Quantitative measure of the electron localization in disordered systems with long-range hopping

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Exact numerical solution of a chain of 340 atoms has been obtained to study the electron localization in a disordered system with long-range hopping. The moment and the inverse participation ratio are calculated to check the electron localization and then compared with the end component ratio. In contrast to the random system with short-range hopping, we discover that the states in the bulk part of the density of states are mostly localized while those in the tail are mostly extended.

Although much is known concerning the qualitative feature of electron localization in disordered systems, a quantitative measure of the electron localization in bulk systems which requires the knowledge of eigenstates is an almost impossible task. With sophisticated computational technique applied to finite disordered systems, quantitative investigations on the electron localization have been carried out by many authors.[1–9] Most of these works study the Anderson model with short-range hopping. Recently, the Anderson model with long-range hopping has been investigated by Day and Martino[10] and by Ching and Huber.[11]

The density of states (DOS) of a disordered system, as compared to that of a regular one, is characterized by the irregular structure in the bulk part of the DOS and the presence of tails the states in which are localized. While these features are well established for disordered systems with short-range hopping, disordered systems with long-range hopping (LRH) may behave rather differently. For example, the states in the low-energy tails of the DOS obtained by Day and Martino[10] (DM) and Ching and Huber[11] (CH) are mostly extended states.

In this paper we will present the results of a quantitative measure of the electron localization in a finite chain with LRH. Let us consider the tight-binding Hamiltonian for a one-dimensional system

$$H=\sum_{i=1}^{N}|i\rangle\epsilon_i\langle i|+\sum_{i\neq j}^{N}|i\rangle t_{ij}\langle j|, \tag{1}$$

where the basis functions $|i\rangle$ are assumed to be orthonormal. DM have used a power-law LRH

$$t_{ij}=-\frac{2}{|i-j|+1}$$

for $|i-j|\leq M$ and $t_{ij}=0$ otherwise. On the other hand, CH have assumed an exponential law LRH

$$t_{ij}=-t_0\exp(-\alpha|i-j|)$$

and constant ϵ_i.

Before introducing the random character to the site energy ϵ_i, it will be helpful to analyze a periodic chain. For given value of the cutoff M in the power-law LRH or the value α in the exponential law LRH, the tight-binding energy band $E(k)$ of an infinite chain $N\rightarrow 0$ can be derived easily. Figure 1 shows the $E(k)$ in the first Brillouin zone for the power law LRH with $M=2$, 3, 4, 5, 6, 8, 11, and 15. Because of the symmetry, for each value of M the $E(k)$ is plotted in half of the first Brillouin zone. The two insets illustrate the $E(k)$ and the corresponding density of states for $M=5$ and 6, respectively. The DOS exhibits rich structures and a long tail. The formation of the long tail is due to the long-range hopping, as can be detected from the figure in which the tail grows with increasing value of M. When disorder is introduced into the system, if the disorder is not strong enough, it will not be able to localize the states in the tail. This is the reason why DM and CH found extended states in the DOS tails in their calculations.

Since exact solutions of disordered chains can be obtained only for finite-chain length, it will help our future discussions if we know the characteristic features of a finite periodic chain. Figure 2 shows a series of DOS of a chain of 340 atoms with the power-law LRH. The corresponding value of M for each DOS is marked at the left end. For $M\geq 6$, we see tuning-fork structures appear. The origin of such structure can be traced back from the $E(k)$ in Fig. 1. Each $E(k)$ curve starts at $k=0$ with a minimum and then oscillates toward the zone boundary. If the lth local maximum counting from $k=0$ is lower than the $(l+2)$th local minimum, then a tuning-fork structure occurs. Once the μth local maximum gets higher than the $(\mu+2)$th local

