PHYSICAL REVIEW B VOLUME 61, NUMBER 21 1 JUNE 2000-I

Dynamical behavior of the random-bond transverse Ising model with four-spin interactions

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(Received 12 November 1999; revised manuscript received 8 February 2000)

We study the time evolution of the one-dimensional random-bond transverse Ising model with four-spin interactions. We calculate the time-dependent correlation function as well as the longitudinal relaxation function of the infinite chain. We analyze how the presence of disorder affect the dynamical behavior of the system in comparison with the pure model. We find that the main effect of disorder is to produce a crossover from a central mode to a collective-mode type of dynamics, as the concentration of weaker bonds is enhanced. Such crossover is also present in the case of an increase in bond dilution.

The role of time evolution of one-dimensional quantum spin systems has been a long-standing theoretical and experimental problem.[1] Among them, the transverse Ising model with multispin interactions, regarded as one of the simplest with a nontrivial dynamics, has attracted considerable interest in recent years.[2,3] On the other hand, the presence of bond randomness has been shown to affect the behavior of magnetic materials in a drastic way providing a very rich area of investigation. In some materials it is present in the form of dilution caused by missing magnetic bonds or sites. In other class of systems it manifests itself through fluctuations in the magnitude of the exchange couplings due to structural disorder, as in glassy materials. Most of the research in disordered systems have been concentrated on obtaining phase diagrams and thermodynamic functions.[3] Much less effort has been made to obtain the dynamical behavior of these systems. Recently, the time evolution of the usual two-body random transverse Ising system was carried out by means of the method of recurrence relations.[4] The crossover from a central peak behavior onto a collective mode behavior was observed as a function of disorder.

In addition to the usual two-spin model, the four-spin quadrilinear transverse Ising system[5] has attracted considerable interest in recent years. The model with zero magnetic field[6] has been studied by several techniques such as mean-field theories,[7,8] renormalization-group,[9] series expansions,[10] and Monte Carlo simulations.[8,11] The phase diagram presents a tricritical point which separates regions of first- and second-order transitions. More recently, a model with four-spin interactions was employed to describe the phase transition in poly(vinylidene fluoride-trifluoroethylene) [P(VDF-TrFE)] copolymers.[12] One study carried out on the dynamics of the pure transverse Ising (TI) model with four-spin interaction showed that the system undergoes a crossover from a collective-mode excitation regime to a central mode type of dynamics as the strength of field is lowered.[5] Differently from the usual two-body model,[13,14] the four-spin interaction model does not allow a Gaussian decay for the correlation function. The crossover from the collective-mode excitation regime to a central mode behavior was observed as function of the transverse field strength. Such behavior has also been observed, for instance, in the $s=1$ Blume-Capel model in the presence of a transverse field.[15]

In this work we shall focus our attention on the time evolution of the one-dimensional disordered TI model with four-spin interaction, at the high-temperature limit. The main purpose of our work is to analyze the effect of the random energy couplings on the dynamical behavior of this model.

We consider a spin-1/2 TI model with a four-body interaction term, in the form

$$H=-8\sum_{i=1}^{L} J_i S_i^z S_{i+1}^z S_{i+2}^z S_{i+3}^z - B\sum_{i=1}^{L} S_i^x, \tag{1}$$

where S_i^α ($\alpha=x,y,z$) is the spin-1/2 operator at site i, B is the uniform transverse magnetic field, and L is the number of sites of the lattice. The periodic boundary conditions $S_{i+L}^\alpha = S_i^\alpha$ are enforced in our calculation. The four-spin interactions J_i are uncorrelated variables chosen at random from a given probability distribution $P(J_i)$.

