

## Coarse-Grained Quantities and Local Environment Effects in Disordered Systems. II

— A Refined Effective Distance —

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Existence of a refined effective "distance"  $\bar{m}(\epsilon + i\Gamma)$  ( $\epsilon$ ; energy,  $\Gamma$ ; degree of coarse-graining) is conjectured in infinite systems to measure, more precisely than the effective "distance"  $\bar{m}(E)$  ( $E = \epsilon + i\Gamma$ ) does, the contribution of local environment around the sites  $l$  and  $l'$  to the Green function  $G_{l,l'}(E)$ . The effective "distance"  $\bar{m}(E)$  is numerically observed in some simple finite sample systems of 1-, 2- and 3-dimension. If the quantity  $2\bar{m}(E)$  exists, it is expected to be an analytic continuation of the localization length  $l(\epsilon)$  on the upper half of the complex energy plane.

### § 1. Introduction

Any quantity observed with instruments is more or less coarse-grained and the coarse-graining is related to throwing away some information of the system  $H$  under observation. What kind of information of  $H$  do we need and what kind of information can we throw away when, contrary to the above, some accuracy (degree of coarse-graining) is required to a quantity? We have known very little on the detailed relation between the degree of coarse-graining and the information of the system we need or the information we can throw away, although we have a lot of good examples<sup>1)~6)</sup> which suggest that a local character of the system determines the approximated (coarse-grained) quantities.

In a previous paper<sup>7)</sup> (hereafter referred to as I) we discussed the above-mentioned relation about quantities derived from the one-particle Green function. The coarse-grained quantities, with respect to energy  $\epsilon$  by  $\Gamma$  (degree of coarse-graining), are derived from the coarse-grained Green function  $G(E) \equiv (H - E)^{-1}$  with the complex energy  $E \equiv \epsilon + i\Gamma$ . We proved the existence of the effective "distance"  $\bar{m}(E)$ , which was a measure of the range of local environment of the system which determined the coarse-grained quantities for given  $\epsilon$  and  $\Gamma$ , in a disordered system of any desired dimension described by a bounded Hamiltonian

$$H = \sum_l^{N_0} |l\rangle \epsilon_l \langle l| + \sum_{l \neq l'} |l\rangle t_{l,l'} \langle l'| \quad (1.1)$$

with short-range interaction. The proof was a generalization of Matsuda's one<sup>8)</sup> on a linear chain model with nearest-neighbour interaction. This guaranteed that the Green function  $G_{l,l'}(E) \equiv \langle l|G(E)|l'\rangle$ , decayed exponentially with the decaying factor  $1/(2\bar{m}(E))$  for increasing  $m(l, l')$  (a "distance" between the sites  $l$  and  $l'$  defined in I) and that the value of  $G_{l,l'}(E)$  was essentially determined by the local environment of  $H$  of the range  $\bar{m}(E)$  around the sites  $l$  and  $l'$ . More precisely,

$$(1) \quad |G_{l,l'}(E)| \leq \min\{|G_{l,l}(E)|, |G_{l',l'}(E)|\} \\ \times (\bar{m}(E)/(1 - \exp\{-1/\bar{m}(E)\}))^{1/2} \\ \times \exp\{-m(l, l')/2\bar{m}(E)\}.$$

(2) The contribution of (the matrix elements of)  $H$  outside two spheres, centered by  $l$  and  $l'$  with a radius  $n \times \bar{m}(E)$ , to the value of  $G_{l,l'}(E)$  was less than  $C/\exp\{n\}$  ( $C$ ; some constant) for any  $n > 0$ .

The "distance"  $\bar{m}(\varepsilon + i\Gamma)$  would be a monotonically increasing function with decreasing  $\Gamma$ , because less coarse-grained Green function needs more information of the environment.

