Finite size effects in infinitely large electronic systems with correlated disorders

Shinya Nishino, Kousuke Yakubo, and Hiroyuki Shima
Department of Applied Physics, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan
(Received 11 December 2008; published 23 January 2009)

We investigate localization properties of one-dimensional electronic systems with long-range correlated disorders characterized by a power-law spectral density. An abrupt change from extended to gradon states is found to occur in individual samples independently of system sizes. This abrupt change differs from the ordinary Anderson transition in the sense that the former accompanies strong sample fluctuations that remain significant even in the thermodynamic limit. We further observe that sample-averaged quantities such as the inverse participation ratio and the level-spacing distribution exhibit nontrivial crossover behaviors from extended states to gradon states.

DOI: 10.1103/PhysRevB.79.033105 PACS number(s): 72.15.Rn

The role of spatial correlation of disorders in electronic properties of inhomogeneous systems has attracted much interest for the last decade. Successive studies have claimed that one-dimensional electronic systems with long-range correlated disorders exhibit nontrivial behavior distinct from the case of uncorrelated disorders.[1–9] Of special interest is correlated disorders with a power-law spectral density, $S(k) \propto k^{-\alpha}$. This type of correlation is generated by the trace of a fractional Brownian motion[10] and may lead a continuum phase of extended states near the band center when α is larger than a critical value α_c.[1] The presence of the extended phase implies the occurrence of the delocalization transition in one-dimensional systems, which conflicts with the conclusion of the well-established scaling theory of the Anderson transition.[11] The existence of mobility edges in one-dimensional systems has been experimentally observed via microwave transmission spectra of single-mode wave guides[12] and in random dimer superlattices.[13] It has been also argued that the long-range correlation of inhomogeneous potentials in the base sequence of a DNA molecule is responsible for its electronic transport.[14–16]

When the correlation length ξ_d of disorder is much shorter than a system size L, physical quantities are usually self-averaged over many subsystems of size ξ_d. This is due to the assumption that the relative variance of observables converge to zero in the thermodynamic limit. However, this assumption is less obvious for systems with long-range correlated disorders. For $\xi_d \gg L$, quantities observed in an experiment strongly depends on samples. In particular, if ξ_d is such an increasing function of L that satisfies $\xi_d(L) \gg L$ for any L, as in the case of correlated disorders with the power-law spectral density, sample-to-sample fluctuations may survive even in the thermodynamic limit. Therefore, it is necessary to confirm the self-averaging property of observed quantities when we discuss the metal-insulator transition in such systems on the basis of sample-averaged quantities. Nevertheless, many previous studies paid little attention to this issue. In addition, the physical origin of the one-dimensional delocalization transition inconsistent with the scaling theory has not been clarified. It is quite important to resolve the contradiction between numerically observed extended states and the scaling argument. Furthermore, an interpretation of the metal-insulator transition from the viewpoint of the self-averaging property provides deep insight into the nature of electronic states in the disordered system with a long-range correlation.

In this Brief Report, we investigate localization properties of one-dimensional electronic systems with long-range correlated disorders. We treat separately physical quantities obtained in individual samples and those averaged over many samples. It is found that each sample undergoes an abrupt change in the degree of localization, the so-called gradon transition, which differs inherently from the ordinary Anderson transition in systems with uncorrelated disorders. The energy giving rise to the abrupt change largely fluctuates from sample to sample, which shows that the sample fluctuation remains significant however large system size we consider so that finite size effects survive even in the thermodynamic limit. We also observe nontrivial crossover behaviors of sample-averaged quantities such as the inverse participation ratio and the variance of the level-spacing distribution.