In the presence of quenched disorder the physical quantities of interest must be averaged in the statistical ensemble of realizations specified by the distribution of exchange couplings $P(J_i)$. Formally, the dynamics of the four-spin model is obtained by calculating the averaged time-dependent autocorrelation function of S_i^z defined by

$$\overline{C(t)} = \int C(t) P(J_i) dJ_i, \tag{2}$$

where

$$C(t) = \frac{\langle S_i^z S_i^z(t) \rangle}{\langle S_i^z S_i^z \rangle}. \tag{3}$$

In the high-temperature limit the autocorrelation function takes the following form:

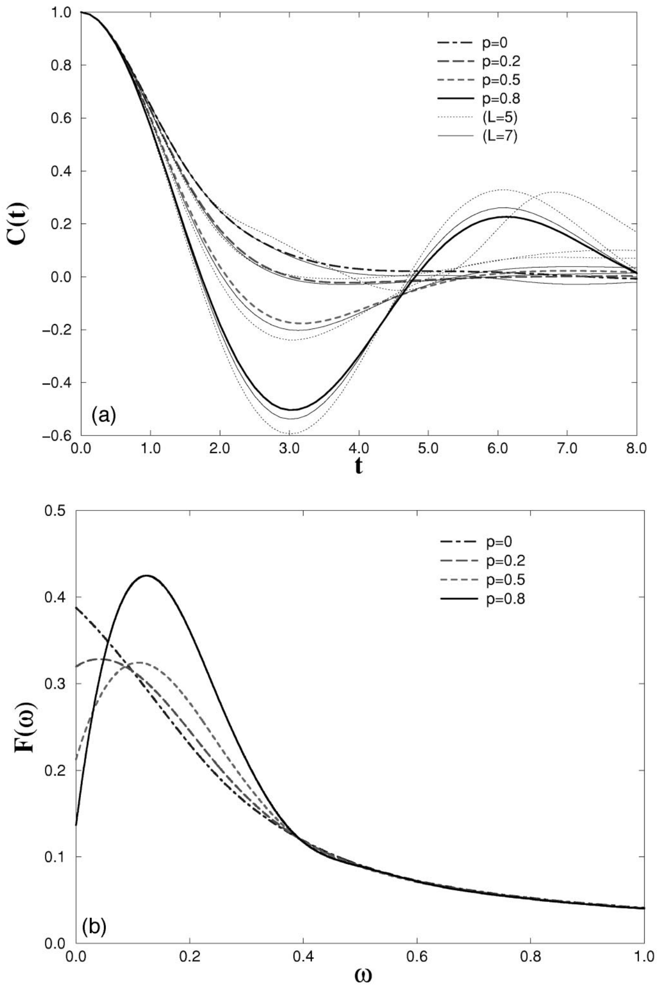

FIG. 1. Dynamic correlation functions for the random-bond transverse Ising model with four-spin interactions in the case of bond dilution. The transverse field is uniform and the coupling energies can take the values 0 and 1 with probabilities p and $1-p$. In our system of units, $\hbar=1$, and the energies are given in units of the transverse field B, which also sets the time scale. The system undergoes a crossover between a central mode to a collective-mode dynamics as the concentration of dilution increases. (a) Time-dependent correlation functions. For each value of p the dotted (thin solid) curve corresponds to $L=5$ ($L=7$) and are displayed to convey the trend toward convergence. For a given p the curves for the cases $L=9$ and $L=11$ lie on top of each other. (b) Longitudinal relaxation function (in arbitrary units) vs frequency.

$$\langle S_i^z S_i^z(t)\rangle=\frac{1}{2^L}\mathrm{Tr}\,S_i^z e^{iHt}S_i^z e^{-iHt}. \tag{4}$$

In our approach the mean autocorrelation function $\overline{C(t)}$ is obtained as follows. We first diagonalize the full Hamiltonian to determine the eigenenergies ϵ_n and eigenvectors $|n\rangle$ for a large number of realizations in the statistical ensemble of energy coupling randomness. We employed between 1000 and 10000 configurations to obtain the averages over the random variables, so that the error bars fall within the thickness of the curves presented. Those results are used to determine the mean autocorrelation function, which is then cast in the following form:[16]

