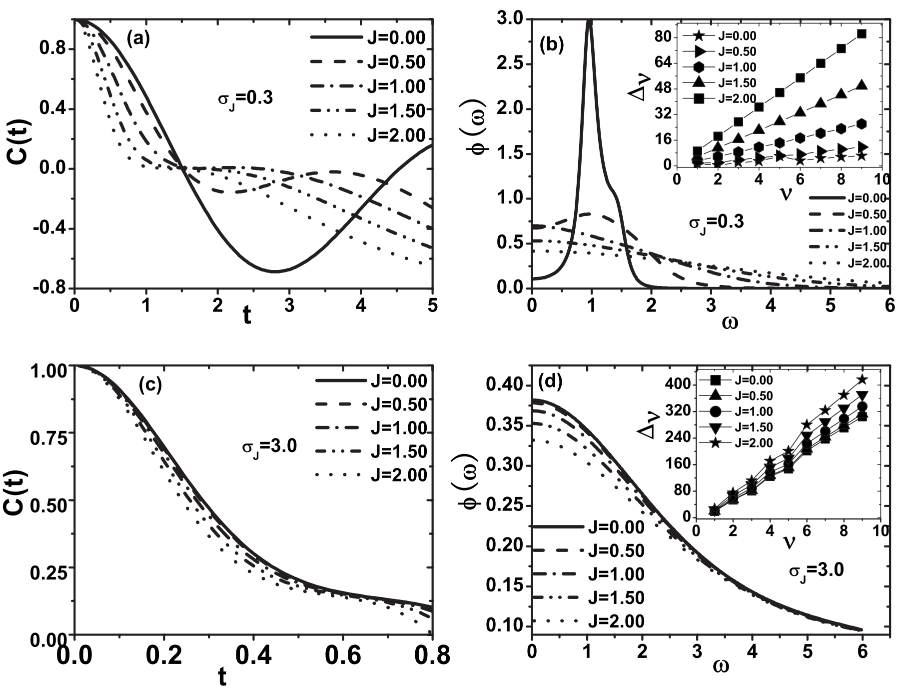

FIG. 5. Autocorrelation functions and the corresponding spectral densities for both cases of σ_J =0.3 and 3.0. When the standard deviation σ_J is small [σ_J=0.3, (a) and (b)], the system undergoes a crossover from a collective-mode behavior to a central-peak behavior as the mean value J varies from 0 to 2.0, but the crossover vanishes when σ_J is large [(c) and (d)].

most disordered behavior or a central-peak behavior for large σ_B or σ_J, respectively.

It is not difficult to find that for the bimodal and Gaussian disorders, the dynamics of the *XY* chain is similar to that of the 1D transverse Ising model.[10,21] This behavior can be understood from the work of Florencio and Lee[7] that the Hilbert spaces of σ_j^x for the *XY* and transverse Ising models have the same geometric structure.

All of the above results are for the cases of isotropic *XY* model. When $J_i \neq K_i$, it corresponds to the anisotropic *XY* model. Especially when $K_i = 0$, the anisotropic *XY* system becomes the Ising system, and we find that the results of the transverse correlation function are the same as those in Ref. 21, in which the random fields or exchange couplings satisfy the Gaussian distribution.

IV. CONCLUSIONS

We have investigated the dynamics of the random isotropic *XY* system in the high-temperature limit by the recurrence relation method. By considering the case that the disordered fields or exchange couplings satisfy the double-Gaussian distribution, we find that not only the standard deviations (σ_B and σ_J) but also the mean values J and B can affect the dynamics of such system. To conclude, when σ_B or σ_J is small, the system undergoes a crossover from a collective-mode behavior to a central-peak one as J/B increases, but for large σ_B or σ_J, it exhibits a most disordered behavior or a central-peak behavior, respectively. We also investigate the two limiting cases of the double-Gaussian distribution, i.e., bimodal distribution and Gaussian distributions. It is found that the dynamics of the *XY* chain are similar to that of 1D Ising system. By comparing to the previous result of the longitudinal correlation function when the magnetic fields satisfy the bimodal distribution, we find that the effects of the disordered fields on the longitudinal and transverse correlation functions are different.

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