Let us consider the one-dimensional tight-binding model described by

$$H = \sum_{n=1}^{N} \varepsilon_n |n\rangle\langle n| - t\sum_{n=1}^{N} (|n\rangle\langle n+1| + |n\rangle\langle n-1|), \qquad (1)$$

where ε_n is the on-site potential at the site n, $|n\rangle$ is the corresponding Wannier basis, and t is the transfer integral between nearest-neighbor sites. Hereafter t is taken to be unity thus fixing the energy scale. The random sequence of $\{\varepsilon_n\}$ is determined by[1]

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

which gives the Fourier transformation of the two-point correlation function of ε_n, namely, the spectral density $S(k)$, proportional to $k^{-\alpha}$. Here, ϕ_k is a random number uniformly distributed in the interval $[0, 2\pi]$, and $C_{N,\alpha}$ is a constant characterizing the strength of disorder. In this work, we fix $\alpha = 4.0$ and the value of $C_{N,\alpha}$ so as to yield $\langle \varepsilon_n^2 \rangle = 0.2$. Typical on-site energy landscapes are shown in Fig. 1. Although actual one-dimensional electronic systems with correlated disorders can be found as we mentioned, the present model has a weak direct relevance to realistic systems due to the

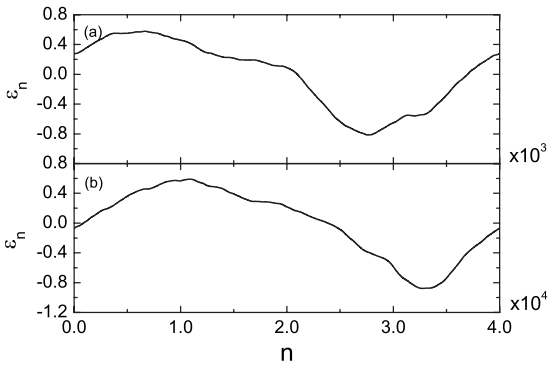

FIG. 1. Typical on-site energy landscapes described by Eq. (2) with (a) $N=4000$ and (b) $N=40\,000$. Parameters are set to be $\alpha=4.0$ and $\langle\varepsilon_n^2\rangle=0.2$.

N-dependent $C_{N,\alpha}$ in Eq. (2). Nevertheless, understanding electronic states in this system is crucial to clarify whether the scaling theory of the Anderson transition should be revised due to the existence of extended states in disordered one-dimensional systems.

In order to examine spatial extents of eigenstates, we numerically calculate the eigenfunction $\psi(n,E)$ belonging to energy E by diagonalizing Hamiltonian (1). The degree of the extent of $\psi(n,E)$ is evaluated by the inverse participation ratio (IPR) (Refs. 17 and 18) defined by

$$I(E,N)=\sum_{n=1}^{N}|\psi(n,E)|^4, \tag{3}$$

which is proportional to $1/N$ for extended states while constant for localized states. Figure 2 shows the energy dependences of $I(E,N)$ for $N=4000$. We have the same profile of $I(E,N)$ for negative E. Three plots correspond to different realizations of random-potential sequences $\{\varepsilon_n\}$. The constant region near the band center ($E\lesssim 1.0$) indicates the continuum extended phase, and the moderate increase after a sharp peak

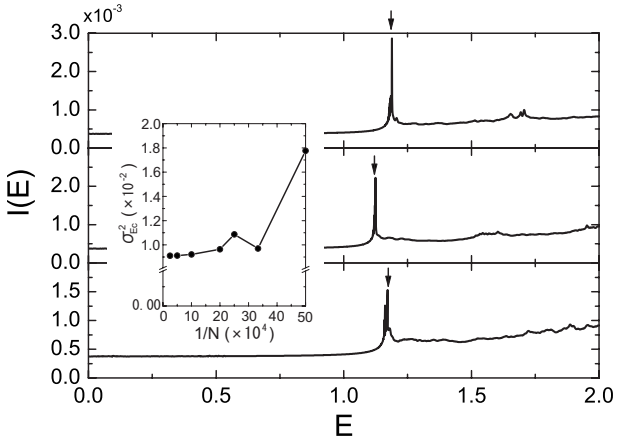

FIG. 2. Energy dependence of the inverse participation ratio $I(E,N)$ for three different realizations of random potentials. The system size is $N=4000$. Sharp peaks indicated by arrows give the transition points. The inset shows the system-size dependence of the variance of the mobility edge E_c.

