Delocalization in harmonic chains with long-range correlated random masses

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We study the nature of collective excitations in harmonic chains with masses exhibiting long-range correlated disorder with a power spectrum proportional to $1/k^{\alpha}$, where k is the wave vector of the modulations on the random masses landscape. Using a transfer-matrix method and exact diagonalization, we compute the localization length and participation ratio of eigenmodes within the band of allowed energies. We find extended vibrational modes in the low-energy region for $\alpha>1$. In order to study the time evolution of an initially localized energy input, we calculate the second moment $M_2(t)$ of the energy spatial distribution. We show that $M_2(t)$, besides being dependent of the specific initial excitation and exhibiting an anomalous diffusion for weakly correlated disorder, assumes a ballistic spread in the regime $\alpha>1$ due to the presence of extended vibrational modes.

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I. INTRODUCTION

The role played by disorder on the nature of collective excitations in condensed-matter physics has been the subject of intensive studies due to its relevance in defining general transport characteristics.[1] Usually, disorder induces localization of collective excitations, thus degrading transport properties, an effect that is largely pronounced in low dimensions. In particular, the one-electron eigenstates in the one-dimensional Anderson model with site-diagonal uncorrelated disorder are exponentially localized for any degree of disorder.[2] However, several one-dimensional models with correlated disorder have been proposed which exhibit delocalized states.[3–5] It has been recently shown that the one-dimensional Anderson model with long-range correlated disorder presents a phase of extended electronic states.[6–8] These results have been confirmed by microwave transmission spectra of single-mode waveguides with inserted correlated scatters.[9] More recently, it has been conjectured that long-range correlations may strongly affect the electronic transport properties in DNA, although in this case the metallic phase is in fact induced by an order-disorder transition.[10]

The above results have motivated the study of further model systems that can be mapped onto the Anderson model and are, therefore, expected to present a similar transition between localized and extended collective excitations. Recently, studies concerning the one-dimensional quantum Heisenberg ferromagnet with exchange couplings exhibiting long-range correlated disorder reported the emergence of a phase of extended spin waves.[11,12] It was also shown that, associated with the emergence of extended spin waves in the low-energy region, the wave-packet mean-square displacement exhibits a long-time ballistic behavior.[12] The effect of correlated disorder has also been studied in other random magnets in which it was shown that long-range correlations change the universality class of quantum critical points.[13] In addition, a criterion for determining the kind of diffusion in systems governed by a generalized Langevin equation with long-range memory was recently reported.[14]

The collective vibrational motion of one-dimensional disordered harmonic chains can also be mapped onto a one-electron tight-binding model.[15] Most of the normal vibrational modes are localized. However, there are a few delocalized low-frequency modes, whose number is of the order of $\sqrt{N}$, in which case the disordered chains behave like the disorder-free system.[15,16] Further, it was shown that correlations in the mass distribution produce a new set of nonscattered modes in this system.[17,18] The transport of energy in mass-disordered (uncorrelated and correlated) harmonic chains is strongly dependent on nonscattered vibrational modes as well as on the initial excitation.[19] For impulse initial excitations, uncorrelated random chains have a superdiffusive behavior for the second moment of the energy distribution $[M_2(t)\propto t^{1.5}]$, while for initial displacement excitations a subdiffusive spread takes place $[M_2(t)\propto t^{0.5}]$. The dependence of the second moment spread on the initial excitation was also obtained in Ref. 20. Correlations induced by thermal annealing have been shown to enhance the localization length of vibrational modes, although they still present an exponential decay for distances larger than the thermal correlation length.[21] Recently the thermal conductivity of harmonic and anharmonic chains with uncorrelated random masses,[22] as well as that of a chain of hard-point particles with alternate masses,[23] have been numerically investigated in detail. In such cases, the main issue is whether the systems display finite thermal conductivity in the thermodynamic limit, a question that remains controversial.[24]

In this paper we extend the study of collective modes in the presence of long-range correlated disorder for the case of vibrational excitations. We consider harmonic chains with long-range correlated random masses assumed to have spectral power density $S\propto 1/k^{\alpha}$. By using a transfer-matrix calculation, we obtain accurate estimates for the Lyapunov exponent, defined as the inverse of the degree of localization λ_c.

We show that, for $\alpha>1$, this model also presents a phase of extended modes in the low-frequency region. This result is confirmed by participation ratio measurements from an exact diagonalization procedure and finite-size scaling arguments. The spatial evolution of an initially localized excitation is also studied by computing the spread of the second moment of the energy distribution, $M_2(t)$. We find that, associated with the emergence of a phase of delocalized modes, a ballistic energy spread takes place.

