Delocalization and spin-wave dynamics in ferromagnetic chains with long-range correlated random exchange

F. A. B. F. de Moura, M. D. Coutinho-Filho, and E. P. Raposo

Laboratório de Física Teórica e Computacional, Departamento de Física, Universidade Federal de Pernambuco, 50670-901 Recife, PE, Brazil

M. L. Lyra

Departamento de Física, Universidade Federal de Alagoas, Br 101 Km 14, Cidade Universitária, Maceió, AL, 57072-970, Brazil (Received 18 December 2001; published 8 July 2002)

We study the one-dimensional quantum Heisenberg ferromagnet with exchange couplings exhibiting longrange correlated disorder with power spectrum proportional to $1/k^{\alpha}$, where k is the wave vector of the modulations on the random coupling landscape. By using the renormalization group, integration of the equations of motion, and exact diagonalization, we compute the spin-wave localization length and the mean-square displacement of the wave packet. We find that, associated with the emergence of extended spin waves in the low-energy region for $\alpha > 1$, the wave-packet mean-square displacement changes from a long-time super diffusive behavior for $\alpha < 1$ to a long-time ballistic behavior for $\alpha > 1$. At the vicinity of $\alpha = 1$, the mobility edge separating the extended and localized phases is shown to scale with the degree of correlation as E_c $\propto (\alpha - 1)^{1/3}$.

DOI: 10.1103/PhysRevB.66.014418

PACS number(s): 75.10.Jm, 75.30.Ds, 75.50.Lk

I. INTRODUCTION

It is well established that one-electron eigenstates in chains with uncorrelated disorder are exponentially localized.¹ However, several theoretical investigations have shown that a series of one-dimensional versions of the Anderson model exhibit a breakdown of the Anderson's localization induced by internal short-range correlations on the disorder distribution, including hopping and on-site energy correlations² or just on-site energy correlations.^{3,4} Recently, it has been shown that the one-dimensional Anderson model with long-range correlated disorder can display a phase of extended electronic states.^{5,6} These results have been confirmed by microwave transmission spectra of single-mode waveguides with inserted correlated scatterers.⁷ The influence of long-range disorder on the electron motion in two dimensions has been recently investigated⁸ and a twodimensional layered Anderson model with long-range correlated disorder has been shown to exhibit a Kosterlitz-Thouless-type metal-insulator transition.⁹

It is also known that the magnon equation of motion for ferromagnetic spin chains with uncorrelated random nearestneighbor exchange couplings can be exactly mapped onto an electronic chain with a particular form of off-diagonal disorder where the random hopping integrals appear correlated in pairs.^{10,11} By using a perturbation approach combined with a scaling hypothesis it was demonstrated¹⁰ that the singularities of the density of states and the localization length of a random ferromagnetic Heisenberg chain depend on the distribution of exchange couplings. For uncorrelated random exchange couplings $J \in [0,1]$ with a probability distribution function $P(J) = (1 - \delta)J^{-\delta}$, it was predicted that for $\delta < -1$, which implies $\langle 1/J \rangle$ and $\langle 1/J^2 \rangle$ finite, the density of states $\rho(E)$ diverges as $1/E^{1/2}$ and the localization length as 1/E. Distinct regimes emerge when either of the above two moments diverges, thus generalizing other studies.¹² Moreover, in order to elucidate doubts raised in the literature,¹³ the spin-wave dynamics of the one-dimensional Heisenberg ferromagnet was investigated¹¹ for the above power-law distribution of exchange couplings J. The mean-square displacement of the wave packet asymptotically displays super diffusion dynamics $[\sigma(t)^2 \propto t^{3/2}]$ for weak disorder ($\delta < 0$), diffusive behavior $[\sigma(t)^{2} \propto t^{1}]$ for $\delta = 0$, and localization $[\sigma(t)^2 \propto \text{const}]$ for strong disorder ($\delta > 0$). Therefore, the uncorrelated Heisenberg ferromagnet with random exchange couplings can display a superdiffusive dynamics if $\langle 1/J \rangle$ is finite. In all three cases, a ballistic regime $[\sigma(t)^2 \propto t^2]$ emerges for initial times. By using the transfer matrix technique, the singularities of the density of states and localization length were verified. The superdiffusive behavior is closely related to the one found in the random-dimer version of the Anderson model.³