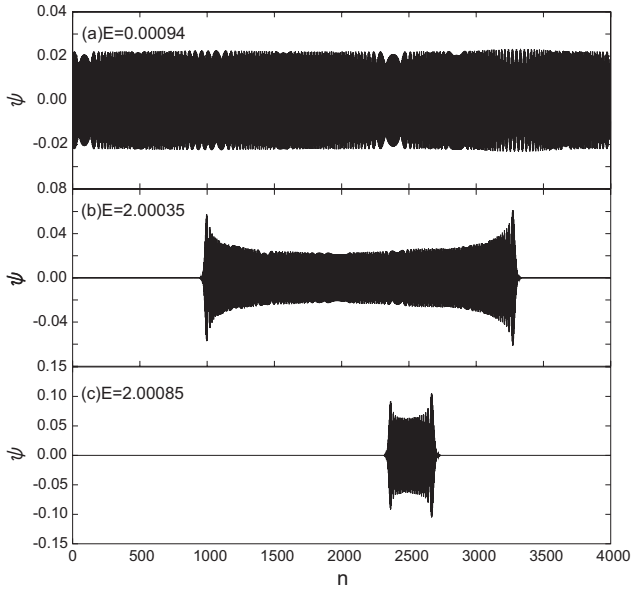

FIG. 3. Spatial profiles of eigenmodes in correlated disordered systems. The eigenmodes (a) and (b) are excited in the same realization of random potentials, while (c) is prepared in a different random-potential configuration. The profiles of (b) and (c) are quite different though these belong to almost the same energy.

at around $E\sim 1.0$ implies the existence of localized states. These results are consistent with the previous work by Russ *et al.*[4] showing the presence of extended states within $|E|\lesssim 1.25$ for $\alpha=4.0$ and $\langle\varepsilon_n^2\rangle=0.2$. We see from Fig. 2 that the localized phase is always separated from the extended phase by the sharp peak of I. We thus define the value of the mobility edge E_c for each sample by the energy giving the sharp peak of $I(E,N)$, whose validity will be proven later.

Figures 3(a) and 3(b) illustrate typical spatial profiles of extended and localized eigenstates, respectively, under the same numerical conditions as those for Fig. 2. The localized mode exhibits a butterflylike form, which totally differs from exponentially localized modes excited in systems with uncorrelated disorders. Such unusual localized modes have been earlier found in graded elastic systems, in which masses or force constants gradually change in a uniaxial direction.[19–22] Butterflylike localized modes in graded lattices are referred to as "gradons," identified with a special kind of light-mass-impurity vibration modes. Intriguingly, graded lattices can exhibit a sharp transition from gradons to extended phonons even in one dimension. In this context, the abrupt change in the localization length in our system can be considered as a sort of the gradon transition.

The similarity between profiles of elastic gradon and our localized modes is not fortuitous because of the following three reasons. First, the potential landscape of the present electron system depicted in Fig. 1 is quite similar to that of graded elastic systems. Second, amplitudes $|\psi(n,E)|$ of a localized electronic mode concentrate onto the region with small (large for holes) ε_n, similar to the case of elastic gradons whose vibrational amplitudes are confined into light-mass regions. Finally, as shown in Fig. 4, the system-size dependence of the sample-averaged IPR $\langle I(E,N)\rangle$ for localized states is described by $\langle I\rangle=(c_1+c_2\log N)/N$ as same as

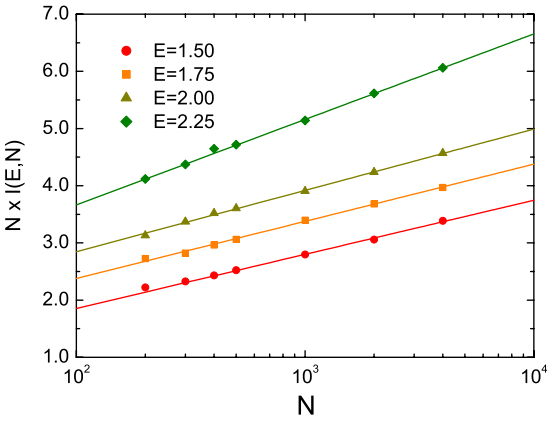

FIG. 4. (Color online) System-size dependence of the inverse participation ratio $I(E,N)$ for various energies. The functional form coincides with that of elastic gradon states (see text).