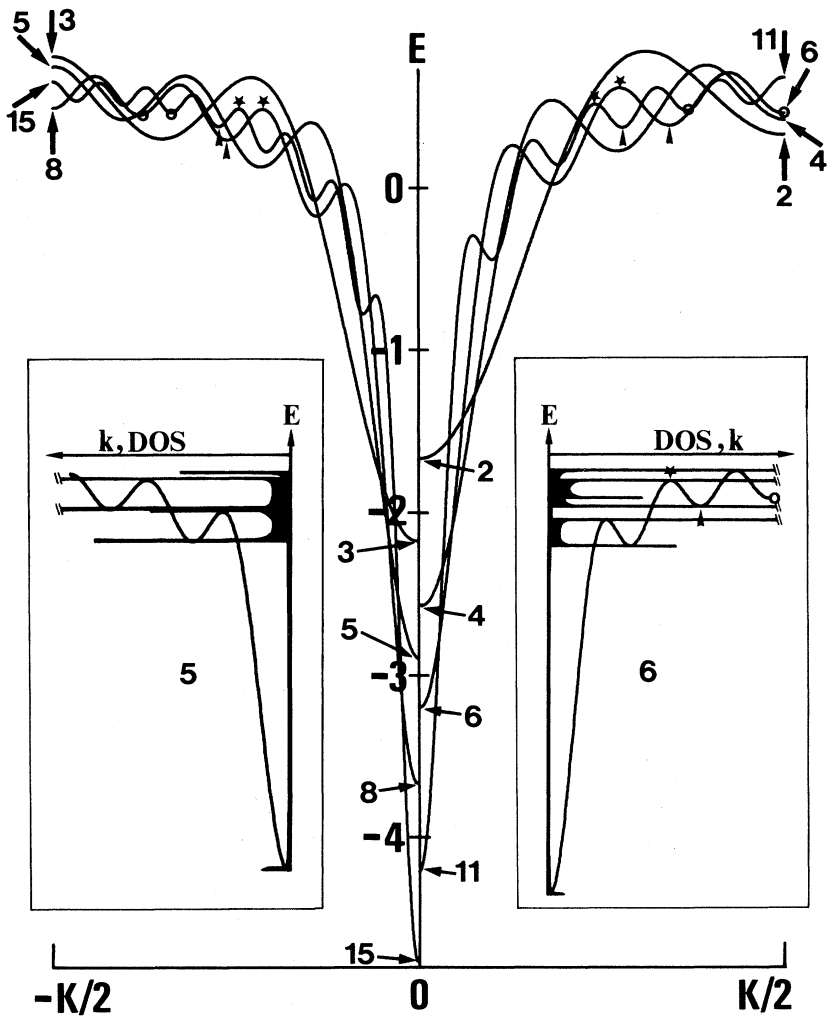

FIG. 1. Band energy $E(k)$ of an infinite periodic chain with the power-law long-range hopping. Each curve corresponds to a maximum hopping range (M value) marked by the number. Insets are the density of states.

minimum, from there on there is no more tuning-fork structure. Such specific μth local maximum and $(\mu+2)$th minimum of each $E(k)$ curve are marked in Fig. 1 with a star and a circle, respectively. The energy corresponding to the k vector indicated by an arrow head in Fig. 1 is defined as the threshold energy. For an infinite periodic chain with given value of M, the number of tuning-fork structures, the value of the threshold energy, and the corresponding threshold k vector can be derived analytically. Table I lists the results for M up to 40.

A chain of 340 atoms is almost the largest system an ordinary computer (for example, DEC10 or IBM370) can solve exactly, not only to solve for eigenenergies but also for eigenstates of a disordered system without specific restrictions. Usually, exact numerical solutions are obtained for a disordered system containing less atoms. The DOS similar to those in Fig. 2 are shown in Fig. 3 for a periodic chain of 160 atoms. Although the general structures still remain when the number of atoms decreases from 340 to 160, the DOS for $6 \leq M \leq 15$ have the characteristic features of a disordered chain, except for the sharp edge at the high-energy end. Such features are introduced artificially by the cutoff of the LRH at $|i-j|=M$, but disappear if $M=100$ for which the hopping t_{ij} for $|i-j|>M$ is already negligibly small. We can demonstrate this point