In this paper, we study the nature of the spin-wave modes of a quantum Heisenberg ferromagnetic chain with longrange correlated random exchange couplings J_n assumed to have spectral power density $S \propto 1/k^{\alpha}$. A previous study reported some finite-size scaling evidence of the emergence of a phase of extended low-energy excitations.¹⁴ Here, we will use a renormalization group technique to provide accurate estimates for the mobility-edge energy as a function of the degree of correlation and to obtain the scaling behavior governing the vanishing of the mobility edge in the vicinity of $\alpha = 1$. Further, we also study the quantum diffusion of the wave packets in these chains using direct integration of the motion equations and exact diagonalization to investigate the possible emergence of a new dynamical regime associated with the occurrence of extended low-energy spin waves for $\alpha > 1.$

II. MODEL AND RENORMALIZATION-GROUP CALCULATION

We consider a Hamiltonian model describing a spin-1/2 quantum ferromagnetic Heisenberg chain of N sites with random exchange couplings J_n :

$$H = \sum_{n=-N/2}^{N/2} J_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \qquad (1)$$

where S_n represents the quantum spin operator at site *n* and open boundary conditions are used. We take the exchange couplings J_n connecting sites *n* and n+1 to be correlated in such a sequency to describe the trace of a fractional Brownian motion:^{15–17}

$$J_n = \sum_{k=1}^{N/2} \left[k^{-\alpha} \left(\frac{2\pi}{N} \right)^{(1-\alpha)} \right]^{1/2} \cos \left(\frac{2\pi nk}{N} + \phi_k \right), \quad (2)$$

where *k* is the wave vector of the modulations on the random coupling landscape and ϕ_k are N/2 random phases uniformly distributed in the interval $[0,2\pi]$. The exponent α is directly related to the Hurst exponent $H(\alpha = 2H+1)$ of the rescaled range analysis, which describes the self-similar character of the series and the persistent character of its increments: for $\alpha > 2$ (H>1/2) the increments are persistent, while for $\alpha < 2$ $(H \le 1/2)$ they are antipersistent. In the case of $\alpha = 2$ (H = 1/2) the sequence of exchange couplings resembles the trace of the usual Brownian motion, while for $\alpha=0$ (H =-1/2) one recovers the uncorrelated random exchange Heisenberg model. The coupling distribution is Gaussian for $\alpha=0$ but assumes a non-Gaussian form for finite α once the presence of long-range correlations is implied in the lack of self-averaging and the breakdown of the central limit theorem. In order to avoid a vanishing exchange coupling we shift all couplings generated by Eq. (2) such to have average value $\langle J_n \rangle = -4.5$ and variance $\langle \Delta J_n \rangle = 1$. Note that, in such a case, all moments of the resulting distribution are finite. In order to keep the variance size independent, the normalization factor scales with the chain size. A detailed finite-size scaling analysis has shown how such a normalization procedure is reflected in the main character of the one-magnon excitations.14 Indeed, without such a rescaling of the potential the disorder width diverges for any $\alpha \neq 0$ and all states are expected to remain localized.¹⁸

The ground state of the system contains all spins pointing in the same direction. If a spin deviation occurs at a site n, this excited state is described by

$$\phi_n = S_n^+ |0\rangle, \tag{3}$$

where the operator S_n^+ creates a spin deviation at site *n* and $|0\rangle$ denotes the ground state. The eigenstates of the Hamiltonian are therefore a linear combination of ϕ_n , i.e., $\Phi = \sum_n c_n \phi_n$, the coefficients c_n satisfying the equation¹¹⁻¹³

$$(J_{n-1}+J_n)c_n - J_{n-1}c_{n-1} - J_n c_{n+1} = 2Ec_n, \qquad (4)$$

where E is the excitation energy.

In order to study the properties of one-magnon states, we apply a decimation renomalization-group technique. The

method is based on the particular form assumed by the equation of motion satisfied by the Green's operator matrix elements $[G(E)]_{i,j} = \langle i | 1/(E-H) | j \rangle$ (Refs. 5 and 19):

$$(E - \epsilon_{n+\mu}^{0})[G(E)]_{n+\mu,n} = \delta_{\mu,0} + J_{n+\mu,n+\mu-1}^{0}[G(E)]_{n+\mu-1,n} + J_{n+\mu,n+\mu+1}^{0}[G(E)]_{n+\mu+1,n},$$
(5)

where $\epsilon_n^0 = (J_{n-1} + J_n)/2$ and $J_{n,n+1}^0 = J_{n+1,n}^0 = J_n/2$. After eliminating the matrix elements associated with a given site, the remaining set of equations of motion can be expressed in the same form as the original one, but with renormalized parameters

$$\boldsymbol{\epsilon}_{N}^{(N-1)}(E) = \boldsymbol{\epsilon}_{N} + J_{N-1,N} \frac{1}{E - \boldsymbol{\epsilon}_{N-1}^{(N-2)}(E)} J_{N-1,N}, \quad (6)$$

$$J_{0,N}^{(eff)}(E) = J_{0,N-1}^{(eff)} \frac{1}{E - \epsilon_{N-1}^{(N-2)}(E)} J_{N-1,N},$$
(7)

where, after N-1 decimations, ϵ_N^{N-1} denotes the renormalized diagonal element at site N and $J_{0,N}^{(eff)}$ indicates the effective renormalized exchange coupling connecting the sites 0 and N.