When we introduce a set of orthonormalized bases  $\{|n\rangle, n=1, 2, \dots, N \leq N_0\}$  starting from an arbitrary state  $|1\rangle$  by recursion method,<sup>(9,6)</sup> the Green function satisfies the following equation in this new representation in the subspace  $\{|n\rangle\}$  (see I in detail)

$$\beta_n^- G_{n-1,n'}(E) + (\alpha_n - E) G_{n,n'}(E) + \beta_n^+ G_{n+1,n'}(E) = \delta_{n,n'}, \quad (n, n'=1, \dots, N) \\ \beta_1^- = \beta_N^+ = 0. \quad (1.2)$$

This pseudo-one-dimensional representation may be called "polar representation" in contrast with the original one ( $\{|l\rangle\}$ ) as the new  $|n\rangle$  spreads, in the original space, over a sphere with the radius  $\sim n$  as if it were a scattered wave from a "pole" in the support of  $|1\rangle$ . In this new representation (denoted by  $n, n', m$  and  $m'$ ) we have two independent solutions  $\{U_n^+(E, N)\}$  (increasing solution with increasing  $n$ ) and  $\{U_n^-(E, N)\}$  (decreasing solution with increasing  $n$ ) of the homogeneous equation such that

$$U_1^+(E, N) = U_N^-(E, N) \neq 0, \\ U_0^+(E, N) = U_{N+1}^-(E, N) = 0. \quad (1.3)$$

Then we can claim that the effective distance  $\bar{m}(E)$  is the inferimum of  $m(E)$  that satisfies

$$\left| \frac{U_{n+m}^+(E, N)}{U_n^+(E, N)} \right|^2 \geq \frac{\exp\{m/\bar{m}(E)\}}{\bar{m}(E)} \left( \frac{\gamma}{\Gamma} \right), \\ \left| \frac{U_{n-m}^-(E, N)}{U_n^-(E, N)} \right|^2 \geq \frac{\exp\{m/\bar{m}(E)\}}{\bar{m}(E)} \left( \frac{\gamma}{\Gamma} \right) \quad (1.4)$$

for any choice of  $m, n$  and of the initial base  $|1\rangle$ , where  $\gamma (> \Gamma)$  is some constant. This is just the definition of the effective "distance"  $\bar{m}(E)$  and the inequalities are essential to guarantee the concluding inequalities in I((1) and (2) in this section).

The "distance"  $\bar{m}(\varepsilon + i\Gamma)$  would diverge for  $\Gamma \rightarrow 0$  in infinite systems because the solution  $\{U_n^+(\varepsilon + i0, N \rightarrow \infty) \mid n=1, 2, \dots\}$  has nodes for real  $H$ .

Now we have the following question concerning infinite systems. Is it necessary to require an infinite range of environment to determine  $G_{l,l'}(\varepsilon + i0)$  even when the eigenfunctions of  $H$  at the energy  $\varepsilon$  are localized? In this case our intuition suggests that especially for  $E = \varepsilon + i0$  the localization-length  $l(\varepsilon)$  ( $< \infty$ ) of the eigenfunctions should govern, instead of  $\bar{m}(\varepsilon + i0)$ , some characteristics like (1) and (2), namely,  $G_{l,l'}(\varepsilon + i0) \propto \exp\{-m(l, l')/Al(\varepsilon)\}$ , ( $A$ : some constant) and finite size ( $\propto l(\varepsilon)$ ) environment effects. On the other hand, it is easy to show that the above characteristics are derived if we replace  $m(E)$  in the two exponents in (1.4) by  $l(\varepsilon)/2$ . That is, the exponential increas-

ing (decreasing) characteristic of  $U_n^+(U_n^-)$ , in statistical sense, determines the exponential decay of  $G_{i,i'}$  and its environment effect.

The above consideration is a principal motive of this paper leading to a concept of refined effective "distance"  $\bar{m}(E)$ . The "distance"  $\bar{m}(E)$  is defined in §2 assuming its existence and some qualitative characteristics are derived.

The existence of  $\bar{m}(E)$  is numerically suggested in §3 in some simple examples of 1-, 2- and 3-dimensional binary alloys.

The final section is devoted to the concluding remarks.

## § 2. Existence of a refined effective "distance" $\bar{m}(E)$

Let us consider an ensemble of 1-dimensional (1-D), 2-D or 3-D systems with the number of lattice points  $N_0 (\geq N)$  of the order of  $M^d$  ( $d$ : dimension,  $M \gg 1$ ). We restrict in this paper that the random variables  $\{\epsilon_i\}$  and  $\{t_{i,i'}\}$  constitute, respectively, stationary processes. That is, the system is statistically homogeneous in the original ( $\{|l\rangle\}$ ) representation.