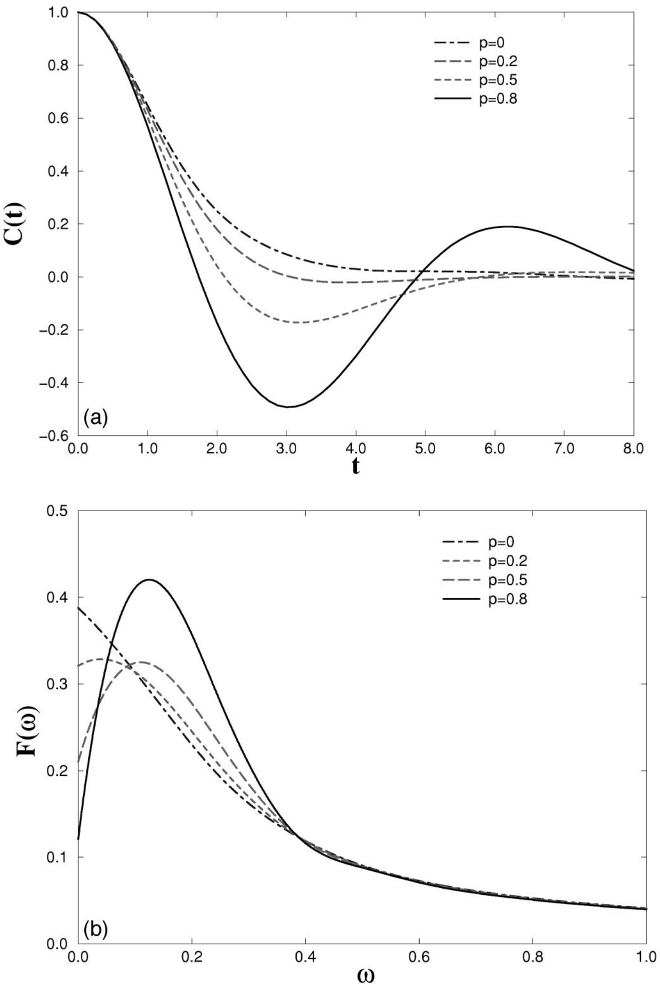

FIG. 2. Dynamic correlation functions for the case where the coupling energies can assume the values 0.1 and 1, with probabilities p and $1-p$. The couplings are given in units of the uniform transverse field B. Note that the dynamics is almost identical to that of the case of dilution, depicted in Fig. 1. (a) Time-dependent correlation functions. (b) Longitudinal relaxation function.

$$\overline{C(t)}=\frac{4}{2^L}\sum_{n,m}\overline{\cos(\epsilon_n-\epsilon_m)t|\langle n|S_i^z|m\rangle|^2}, \tag{5}$$

where the configurational average is also performed.

We are also interested in the averaged longitudinal relaxation shape function, defined as

$$\Psi(\omega)=\int_0^\infty \overline{C(t)}e^{-i\omega t}dt, \tag{6}$$

where $\overline{C(t)}$ is given by Eq. (2). The real part of $\Psi(\omega)$ gives directly a physically accessible quantity, the so-called longitudinal relaxation function, $F(\omega)=\mathrm{Re}\,\Psi(\omega)$, which can be measured directly in nuclear magnetic resonance (NMR) experiments —the so-called NMR line shape.[17] The features of the longitudinal relaxation function are also very useful in the understanding of the dynamics of the system, since different dynamic behaviors have distinct signatures in that quantity.[18]

We studied the four-body TI model chain considering the following energy coupling probability distribution