To investigate the localized-delocalized nature of the spinwave modes, we compute the inverse of the excitation width or the Lyapunov coefficient $\gamma(E)$ (inverse localization length). The Lyapunov coefficient is asymptotically related to the effective exchange coupling by^{5,19}

$$\gamma(E) = -\lim_{N \to \infty} \left[\frac{1}{N} \ln \left| J_{0,N}^{(eff)}(E) \right| \right].$$
(8)

After a linear regression of $\ln |J_{0,N}^{(eff)}(E)|$ versus *N* we have a direct extrapolation of the Lyapunov coefficient in the thermodynamical limit. We computed $\gamma(E)$ for distinct values of the exponent α and $N=10^5$ sites. In addition, the density of states (DOS) was calculated by using the numerical Dean's method.²⁰ In Fig. 1 we show the normalized DOS for chains with $N=10^5$ sites. Notice that it becomes less rough as α is increased and its singularity at the bottom of the band is not affected by the imposed long-range correlation in the coupling constants (see insets). For $\alpha=1.5$ it consists of a nonfluctuating part near the bottom of the band with the same form as that of the pure chain ($J_n = \text{const}$). Previous studies have pointed out that the smoothing of the DOS is usually connected with the emergence of delocalized states.²¹

In Fig. 2 we show the plot of γ versus E for $\alpha=0$ (uncorrelated random exchanges). In this case, the Lyapunov coefficient is finite for all energies, except for E=0 as usual. This behavior remains qualitatively unaltered for $0 < \alpha \leq 1$, therefore implying the absence of extended spin waves in this regime. For $\alpha=0$, we have also observed that, near the bottom of the band, the Lyapunov coefficient vanishes as $\gamma \propto E^{\nu}$ with $\nu=1.0$, in agreement with Ref. 10 for probability distribution functions with finite $\langle 1/J \rangle$ and $\langle 1/J^2 \rangle$ (see inset of Fig. 2). The picture is qualitatively different for $\alpha>1$. In Fig. 3(a) we plot γ versus E for $\alpha=1.5$. The Lyapunov co-



FIG. 1. The spin-wave density of states (DOS) for chains with $N=10^5$ sites using Dean's method. The DOS becomes less rough as α is increased and its singularity at the bottom of the band is not affected by the imposed long-range correlation in the coupling constants (insets). For $\alpha=1.5$ it consists of a nonfluctuating part near the bottom of the band with the same form as that of the pure chain $(J_n = \text{const})$.

efficient vanishes within a finite range of energy values, thus confirming the presence of low-energy extended spin waves. In all chains studied with sizes ranging from 10^5 up to 10^6 sites, the $\gamma(E)$ curves appear to be the same, indicating that the extended phase of magnons is stable in the thermodynamical limit. The phase diagram in the (E_c, α) plane is shown in Fig. 3(b), with E_c (given in units of ΔJ) denoting the mobility edge and statistical errors are smaller than the symbol sizes. The data analysis (see inset) suggests that, at the vicinity of $\alpha=1$, the mobility edge depends on the correlation exponent as $E_c \propto (\alpha-1)^{\gamma}$, with $\gamma=1/3$.

III. SPIN-WAVE DYNAMICS

In order to investigate the spin-wave dynamics, we compute the time dependence of the mean-square displacement of the wave packet. Let us consider an excitation initially



FIG. 2. Lyapunov coefficient γ vs energy *E* for $\alpha=0$ (uncorrelated random-exchange model) and $N=10^5$ sites from the renormalization procedure. The Lyapunov coefficient is finite for nonzero energies (localized states) and vanishes as $\gamma \propto E^{\nu}$, $E \rightarrow 0$, with $\nu=1.0$ (inset).