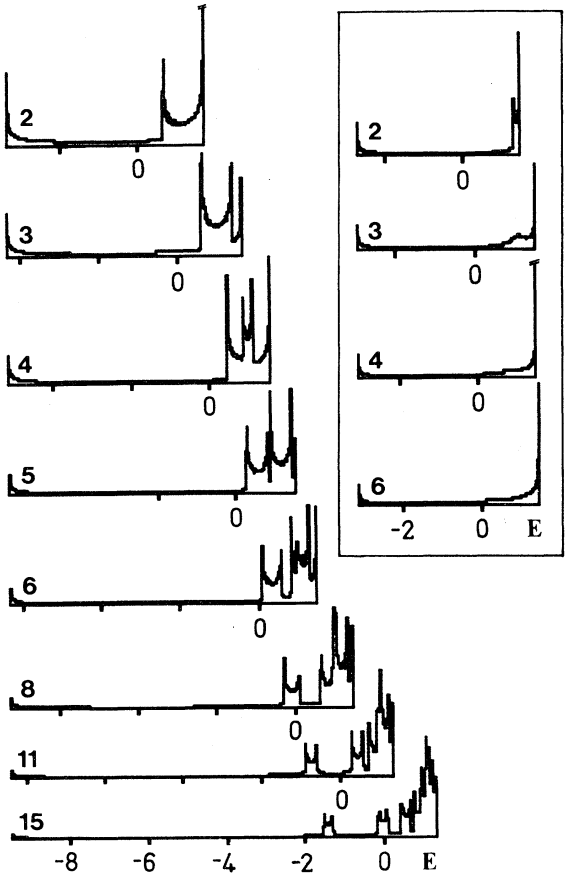

FIG. 2. Numerical solutions of the DOS for a finite periodic chain of 340 atoms with the power-law long-range hopping. Inset is the DOS of the same chain but with the exponential law LRH.

more clearly by considering the exponential law LRH $t_{ij} = -\exp(-|i-j|)$. The so obtained DOS are shown as insets in Fig. 2 for $N = 340$ and in Fig. 3 for $N = 160$. In this case, the irregular structures in the DOS can be detected only for $M < 4$.

By now it is obvious that if one investigates numerically a finite disordered system with LRH, the DOS gives very little information. It is necessary to have a quantitative measure on the localization of each eigenstate. One quantitative measure is the inverse participation ratio (IPR) which was introduced by Bell *et al.*[1] and has been used by Ching[9] and CH.[11] On the other hand, DM (Ref. 10) has used the end component ratio (ECR) to measure the electron localization. In this paper, in addition to the IPR and the ECR we will perform the moment analysis to check the electron localization in a random system with LRH.

We must first show that the disordered chain we are going to investigate is long enough to yield reliable results. Figure 4 demonstrates a series of DOS for a periodic chain with the power-law LRH. The LRH is cut off at $M = 4$, and the number of atoms N for each DOS is marked next to the plot. Similar results are given in Fig. 5 for the exponential law LRH with

$$t_{ij} = -\exp(-|i-j|).$$

We see that the results begin to converge when N increases to 160.

In order to compare our result with that of DM, we will introduce the same types of disorder in the site energy ϵ_i as DM have done. For the first case of uniformly (U) distributed disorder, ϵ_i is a random number distributed uniformly on the interval (-1, 1).