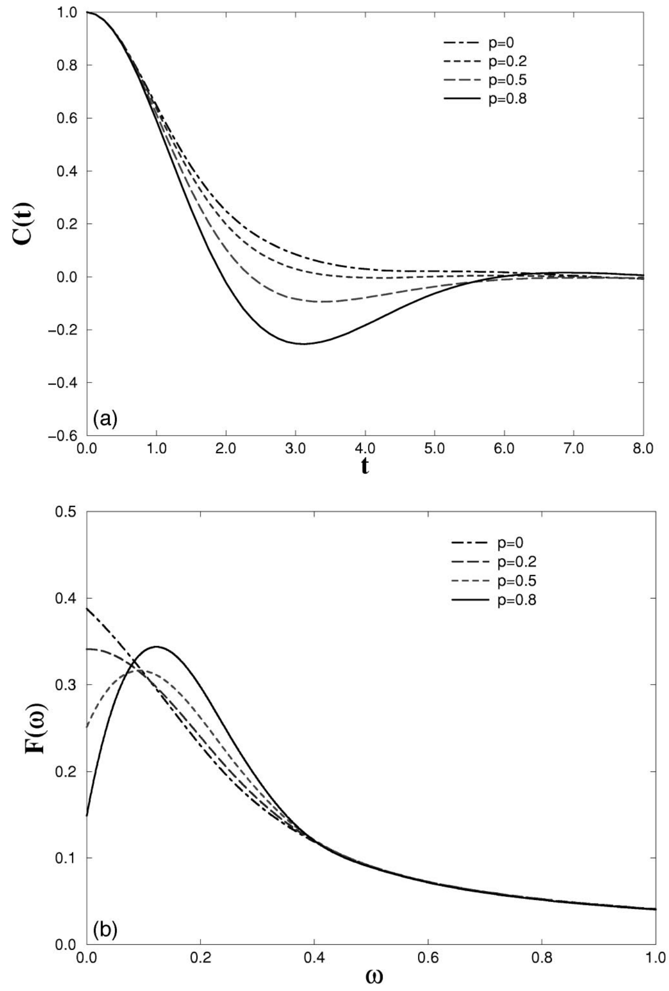

FIG. 3. Dynamic correlation functions where the coupling energies are either 0.5 or 1 in units of the transverse field, with probabilities p and $1-p$. The crossover from central mode to collective-mode behavior is somewhat less intense than in the previous cases. (a) Time-dependent correlation functions. (b) Longitudinal relaxation function.

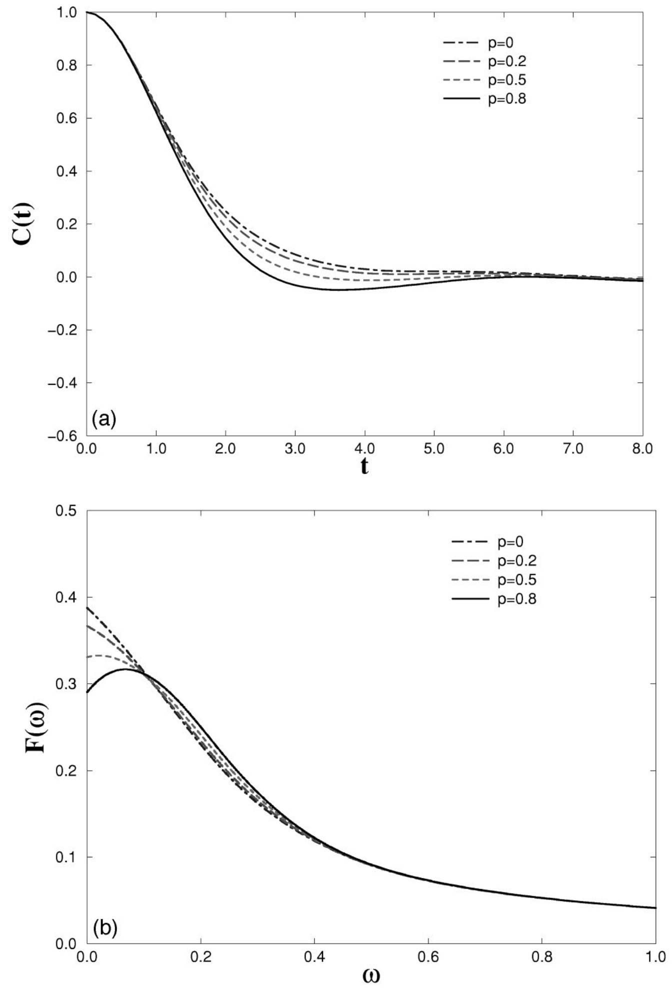

FIG. 4. Dynamic correlation functions for the case where the coupling energies are either 0.8 or 1 in units of the transverse field, with probabilities p and $1-p$. The crossover between central mode to collective-mode dynamics is much less intense than in the previous cases, which have lesser values of J_2. (a) Time-dependent correlation functions. (b) Longitudinal relaxation function.

$$P(J_i)=(1-p)\,\delta(J_i-J_1)+p\,\delta(J_i-J_2), \qquad (7)$$

where p is the concentration of couplings of type J_2. In our analysis we keep $J_1=B=1$, which sets the energy and time scales, and let J_2 take several values. For each value of J_2 we determine the time-dependent autocorrelation function and the longitudinal relaxation function for several values of p. Since we keep the transverse field constant throughout the chain, we are able to focus on the effects of disorder due to the random replacement of the interaction energies.