II. VIBRATIONAL MODES

We consider a disordered harmonic chain of N masses, for which the equation of motion for the Fourier transform u_n of the spatial displacement $Q_n=u_n e^{-i\omega t}$ of the nth mass with vibrational frequency ω is[16,18]

$$(\beta_{n-1}+\beta_n-\omega^2 m_n)u_n=\beta_{n-1}u_{n-1}+\beta_n u_{n+1}. \qquad (1)$$

Here m_n is the mass at the nth site and β_n is the spring constant that couples the masses m_n and m_{n+1}. In what follows, we use units in which $\beta_n=1$. In the present harmonic chain model, we take the masses m_n following a random sequence describing the trace of a fractional Brownian motion:[25]

$$m_n=\sum_{k=1}^{N/2}\rho(k)\cos\left(\frac{2\pi nk}{N}+\phi_k\right), \qquad (2)$$

where k is the wave vector of the modulations on the random mass landscape and ϕ_k are $N/2$ random phases uniformly distributed in the interval $[0,2\pi]$. The amplitude of each Fourier component can be written as $\rho(k)=[S(k)\times(2\pi/N)^{(1-\alpha)}]^{1/2}$, where $S(k)$ is the power spectrum. A long-range correlated mass sequence can be generated by imposing the power spectrum to obey a power law $S(k)=Ck^{-\alpha}$, where $C=\mathcal{C}(N/2\pi)^{(1-\alpha)}$ and $\mathcal{C}$ is chosen to give a unitary mass variance $\Delta m_n=1$. The exponent α is directly related to the Hurst exponent H of the rescaled range analysis $\alpha=2H+1$.[25] In order to avoid vanishing masses we shift all masses generated by Eq. (2) to have an average value $\langle m_n\rangle=5$. Using matrix formalism, Eq. (1) can be rewritten as

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix}=\begin{pmatrix} 2-m_n\omega^2 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}=T_n\begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}. \qquad (3)$$

Once the initial values for u_0 and u_1 are known, the value of u_n can be obtained by repeated iterations along the chain, as described by the product of transfer matrices $M_N=\Pi_{n=1}^{N}T_n$. The localization length of each vibrational mode is taken as the inverse of the Lyapunov exponent γ defined by[16,18,26,27]

$$\gamma=(1/N)\lim_{N\to\infty}\log[|M_N c(0)|/|c(0)|], \qquad (4)$$

where $c(0)=\binom{u_1}{u_0}$ is a generic initial condition. The nature of the vibrational modes can also be investigated by computing the participation ratio ξ, since it displays a dependence on the chain size for extended states and is finite for exponentially localized ones. ξ is defined by $\xi(\omega)=\Sigma_{n=1}^{N}u_n^2/\Sigma_{n=1}^{N}u_n^4$,[17,21] where the Fourier transforms u_n are those associated with an eigenmode ω of a chain of N masses and are obtained by direct diagonalization of the $N\times N$ secular matrix A defined by $A_{i,i}=2/m_i$, $A_{i,i+1}=A_{i+1,i}=1/(m_i m_{i+1})^{1/2}$, and all other $A_{i,j}=0$.[15,18] The participation ratio calculations were averaged over 100 samples.