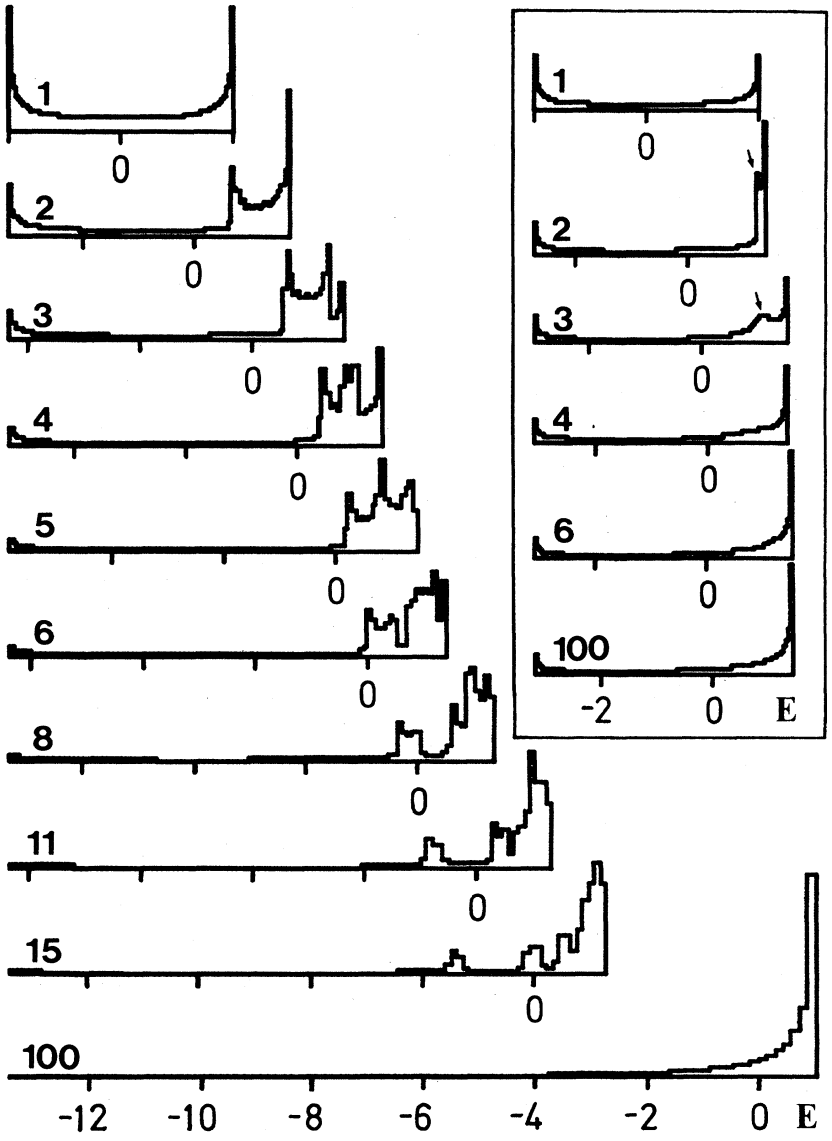

FIG. 3. Same as in Fig. 2 but for a chain of 160 atoms.

For the second case of percolation (P) distribution, ϵ_i can be either -0.9 or 0.9 and are distributed randomly. We consider both the power-law LRH

$$t_{ij} = -\frac{2}{|i-j|+1}$$

with $M=4$, and the exponential law LRH

$$t_{ij} = -\exp(-|i-j|)$$

with the same cutoff at $|i-j|=4$. Finally, two different chain lengths are studied: a long chain of 340 atoms and a shorter chain of 160 atoms.

The normalized eigenstates can be expressed as

$$|\Psi_i\rangle = \sum_{j=1}^{N} B_{ji} |j\rangle \tag{2}$$

and the corresponding IPR is defined as

$$\mathcal{R}_i = \sum_{j=1}^{N} |B_{ji}|^4. \tag{3}$$

If we take the nearest-neighbor distance along the chain as the unit of length, then the second moment