FIG. 3. (a) Lyapunov coefficient γ vs energy *E* for α =1.5 and N=10⁵ sites from the renormalization procedure. The Lyapunov coefficient vanishes within a finite range of energy values revealing the presence of extended low-energy spin waves. (b) (E_c , α) phase diagram, where E_c is the mobility edge (in units of ΔJ) for N = 10⁵ sites. The phase of extended spin waves emerges for α >1 and $E < E_c$.

localized at site n_0 , represented at t=0 by its eigenfunction $\phi_n(t=0) = \delta_{n,n_0}$. Its time evolution is described by the Schrödinger equation $(\hbar=1)$

$$i\frac{d\phi_n(t)}{dt} = H\phi_n(t), \qquad (9)$$



FIG. 4. Mean squared displacement σ^2 vs time t for $\alpha=0$ from the integration of the equations of motion. The self-expanded chain was used to minimize end effects. The spread of the wave packet depicts a crossover from a initial ballistic ($\sigma^2 \propto t^2$) to a superdiffusive ($\sigma^2 \propto t^{3/2}$) behavior.



FIG. 5. Mean-squared displacement σ^2 vs time *t* for α =0.5 and N=20 000 sites from the integration of the equations of motion. A longer-living ballistic motion ($\sigma^2 \propto t^2$) is found but still followed by a crossover to the superdiffusive regime ($\sigma^2 \propto t^{3/2}$).

whose time-dependent wave function can be written in terms of the computed eigenvectors $V^{(j)}$ and eigenvalues E_j of H as¹¹

$$\phi_n(t) = \sum_{j}^{N} V_n^{(j)} V_{n_0}^{(j)} \exp(-iE_j t).$$
(10)

The same time-dependent wave function can be obtained by integrating the equations of motion. The second moment of the corresponding spatial probability distribution is then given by

$$\sigma^{2}(t) = \sum_{n} (n - n_{0})^{2} \phi_{n}(t) \phi_{n}^{*}(t).$$
(11)

From the mean-square displacement $\sigma^2(t)$ we can estimate the wave packet spread in space at a time t. For any $\alpha \ge 0$, we find ballistic behavior $[\sigma(t)^2 \propto t^2]$ for initial times, indicating that disorder has not yet been realized by the spin waves.¹¹ In the case of uncorrelated random exchange ($\alpha=0$) the self-expanded chain was used to minimize end effects. When the probability of finding the particle at the ends of the chain exceeded 10^{-100} we added new sites thus expanding the chain. In Fig. 4 we show the mean-squared displacement versus time for $\alpha = 0$ as obtained by integrating the equations of motion. In this case, for longer times the wave packet presents a super diffusive spread $[\sigma(t)^2 \propto t^{3/2}]$ in agreement with previous studies¹¹ for an uncorrelated random exchange distribution with $\langle 1/J \rangle$ finite. In Fig. 5 we plot the data obtained by integrating the equations of motion for $\alpha = 0.5$ and 20 000 sites. As indicated, the initial ballistic motion extends over longer times, although a super diffusive motion still takes place after this initial transient. Finally, Fig. 6 shows that for $\alpha = 1.5$ the wave packet displays only a ballistic spread. In this case our calculation was performed by using both numerical integration of the equations of motion for N $= 20\,000$ sites and exact diagonalization for N = 2000, 4000,and 8000 sites, in which case the end effect is present (see inset).

In contrast with the case of uncorrelated random exchange couplings,¹¹ in which an asymptotic superdiffusive behavior



FIG. 6. Mean-squared displacement σ^2 vs time t for $\alpha = 1.5$ for $N = 20\,000$ sites from the integration of the equations of motion. Inset: results using exact diagonalization for N = 2000 (dotted line), 4000 (dashed line), and 8000 (dot-dashed line) sites. Ballistic behavior $(\sigma^2 \propto t^2)$ is found for all times.

sets up whenever $\langle 1/J \rangle$ is finite, we find a crossover with increasing α from superdiffusive to ballistic asymptotic regimes induced by long-range correlations in the exchange couplings. The ballistic regime for $\alpha > 1$ can be understood following arguments similar to those used in Refs. 3 and 11. Exploring the exact mapping of the magnon problem onto a paired electronic one, the diffusion coefficient D can be estimated by integrating $v(k)\lambda(k)$ over the extended states that effectively participate in the transport, where v(k) and $\lambda(k)$ are, respectively, the velocity and mean free path of the excitation mode with wave number k. In a finite chain all extended modes have $\lambda(k) \simeq N$ and travel with finite velocity since in the electronic problem the DOS is nonsingular near the band center. Once there is a finite fraction of states that are delocalized, the integration runs over a finite wave number and, interchanging N and t, the diffusion coefficient results in $D \propto t$. Consequently, the mean-square displacement is $\langle \sigma^2(t) \rangle = Dt \propto t^2$, confirming the ballistic nature of the wave packet spread found in our numerical analysis.