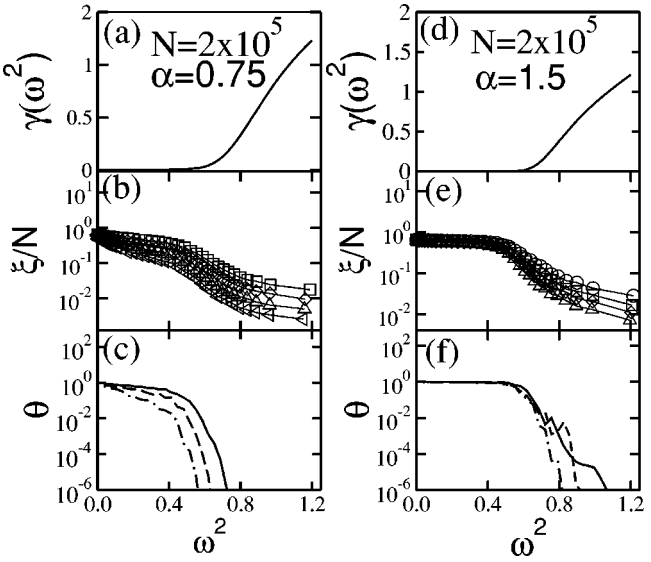

FIG. 1. (a) Lyapunov coefficient γ versus ω^2 for $\alpha=0.75$ and $N=2\times10^5$ sites. (b) Scaled participation ratio ξ/N as a function of ω^2 for $\alpha=0.75$. From top to bottom, $N=200$, 400, 800, and 1600. (c) $\theta(\omega,2N,N)$ function (see text) versus ω^2 for $N=200$ (solid line), 400 (dashed line), and 800 (dot-dashed line). In spite of γ being very small in the bottom of the band, all modes with $\omega>0$ are localized. (d)–(f) The same as in (a)–(c) for $\alpha=1.5$. The Lyapunov coefficient vanishes within a finite range of frequency values, thus revealing the presence of extended vibrational modes. The phase of extended vibrational modes is confirmed by the ξ/N size-independent plateau in the low-frequency region and the scale invariance of $\theta(\omega,2N,N)$.

To investigate the effect of weak long-range correlated disorder, we present in Fig. 1(a) the Lyapunov coefficient as a function of ω^2 for $\alpha=0.75$ and $N=2\times10^5$. In spite of γ being very small in the bottom of the band, ξ/N for $\omega>0$ vanishes in the thermodynamic limit. This trend can be observed in Fig. 1(b) where the participation ratio continuously decreases as longer chains are considered. A more quantitative scaling analysis of such a trend can be derived by introducing the set of auxiliary functions

$$\theta(\omega,N_1,N_2)=\exp\left[-\left|\frac{N_1}{\xi(\omega,N_1)}-\frac{N_2}{\xi(\omega,N_2)}\right|\right], \qquad (5)$$

which is a measure of the difference between data from two consecutive chain sizes investigated, with $N_1=2N_2$ in our simulations. For extended states $\theta\approx1$ for large chain sizes. For localized states $\theta\to0$ in the thermodynamic limit. In Fig. 1(c) one sees clearly the increasing tendency of localization as longer chains are considered. Therefore, all modes with $\omega>0$ are still localized, a feature that holds for any $0\leqslant\alpha\leqslant1$. However, the nature of the low-frequency modes

changes qualitatively for $\alpha>1$. In Fig. 1(d) we show γ versus ω^2 for $\alpha=1.5$ and $N=2\times10^5$ sites. The Lyapunov coefficient vanishes within a finite range of frequency values, thus revealing the presence of extended vibrational modes. The scaled participation ratio ξ/N [see Fig. 1(e)] displays a well-defined data collapse in the low-frequency region. In Fig. 1(f) we can see that the θ versus ω^2 data suggest that the phase of extended low-frequency vibrational modes is stable in the thermodynamic limit.

III. ENERGY TRANSPORT

In order to study the time evolution of a localized energy pulse, we calculate the second moment of the energy distribution.[19,20] This quantity is related to the thermal conductivity by Kubo's formula.[19,28] The classical Hamiltonian H for a harmonic chain can be written as $H=\Sigma_{n=1}^{N}h_n(t)$, where the energy $h_n(t)$ at the site n is given by ($\beta_n\equiv1$)

$$h_n(t)=\frac{P_n^2}{2m_n}+\left[\frac{1}{4}(Q_{n+1}-Q_n)^2+\frac{1}{4}(Q_n-Q_{n-1})^2\right]. \quad (6)$$

Here P_n and Q_n define the momentum and displacement of the mass at the nth site. The fraction of the total energy H at the site n is given by $h_n(t)/H$ and the second moment of the energy distribution, $M_2(t)$, is defined by[19]

$$M_2(t)=\sum_{n=1}^{N}(n-n_0)^2[h_n(t)/H], \quad (7)$$

where an initial excitation is introduced at the site n_0 at $t=0$. Using the fourth-order Runge-Kutta method, we solve Hamilton's differential equations $\dot{P}_n(t)=-\partial H/\partial Q_n$ and $\dot{Q}_n(t)=\partial H/\partial P_n$, and calculate $M_2(t)$. The second moment of the energy distribution $M_2(t)$ has the same status of the mean-square displacement of the wave packet of an electron in a crystal.[19] We calculate $M_2(t)$ for several α values and two kinds of initial excitation: impulse excitation and displacement excitation.