We performed our numerical calculations on systems of sizes $L=5,7,9$, and 11, with periodic boundary conditions. With the exception of Fig. 1(a), which shows results from all chain sizes in order to illustrate convergence of our results as the chain size increases, we will present here only the results obtained with the chain of size $L=11$. In that case the thermodynamic limit is reached in the time domain shown, $0\leqslant t\leqslant 8$. In all cases studied, our calculations also recover the results for the pure TI model with four-spin interactions ($p=0$).[5]

In bond diluted systems the exchange interactions can assume the value $J_2=0$ with concentration p. We consider the cases where $p=0,0.2,0.5$, and 0.8. The time-dependent correlation function is shown in Fig. 1(a). As the dilution concentration increases the dynamics becomes increasingly dominated by the transverse magnetic field. The case $p=0.8$, the highest concentration shown, already has the damped oscillatory behavior which is typical of the collective mode due to the transverse field. As the concentration increases further, the oscillatory behavior becomes more prominent and, at $p=1$, where all the four-spin interaction is gone, the correlation function assumes the form of a cosine function. Note that the other extreme case, $p=0$, corresponds to the pure case with $J=B$ studied in Ref. 5. The longitudinal relaxation function, with same parameter values is depicted in Fig. 1(b). The effect of dilution is to change the central mode type of behavior at $p=0$ onto the collective-mode behavior as p increases. The case $p=0.2$ already shows a depletion of the central mode peak at $\omega=0$ and the appearance of the collective-mode peak at a finite yet small frequency. The cases $p=0.5$ and 0.8 show the building up of the collective-mode behavior and strong suppression of the central mode dynamics. As p increases further, the central peak loses its strength even more, while the collective-mode peak becomes higher while its width decreases to zero as p approaches unity. In that limit, that peak becomes a Dirac δ function and the dynamics is entirely governed by the precessing of the uncoupled spins about the transverse field, since the four-spin interaction is null.

In some physical systems, the distribution of interatomic separations in a noncrystalline material may lead to a distribution of exchange interactions. These interactions can be of both positive and negative signs or they only fluctuate in strength. The interaction energy couplings can be quite smaller than the thermal energy even, say, at room temperature. In those cases where $J_i/kT \ll 1$ one can study the dynamics as if the system is at the infinite temperature limit. At that limit, it is a well-known fact that the dynamics is insensitive to the sign of the interaction, since only even powers of the interaction coupling comes into the moments of the autocorrelation function.[5,14,19] Therefore it suffices to study instances where the coupling energies assume positive values only.

In our analysis for the disordered exchange couplings, we again fixed the values of the transverse field $B=J_1=1$ and then considered the cases where $J_2=0.1,0.5$, and 0.8. We also considered several concentrations for each of these cases. The results for the correlation functions and longitudinal relaxation functions are shown in Figs. 2–4. The effects of disorder is quite similar to the case with dilution, that is, as the concentration of the weaker couplings J_2 increases, there is a crossover where the system departs towards a collective-mode dominated by the transverse field. That effect is most pronounced for low values of J_2, and less so for higher values, such as for the case $J_2=0.8$. In that case, even for high concentrations it is not possible for the collective mode completely overwhelm the central mode behavior.

To summarize, we have studied the effects of bond randomness in the dynamics of the transverse Ising model with four-spin interactions via exact diagonalization of finite chains. We present the time-dependent correlation functions and the longitudinal relaxation functions for a system of size $L=11$. For this system size the dynamic correlation functions have already converged to those at the thermodynamic limit. Our results show that disorder induces a crossover from a central mode behavior to a collective mode type of dynamics, as the concentration of weaker bonds (or bond dilution) is enhanced.

This work was partially supported by CNPq, Finep, MCT, Fapemig and Faperj (Brazilian agencies).

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[1] J. Bernasconi and T. Schneider, *Physics in one Dimension* (Springer, Berlin, 1981); *Magnetic Excitations and Fluctuations II*, edited by U. Balucani *et al.* (Springer, Berlin, 1987); A.S.T. Pires, Helv. Phys. Acta **61**, 988 (1988).