IV. CONCLUSIONS

In summary, we have studied the one-dimensional quantum Heisenberg ferromagnet with exchange couplings exhibiting long-range correlated disorder with spectral power density proportional to $1/k^{\alpha}$. By using a decimation renormalization-group technique we have found further evidence suggesting that this magnetic system displays a phase of extended spin waves in the low-energy region for $\alpha > 1(H>0)$. The mobility edge separating low-energy extended and high-energy localized states was shown to depend on the degree of correlation in a very special manner. Finally, through integration of the equations of motion and exact diagonalization, we have also computed the mean-square displacement of the spin-wave packet. For $0 < \alpha \le 1$, we havefound long-time super diffusion, in agreement with previous DELOCALIZATION AND SPIN-WAVE DYNAMICS IN ...

works for uncorrelated random exchange distribution with $\langle 1/J \rangle$ finite. However, for strong correlations ($\alpha > 1$) a longtime ballistic regime was numerically observed which is associated with the emergence of extended excitations. We believe that the reported results might be useful to stimulate further theoretical and experimental investigations of spinwave dynamics on correlated ferromagnetic chains and nonperiodic ferromagnetic superlattices.

ACKNOWLEDGMENTS

This work was supported by the Brazilian agencies CNPq, Finep, CAPES, FACEPE, and FAPEAL.

- ¹E. Abrahams, P.W. Anderson, D.C. Licciardello, and T.V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979); For a review see, e.g., I.M. Lifshitz, S.A. Gredeskul, and L.A. Pastur, *Introduction to the Theory of Disordered Systems* (Wiley, New York, 1988).
- ²J.C. Flores, J. Phys.: Condens. Matter 1, 8471 (1989).
- ³D.H. Dunlap, H.L. Wu, and P.W. Phillips, Phys. Rev. Lett. 65, 88 (1990); H.-L. Wu and P. Phillips, *ibid.* 66, 1366 (1991); P.W. Phillips and H.-L. Wu, Science 252, 1805 (1991).
- ⁴S.N. Evangelou and A.Z. Wang, Phys. Rev. B 47, 13 126 (1993);
 S.N. Evangelou and E.N. Economou, J. Phys. A 26, 2803 (1993).
- ⁵F.A.B.F. de Moura and M.L. Lyra, Phys. Rev. Lett. **81**, 3735 (1998); Physica A **266**, 465 (1999).
- ⁶F.M. Izrailev and A.A. Krokhin, Phys. Rev. Lett. **82**, 4062 (1999); F.M. Izrailev, A.A. Krokhin, and S.E. Ulloa, Phys. Rev. B **63**, 041102 (2001).
- ⁷U. Kuhl, F.M. Izrailev, A. Krokhin, and H.J. Stöckmann, Appl. Phys. Lett. **77**, 633 (2000).
- ⁸D. Taras-Semchuk and K.B. Efetov, Phys. Rev. B **64**, 115301 (2001).

- ⁹W.S. Liu, T. Chen, and S.J. Xiong, J. Phys.: Condens. Matter 11, 6883 (1999).
- ¹⁰T.A.L. Ziman, Phys. Rev. Lett. **49**, 337 (1982).
- ¹¹S.N. Evangelou and D.E. Katsanos, Phys. Lett. A **164**, 456 (1992); see also S.N. Evangelou, A.Z. Wang, and S.J. Xiong, J. Phys.: Condens. Matter **6**, 4937 (1994).
- ¹²G. Theodorou, J. Phys. C 15, L1315 (1982).
- ¹³M. Cieplak and G. Ismail, J. Phys. C **20**, 1309 (1987).
- ¹⁴R.P.A. Lima, M.L. Lyra, E.M. Nascimento, and A.D. de Jesus, Phys. Rev. B 65, 104416 (2002).
- ¹⁵J. Feder, *Fractals* (Plenum Press, New York, 1988); A. Tsonis, *Chaos: From Theory to Applications* (Plenum Press, New York, 1992).
- ¹⁶A.R. Osborne and A. Provenzale, Physica D 35, 357 (1989).
- ¹⁷N.P. Greis and H.S. Greenside, Phys. Rev. A 44, 2324 (1991).
- ¹⁸S. Russ, J.W. Kantelhardt, A. Bunde, and S. Havlin, Phys. Rev. B 64, 134209 (2001).
- ¹⁹K.A. Chao, R. Riklund, and Y.Y. Liu, Phys. Rev. B **32**, 5979 (1985); see also R. Farchioni *et al.*, *ibid.* **45**, 6383 (1992).
- ²⁰ P. Dean, Rev. Mod. Phys. **44**, 127 (1972).
- ²¹B.L. Altshuler, J. Appl. Phys. 26, 1938 (1987).