A. Impulse excitation

In Fig. 2 we present the scaled second moment $M_2(t)/t^{1.5}$ versus time t for $\alpha=0$ (dotted line), which corresponds to the uncorrelated random chain, and $\alpha=0.75$ (dashed line). These results have been obtained after an initial impulse excitation, $P_{n_0}(t=0)=\delta_{n_0,N/2}$. In our calculations for $\alpha=0$, the self-expanded chain method[4,19] with initial chain size $N=1000$ was used to minimize end effects. Throughout the numerical integration process we kept the fraction of the total energy H at the ends of the chain [$h_0(t)/H$ and $h_N(t)/H$] smaller than 10^{-300} for all times. As shown in Fig. 2(a), we find a long-time superdiffusive behavior for $\alpha=0$, in agreement with Ref. 19. In contrast, for $\alpha>0$ we cannot use the self-expanded chain method due to the long-range character of the mass correlations. Therefore, chains with $N=10\,000$ masses were considered, and the runs stopped whenever the fraction of the total energy at the chain ends achieved 10^{-300}. For $\alpha=0.75$ the time dependence of the scaled energy second moment $M_2(t)/t^{1.5}$ typically represents a weak long-range correlated case. In such a case we also find superdiffusive behavior for long times. On the other hand, in the strong correlated regime, $\alpha>1$, a breakdown in the superdiffusive behavior becomes apparent. Figure 2(b) shows the time dependence of the scaled energy second moment, $M_2(t)/t^2$, for $\alpha=1.5$ (dotted line) and $\alpha=2.0$ (dashed line). Associated with the emergence of extended vibrational modes in the low-energy region, the second moment $M_2(t)$ displays a long-time ballistic behavior.

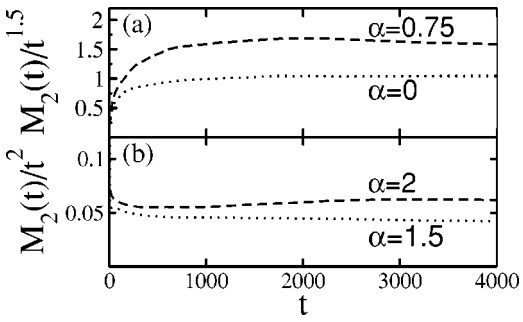

FIG. 2. (a) Scaled energy second moment $M_2(t)/t^{1.5}$ versus time t for $\alpha=0$ (dotted line) and $\alpha=0.75$ (dashed line) with initial impulse excitation. For $0\leqslant\alpha\leqslant1$ only superdiffusive behavior is found for long times. (b) Scaled second moment $M_2(t)/t^2$ versus time t for $\alpha=1.5$ (dotted line) and $\alpha=2.0$ (dashed line) with initial impulse excitation showing long-time ballistic behavior.

B. Displacement excitation

The long-time behavior of the second moment $M_2(t)$ in uncorrelated random chains with initial displacement excitation is significantly different from the corresponding behavior with initial impulse excitation.[19,20] Analytical calculations and numerical techniques predict that $M_2(t)\propto t^{0.5}$.[19] For $\alpha=0$ we indeed reproduce this behavior, as shown in Fig. 3(a), for the scaled second moment $M_2(t)/t^{0.5}$ versus time t with initial displacement excitation $Q_{n_0}(t=0)=\delta_{n_0,N/2}$. We find that this asymptotic subdiffusive behavior remains true for $0\leqslant\alpha<1$ [dashed line in Fig. 3(a)]. Similarly to the pre-

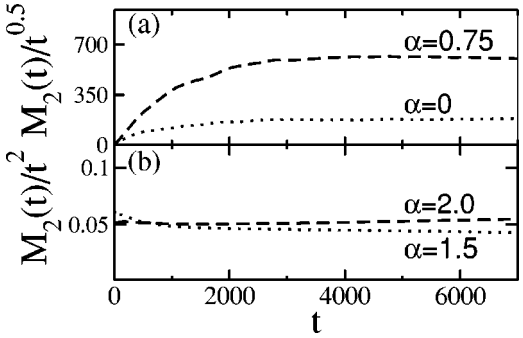

FIG. 3. (a) The scaled second moment $M_2(t)/t^{0.5}$ versus time t for $\alpha=0$ (dotted line) and $\alpha=0.75$ (dashed line) with initially given displacement excitation. The subdiffusive behavior is found for long times. (b) The scaled second moment $M_2(t)/t^2$ versus time t for $\alpha=1.5$ (dotted line) and $\alpha=2.0$ (dashed line) with initially given displacement excitation showing long-time ballistic behavior.

vious case, for strong correlations ($\alpha > 1$), which induce the emergence of new extended vibrational modes in the low-energy region, the energy transport is faster than in the subdiffusive regime and assumes a ballistic nature, as shown in Fig. 3(b).