[2] R.W. Youngblood, G. Aeppli, J.D. Axe, and J.A. Griffin, Phys. Rev. Lett. **49**, 1724 (1982); J. Kötzler, H. Neuhaus-Steinmetz, A. Froese, and D. Gorlitz, *ibid.* **60**, 647 (1988); C. Lee and S.I. Kobayashi, *ibid.* **62**, 1061 (1989); E.H. Lieb, T. Schultz, and D. C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).

[3] B. Boechat, R.R. dos Santos, and M.A. Continentino, Phys. Rev. B **49**, R6404 (1994); **50**, 13 528 (1994).

[4] J. Florencio and F.C. Sá Barreto, Phys. Rev. B **60**, 9555 (1999). For other applications of the method of recurrence relations, see, e.g., M.H. Lee, Phys. Rev. Lett. **49**, 1072 (1982); H. Mori, Prog. Theor. Phys. **33**, 423 (1965); **34**, 399 (1965); M.H. Lee *et al.*, Phys. Scr. **T19B**, 498 (1987); J. Florencio and M.H. Lee, Phys. Rev. A **31**, 3231 (1985).

[5] J. Florencio, O.F. de Alcantara Bonfim, and F.C. Sá Barreto, Physica A **235**, 523 (1997).

[6] R.J. Baxter and F.Y. Wu, Phys. Rev. Lett. **31**, 1294 (1973); M. Yamashita, H. Nakano, and K. Yamada, Prog. Theor. Phys. **62**, 1225 (1979).

[7] O. Mitran, J. Phys. C **12**, 557 (1979); **7**, L54 (1979); B. Frank, and M. Danino, *ibid.* **19**, 2529 (1986).

[8] O.G. Mouritsen, S.J. Knak Jensen, and B. Frank, Phys. Rev. B **23**, 976 (1981); **24**, 347 (1981).

[9] A. Aharony, Phys. Rev. B **9**, 2416 (1974); M. Gitterman and M. Mikulinsky, J. Phys. C **10**, 4073 (1977).

[10] M. Suzuki, Phys. Lett. **28A**, 267 (1972); D.W. Wood and H.P. Griffith, J. Math. Phys. **14**, 1715 (1973); J. Phys. C **7**, L54 (1974); H.P. Griffith and D.W. Wood, *ibid.* **6**, 2533 (1973); **7**, 4021 (1974).

[11] O.G. Mouritsen, B. Frank, and D. Mukamel, Phys. Rev. B **27**, 3018 (1983); B. Frank and O.G. Mouritsen, J. Phys. C **16**, 2481 (1983); F.C. Alcaraz, L. Jacobs, and R. Savit, Phys. Lett. **89A**, 49 (1982).

[12] P.R. Silva, B.V. Costa, and R.L. Moreira, Polymer **34**, 3107 (1993).

[13] U. Brandt and K. Jacoby, Z. Phys. B **25**, 181 (1976); H.W. Capel and J.H.H. Perk, Physica A **87**, 211 (1977).

[14] J. Florencio and M.H. Lee, Phys. Rev. B **35**, 1835 (1987).

[15] F.C. Sá Barreto, Braz. J. Phys. **24**, 1 (1994).

[16] This procedure was employed in the study of the dynamics of the isotropic Heisenberg chain by A. Sur and I.J. Lowe, Phys. Rev. B **11**, 1980 (1975); A. Sur, D. Jasnow, and I.J. Lowe, *ibid.* **12**, 3845 (1975).

[17] M. Engelsberg, I.J. Lowe, and J.L. Carolan, Phys. Rev. B **7**, 924 (1973).

[18] S.W. Lovesey, *Condensed Matter Physics: Dynamic Correlations* (Benjamin/Cummings, Reading, MA, 1986).

[19] S. Sen, M. Long, J. Florencio, and Z.X. Cai, J. Appl. Phys. **73**, 5471 (1993); S. Sen, S.D. Mahanti, and Z.X. Cai, Phys. Rev. B **43**, 10 990 (1991); J. Stolze, G. Müller, and V.S. Viswanath, Z. Phys. B: Condens. Matter **89**, 45 (1992).