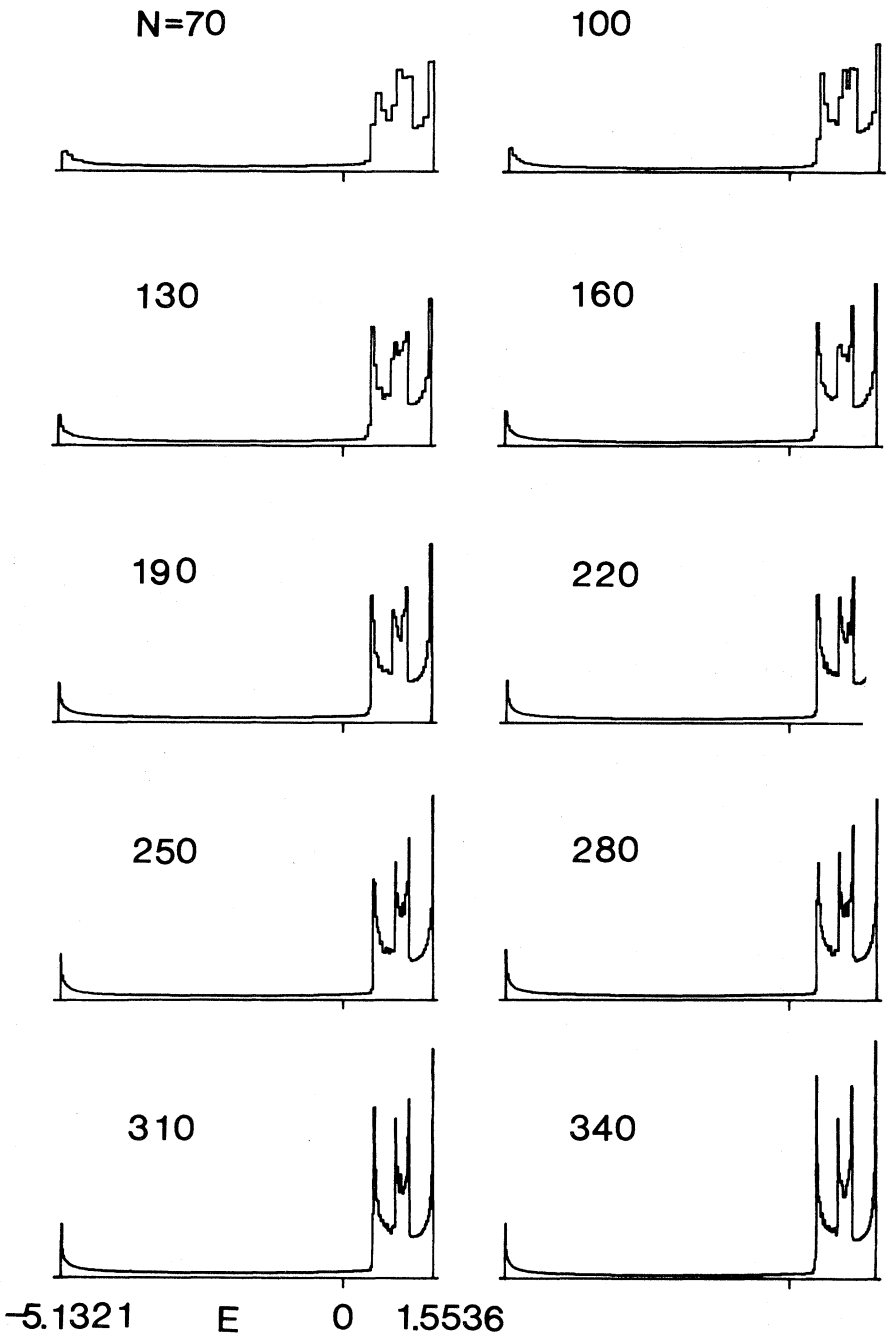

FIG. 4. DOS of a periodic chain with the power-law LRH. The number of atoms in the chain for each DOS is indicated by the number. The maximum range of hopping is $M=4$.

can be defined as

$$\mathscr{L}_i=\frac{1}{N}\left[\sum_{j=1}^{N} j^2 |B_{ji}|^2-\left[\sum_{j=1}^{N} j |B_{ji}|^2\right]^2\right]^{1/2}. \tag{4}$$

The second moment and the IPR will then be used to measure the localization of the eigenstate $|\Psi_i\rangle$.