IV. SUMMARY

In summary, we studied the nature of collective vibrational modes in harmonic chains with long-range correlated random masses m_n, with spectral power density $S \propto 1/k^{\alpha}$. We found that, associated with the emergence of a phase of low-energy extended collective excitations in the strong correlations regime, $\alpha > 1$, the energy second moment $M_2(t)$ displays a crossover from an anomalous subdiffusive or superdiffusive regime (depending on the initial displacement or impulse excitation, respectively) to an asymptotic ballistic behavior. Indeed, this can be understood by the fact that the number of such extended modes is extensive and has a finite width in k space.[19] The above findings indicate that the thermal conductivity can be strongly influenced by the presence of long-range correlations in the random distribution of masses and we hope that the present work stimulates further studies along this direction.

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[1] T.A.L. Ziman, Phys. Rev. Lett. **49**, 337 (1982). For a review see, e.g., B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).

[2] E. 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).

[3] J.C. Flores, J. Phys.: Condens. Matter **1**, 8471 (1989).

[4] D.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).

[5] S.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).

[6] F.A.B.F. de Moura and M.L. Lyra, Phys. Rev. Lett. **81**, 3735 (1998); *ibid.* **84**, 199 (2000); Physica A **266**, 465 (1999).

[7] F.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); F.M. Izrailev and N.M. Makarov, *ibid.* **67**, 113402 (2003).

[8] G.P. Zhang and S.-J. Xiong, Eur. Phys. J. B **29**, 491 (2002).

[9] U. Kuhl, F.M. Izrailev, A. Krokhin, and H.J. Stöckmann, Appl. Phys. Lett. **77**, 633 (2000).

[10] P. Carpena, P. Bernaola-Galán, P.Ch. Ivanov, and H.E. Stanley, Nature (London) **418**, 955 (2002); *ibid.* **421**, 764 (2003).

[11] R.P.A. Lima, M.L. Lyra, E.M. Nascimento, and A.D. de Jesus, Phys. Rev. B **65**, 104416 (2002).

[12] F.A.B.F. de Moura, M.D. Coutinho-Filho, E.P. Raposo, and M.L. Lyra, Phys. Rev. B **66**, 014418 (2002).

[13] H. Rieger and F. Iglói, Phys. Rev. Lett. **83**, 3741 (1999).

[14] R. Morgado, F.A. Oliveira, G.G. Batrouni, and A. Hansen, Phys. Rev. Lett. **89**, 100601 (2002).

[15] P. Dean, Proc. Phys. Soc. London **84**, 727 (1964).

[16] H. Matsuda and K. Ishii, Prog. Theor. Phys. Suppl. **45**, 56 (1970); K. Ishii, *ibid.* **53**, 77 (1973).

[17] F. Dominguez-Adame, E. Macià, and A. Sánchez, Phys. Rev. B **48**, 6054 (1993).

[18] P.K. Datta and K. Kundu, J. Phys.: Condens. Matter **6**, 4465 (1994).

[19] P.K. Datta and K. Kundu, Phys. Rev. B **51**, 6287 (1995).

[20] M. Wagner, G. Zart, J. Vazquez-Marquez, G. Viliani, W. Frizzera, O. Pilla, and M. Montagna, Philos. Mag. B **65**, 273 (1992).

[21] J.C. Cressoni and M.L. Lyra, Phys. Rev. B **53**, 5067 (1996); J. Phys.: Condens. Matter **8**, L83 (1996).

[22] B. Li, H. Zhao, and B. Hu, Phys. Rev. Lett. **86**, 63 (2001); A. Dhar, *ibid.* **86**, 5882 (2001).

[23] P.L. Garrido, P.I. Hurtado, and B. Nadrowski, Phys. Rev. Lett. **86**, 5486 (2001); A.V. Savin, G.P. Tsironis, and A.V. Zolotaryuk, *ibid.* **88**, 154301 (2002).

[24] A. Dhar, Phys. Rev. Lett. **88**, 249401 (2002); P.L. Garrido and P.I. Hurtado, *ibid.* **88**, 249402 (2002); H.B. Li, Y.H. Wang, and H. Zhao, *ibid.* **89**, 079401 (2002); P.L. Garrido and P.I. Hurtado, *ibid.* **89**, 079402 (2002).

[25] J. Feder, *Fractals* (Plenum, New York, 1988); A. Tsonis, *Chaos: From Theory to Applications* (Plenum, New York, 1992).

[26] S.N. Evangelou and E.N. Economou, J. Phys. A **26**, 2803 (1993).

[27] P. Dean, Rev. Mod. Phys. **44**, 127 (1972).

[28] P.B. Allen and J.L. Feldman, Phys. Rev. B **48**, 12 581 (1993).