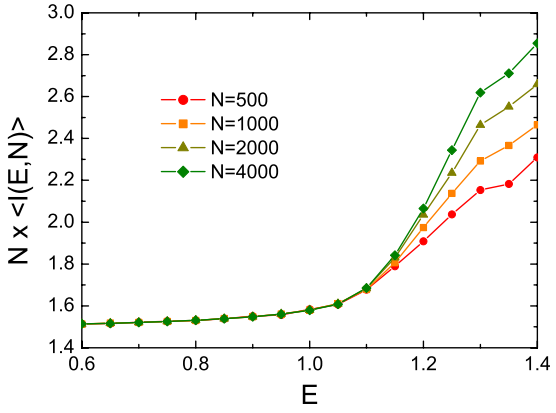

FIG. 5. (Color online) Sample-averaged inverse participation ratio $\langle I(E,N)\rangle$ multiplied by system size N.

those for elastic gradons.[23] We thus conclude that our localized states observed above $|E|\sim 1.0$ are identified with gradons in electron systems. It further follows from Fig. 2 that spatial extents ξ of gradons increase with decreasing $|E|$, and then reaching the system size N at a characteristic energy E_c. This consequences that each sample undergoes the delocalization-gradon transition at E_c. Since immediately above (or just at) E_c, the cusps of $|\psi(n)|$ at the both ends of the butterflylike mode are magnified drastically, $I(E)$ yields a sharp peak just at the transition energy E_c as shown in Fig. 2.

It should be emphasized that the delocalization-gradon transition at E_c differs inherently from the conventional Anderson transition. The latter transition stems from quantum interference due to diffusive scattering in random media, while the gradon transition results from the quantum confinement within low-ε_n (high ε_n for holes) region in a coarse-grained landscape of long-range correlated potentials. The way of the confinement strongly depends on potential profiles as shown in the comparison of Figs. 3(b) and 3(c) and cannot be characterized by the single length scale. Thus, the scaling theory is no longer available for describing the gradon transition.

Another important feature of our electron system is that the finite size effect on localization properties survives however large system size we take. This feature is manifested by the nonvanishing variance $\sigma^2_{E_c}$ of the mobility edge E_c. The inset of Fig. 2 shows the N dependence of $\sigma^2_{E_c}$ evaluated from 100 different realizations of random potentials $\{\varepsilon_n\}$. The nonvanishing $\sigma^2_{E_c}$ at larger N results from the lack of self-averaging properties, attributed to the self-affine character of correlated random potentials given by Eq. (2). It indeed follows from Figs. 1(a) and 1(b) that the coarse-grained profile of the potential sequence for N=4000 is not very different from that for N=40 000, implying the divergent correlation length of disorders. This unusual similarity between Figs. 1(a) and 1(b) is a consequence of the size-dependent $C_{N,\alpha}$ in Eq. (2). Accordingly, large fluctuations in E_c remain significant even in the thermodynamic limit.