The numerical results are shown in Fig. 6 for the case of power-law LRH and in Fig. 7 for the case of exponential law LRH. In each figure the left

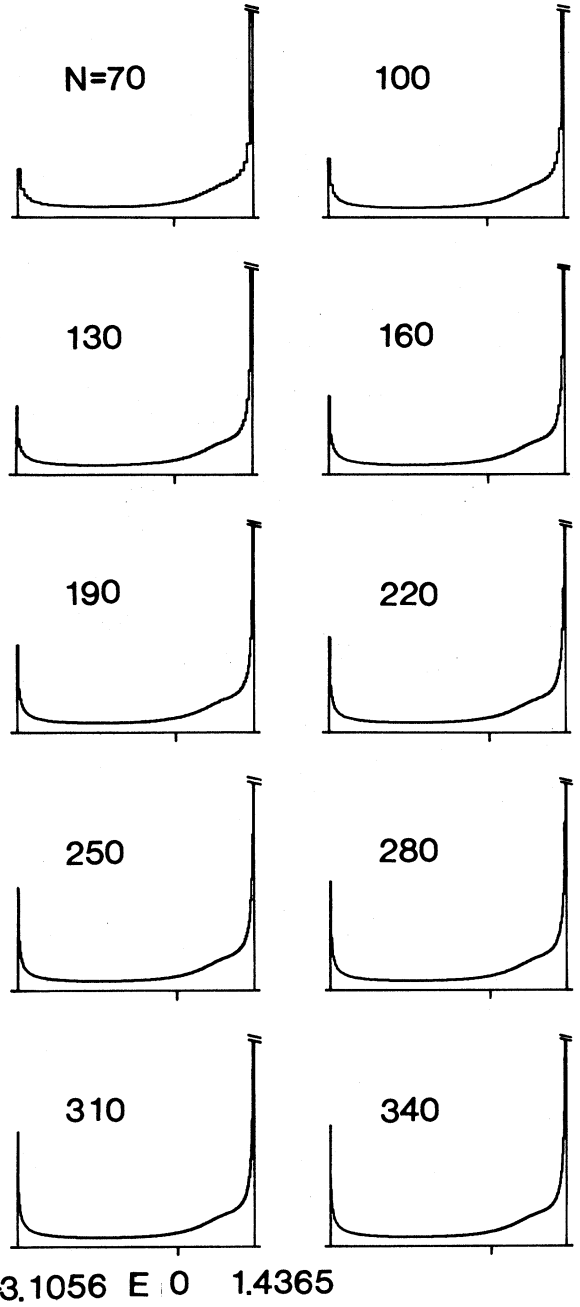

FIG. 5. Same as in Fig. 4 but for the exponential law LRH.

TABLE I. Threshold energy E and the threshold k vector (the point marked by an arrow head in Fig. 1) for given maximum range of hopping M (column under "neighbor"). The number of tuning-fork structures in the DOS is given by the number in the last column under "N."

Neighbor	k vector	Threshold E	N
5	1.0000		0
6	1.0000	0.404 05	1
7	0.8650	0.360 37	1
8	0.7620	0.310 54	1
9	0.8940	0.442 81	2
10	0.8080	0.412 52	2
11	0.7370	0.379 13	2
12	0.6770	0.343 84	2
13	0.7760	0.441 48	3
14	0.7220	0.416 36	3
15	0.6750	0.389 93	3
16	0.6340	0.362 58	3
17	0.7130	0.439 75	4
18	0.6740	0.418 70	4
19	0.6390	0.396 90	4
20	0.6080	0.374 60	4
21	0.6730	0.438 31	5
22	0.6430	0.420 24	5
23	0.6160	0.401 79	5
24	0.5900	0.383 05	5
25	0.6460	0.437 26	6
26	0.6220	0.421 41	6
27	0.5990	0.405 37	6
28	0.5780	0.389 20	6
29	0.6260	0.436 37	7
30	0.6060	0.422 32	7
31	0.5860	0.408 13	7
32	0.5680	0.393 79	7
33	0.6110	0.435 70	8
34	0.5940	0.423 15	8
35	0.5770	0.410 43	8
36	0.5610	0.397 55	8
37	0.5990	0.435 00	9
38	0.5840	0.423 59	9
39	0.5690	0.412 24	9
40	0.5550	0.400 75	9

column is for the longer chain $N=340$, while the right column is for the shorter chain $N=160$. Each column is divided into three parts: The three plots at the bottom marked by S are for the periodic straight chain, the three plots at the middle marked by U are for the uniformly distributed disorder, and the three plots at the top marked by P are for the percolation distribution of the disordered-site energy. For the periodic chain, both the IPR and the moment are typical for extended state. However,

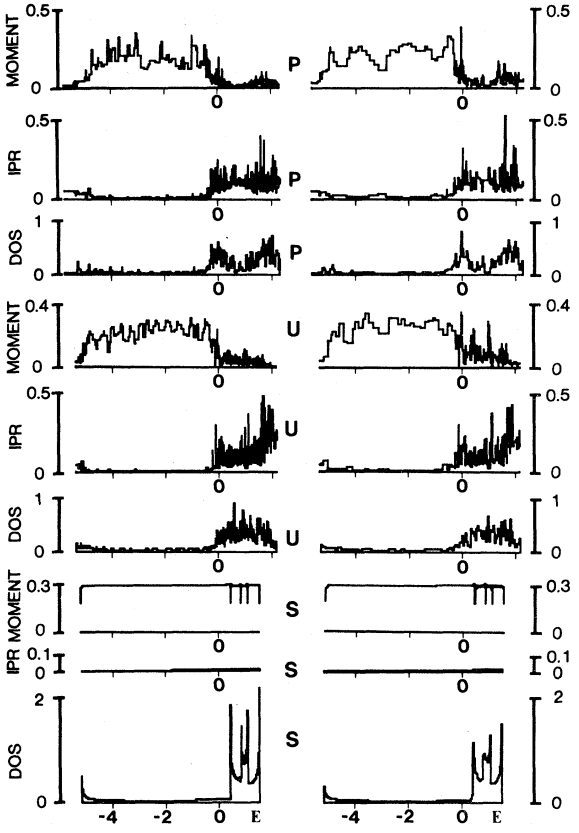

FIG. 6. DOS, IPR, and moment of a periodic chain (S), a disordered chain with uniformly distributed random-site energy (U), and a disordered chain with the percolation distribution of the random-site energy. The long-range hopping is of the power-law type with the maximum range $M=4$. Left column is for a chain of 340 atoms and the right column is for a chain of 160 atoms.

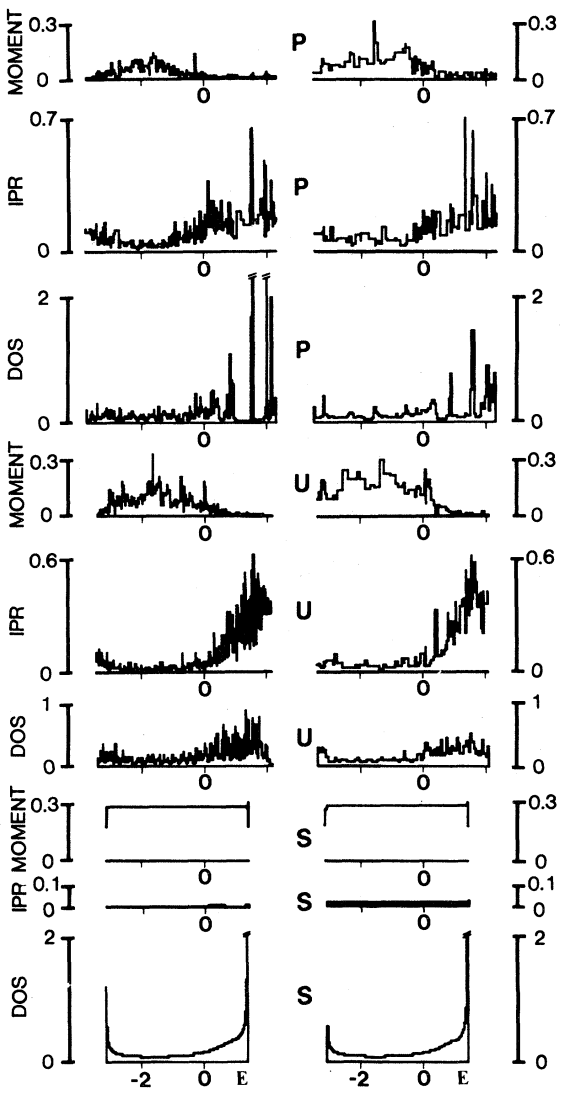

FIG. 7. Same as in Fig. 6 but for the exponential law LRH.