All results presented above are associated with individual samples with different random-potential sequences. The absence of the self-averaging property distinguishes physical quantities in infinite individual systems from sample-averaged ones. This is demonstrated for the energy-dependence of the averaged IPR $\langle I(E,N)\rangle$ depicted in Fig. 5, where the average is taken over 100 samples. The averaged IPR shows no sharp peak at around $E=1.0$ in contrast to the IPR for individual samples. There is, however, a smooth change from the extended behavior below $E=1.0$ to the localized one for $E\gg 1.0$. It should be noted that the energy dependence of the averaged IPR showing the smooth crossover ($0.9\lesssim E\lesssim 1.1$) does not depend on the system size N, which implies the crossover behavior even in the thermodynamic limit.[24] Such a crossover behavior of electronic states has been more clearly found in the level-spacing distribution $P(s)$ for many samples, where s is the nearest-neighbor level spacing rescaled by the averaged spacing $\langle s\rangle$. The random matrix theory states that $P(s)$ should be the Wigner distribution for extended states and the Poissonian distribution for localized states,[25] where the theory assumes that disorders are spatially uncorrelated. Therefore, $P(s)$ for the present system deviate from these two distribution functions as shown in the inset of Fig. 6.[26,27] However, the functional

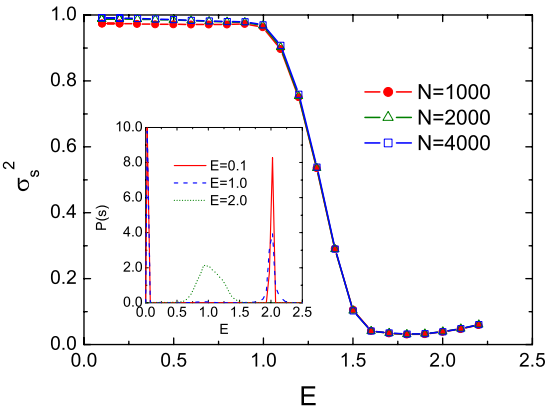

FIG. 6. (Color online) Energy dependence of the variance of the level-spacing distribution $P(s)$ for various system sizes N. For a given E, we use $0.05N$ eigenvalues around E. The number of samples is chosen so that the total number of eigenvalues become no less than 1×10^5. The unfolding procedure is applied to eliminate the energy dependence of the mean level-spacing (Ref. 28). The inset shows functional forms of $P(s)$ for various energies.

form of $P(s)$ reflects spatial extents of wave functions as in the uncorrelated case. In order to characterize the E dependence of $P(s)$, we plot in Fig. 6 the variance $\sigma_s^2(E)$ of the level spacing defined by $\sigma_s^2 \equiv \int_0^\infty (s-\langle s\rangle)^2 P(s)ds$. The value of σ_s^2 for extended states is close to unity, while it becomes very small in the gradon region. Notably, all data for different N's are collapsed onto a single smooth curve, showing a crossover from the extended to the localized gradon regions even for infinitely large system size. This is contrast to a transition behavior where σ_s^2 tends to drop sharply at E_c as increasing N. Our result assures again that considerably large sample fluctuations peculiar to the present system retain the finite size effect even in the thermodynamic limit.

In conclusion, we studied numerically electronic states in one-dimensional systems with long-range correlated disorders. For individual disordered systems, we found the abrupt change in electronic states from extended states around the band center to gradon states near the band edge, which is identified with the delocalization-gradon transition. Due to the lack of the universality of the gradon transition, the existence of the delocalization transition does not conflict with the scaling theory. The transition energy fluctuates from sample to sample even in the thermodynamic limit because the present system does not possess the self-averaging property due to an infinite correlation length of disorder. This remarkable feature is also supported by behaviors of the sample-averaged IPR and $P(s)$. These quantities clearly show the crossover (not the transition) from the extended region ($|E| \lesssim 1.0$) to the gradon region ($|E| \gtrsim 1.0$) independently of the system size. Since sample fluctuation and crossover behavior are intrinsic nature of finite size systems, we conclude that the finite size effect survives in the thermodynamic limit of one-dimensional electron systems with long-range correlated disorders.