when the system becomes disordered for both the U case and the P case, the moment analysis and the IPR result consistently indicate that the states in the bulk part of the density of states are more localized than those in the band tail. This phenomenum is opposite to what one finds in random systems with short-range hopping.

Day and Martino[10] have developed a technique based on the ideas of Herbert and Jones[2] to obtain the end component ratio $G1/G2$ for the eigenstates in some energy region. The ECR can be considered as an approximated value of $|B_{1j}/B_{Nj}|^2$ where j labels one eigenstate with the corresponding eigenenergy lying in this energy region. Since DM can obtain the ECR without solving for the eigenstates, they can study a much longer chain of 1000 atoms. Their results are reproduced in Fig. 8 for the periodic chain (marked as S), the uniformly distributed disorder (marked by U), and the percolation distribution of the random-site energy (marked by P). We should notice that in Fig. 8 $G1/G2$ is plotted in the logarithmic scale. Then, if we compare Fig. 8 to the three moment curves in the left column of Fig. 6, again we see that the ECR, the IPR, and the mo-

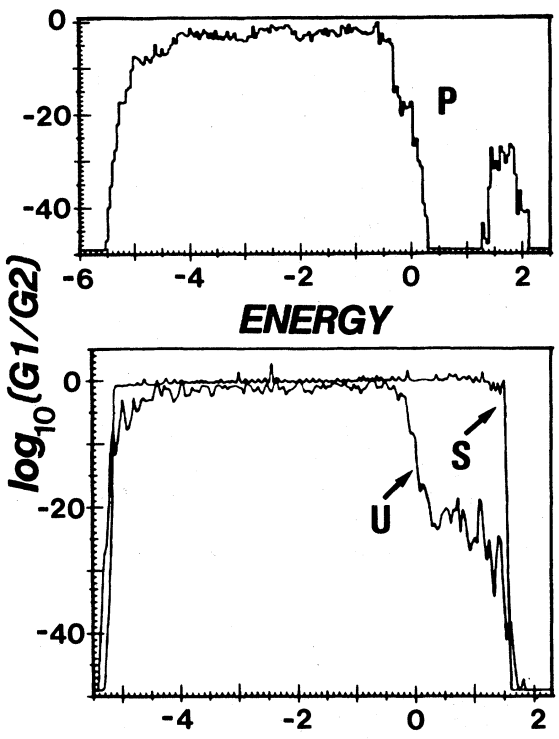

FIG. 8. End component ratio as a measure of the localization (from Ref. 10).

ment analysis give the similar qualitative feature of the electron localization characteristic to the long-range hopping.

To close this paper, we should emphasize that in a system with LRH, the DOS itself is too complicated to tell whether the system is ordered or random. The most important feature in a random system with LRH, as clearly shown in Figs. 6 and 7, is that the states in the bulk part of the DOS are mostly localized while the states in the tail are mostly extended. This is just the opposite of the localization property in a random system with short-range hopping. A similar result has been obtained by Ching and Huber[11] in a three-dimensional system where the site energy is constant and the disorder is introduced with the random placement of the atoms (random long-range hopping). In a system with short-range hopping, the band tail is caused by the disorder effect which also tends to localize the states. On the other hand, in a system with LRH the band-tail formation has its origin in the long-range hopping in the absence of disorder. The long-range hopping makes the electrons in the tail states extremely mobile. Therefore, extremely strong disorder is needed to localize such mobile electrons in the band tail.

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