We would like to thank T. Nakayama, M. Goda, and K. W. Yu for useful discussions. Numerical calculations were performed partially on the HITACHI SR-11000 of Supercomputer Center, Institute for Solid State Physics, University of Tokyo. This work was supported in part by a Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science (Grants No. 18760059, No. 19560001, and No. 19360042) and for the 21st Century COE Program, entitled "Topological Science and Technology," from the Ministry of Education, Culture, Sport, Science and Technology of Japan (MEXT).

[1] F. A. B. F. de Moura and M. L. Lyra, Phys. Rev. Lett. **81**, 3735 (1998).
[2] J. W. Kantelhardt, S. Russ, A. Bunde, S. Havlin, and I. Webman, Phys. Rev. Lett. **84**, 198 (2000).
[3] F. A. B. F. de Moura and M. L. Lyra, Phys. Rev. Lett. **84**, 199 (2000).
[4] S. Russ, J. W. Kantelhardt, A. Bunde, and S. Havlin, Phys. Rev. B **64**, 134209 (2001).
[5] F. A. B. F. de Moura, M. D. Coutinho-Filho, E. P. Raposo, and M. L. Lyra, Phys. Rev. B **68**, 012202 (2003).
[6] H. Shima, T. Nomura, and T. Nakayama, Phys. Rev. B **70**, 075116 (2004).
[7] H. Cheraghchi, S. M. Fazeli, and K. Esfarjani, Phys. Rev. B **72**, 174207 (2005).
[8] T. Kaya, Eur. Phys. J. B **55**, 49 (2007).
[9] I. F. dos Santos, F. A. B. F. de Moura, M. L. Lyra, and M. D. Coutinho-Filho, J. Phys.: Condens. Matter **19**, 476213 (2007).
[10] J. Feder, *Fractals* (Plenum, New York, 1988).
[11] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).
[12] U. Kuhl, F. M. Izrailev, A. Krokhin, and H. J. Stöckmann, Appl. Phys. Lett. **77**, 633 (2000).
[13] V. Bellani, E. Diez, R. Hey, L. Toni, L. Tarricone, G. B. Parravicini, F. Dominguez-Adame, and R. Gomez-Alcala, Phys. Rev. Lett. **82**, 2159 (1999).
[14] P. Carpena, P. Bernaola-Galvan, P. C. Ivanov, and H. E. Stanley, Nature (London) **418**, 955 (2002).
[15] V. M. K. Bagci and A. A. Krokhin, Chaos, Solitons Fractals **34**, 104 (2007).
[16] A.-M. Guo, Phys. Rev. E **75**, 061915 (2007).
[17] S. Yoshino and M. Okazaki, J. Phys. Soc. Jpn. **43**, 415 (1977).
[18] F. Wegner, Z. Phys. B **36**, 209 (1980).
[19] J. J. Xiao, K. Yakubo, and K. W. Yu, Phys. Rev. B **73**, 054201 (2006).
[20] J. J. Xiao, K. Yakubo, and K. W. Yu, Phys. Rev. B **73**, 224201 (2006).
[21] J. J. Xiao, K. Yakubo, and K. W. Yu, J. Phys. Soc. Jpn. **76**, 024602 (2007).
[22] J. J. Xiao, K. Yakubo, and K. W. Yu, J. Phys.: Condens. Matter **19**, 026224 (2007).
[23] M. J. Zheng, M. Goda, K. Yakubo, and K. W. Yu (unpublished).
[24] If we had the transition at a certain energy E_c, the quantity $N\langle I\rangle$ for $E<E_c$ should be a decreasing function of the system size N while it for $E>E_c$ should be an increasing function of N.
[25] M. L. Metha, *Random Matrices* (Academic, Boston, 1990).
[26] P. Carpena, P. Bernaola-Galvan, and P. C. Ivanov, Phys. Rev. Lett. **93**, 176804 (2004).
[27] H. Shima, S. Nishino, and T. Nakayama, J. Phys.: Conf. Ser. **92**, 012156 (2007).
[28] Y. Ono, H. Kuwano, K. Slevin, T. Ohtsuki, and S. Havlin, J. Phys. Soc. Jpn. **62**, 2762 (1993).