The transfer matrix  $t_n$  and a renormalized one  $t_n^*$  of the system in the polar ( $\{|n\rangle\}$ ) representation are defined as

$$\begin{pmatrix} U_{n+1}(E, N) \\ U_n(E, N) \end{pmatrix} \equiv t_n(E) \begin{pmatrix} U_n(E, N) \\ U_{n-1}(E, N) \end{pmatrix},$$

$$t_n^*(E) \equiv ((\beta_n^-/\beta_n^+)^{1/2})^{-1} t_n(E), \quad \det t_n^*(E) = 1. \quad (2.1)$$

Then the strict upper bounds of the average rate of increasing of  $U_n^+(E, N)$  and the average rate of decreasing of  $U_n^-(E, N)$ , over the range  $n=m'$  to  $m$ , are defined

$$\begin{aligned} 1/(2\bar{m}_{(m+1-m')}^+(E)) &\equiv 1/(m+1-m') \cdot \ln \|t_{m--m'}(E)\|, \\ 1/(2\bar{m}_{(m+1-m')}^-(E)) &\equiv 1/(m+1-m') \cdot \ln \|(t_{m--m'}(E))^{-1}\|, \\ t_{m--m'}(E) &\equiv \prod_{n=m'}^m t_n(E) = (\beta_{m'}^-/\beta_m^+)^{1/2} t_{m--m'}^*(E). \end{aligned}$$

$$(1 \leq m', m \leq N-1) \quad (2.2)$$

The subscript  $(m+1-m')$  of  $\bar{m}^\pm$  means that the  $\bar{m}^\pm$  correspond to the product of a sequence of  $(m+1-m')$  adjacent transfer matrices. The  $\bar{m}_{(M)}^\pm(E)$ , ( $M \equiv m+1-m'$ ), depend on the sample system and the initial base  $|1\rangle$ .

To avoid the complicated effect from the boundary of the system an integer  $M$  is selected in this paper such that the support of  $|M+1\rangle$  just touches the boundary of the system in the original ( $\{|l\rangle\}$ ) representation. By using the  $\bar{m}_{(M)}^\pm(E)$ , ( $M \equiv M+1-1$ ), we can construct the following inequalities similar to (1.4)

$$\begin{aligned} \left| \frac{U_{n+m}^+(E, N)}{U_n^+(E, N)} \right|^2 &\geq \frac{(\gamma/\Gamma)}{m_f(E, M)} \exp\{m/\bar{m}_{(M)}^+(E)\}, \\ \left| \frac{U_{n-m}^-(E, N)}{U_n^-(E, N)} \right|^2 &\geq \frac{(\gamma/\Gamma)}{m_f(E, M)} \exp\{m/\bar{m}_{(M)}^-(E)\}, \end{aligned}$$

$$(1 \leq n, n \pm m \leq M+1) \quad (2.3)$$

where the second factors of the right-hand sides represent an average behaviour of  $U_n^+(E, N)$  and  $U_n^-(E, N)$  over the range  $n=1$  to  $M+1$  and the first factors cover the fluctuation of the left-hand sides from the second factors. The  $m_f(E, M)$  has thus been defined as the minimum value which satisfies the inequalities (2.3).

Next we consider an ensemble of infinite ( $N_0, N, M \rightarrow \infty$ ) systems. We have known (from convergent property of  $\zeta_n^-$  in Ref. 8)) that the following limit exists,

$$U_{m+1}^-(E)/U_1^-(E) \equiv \lim_{N \rightarrow \infty} U_{m+1}^-(E, N)/U_1^-(E, N), \quad (\text{for } \Gamma > 0) \quad (2.4)$$

and obviously exists

$$U_{m+1}^+(E)/U_1^+(E) \equiv \lim_{N \rightarrow \infty} U_{m+1}^+(E, N)/U_1^+(E, N). \quad (\text{for } \Gamma > 0) \quad (2.4')$$

Our fundamental assumptions throughout this paper are:

$$(A) \quad \lim_{M' \rightarrow \infty} 1/(2\bar{m}_{(M')}(E)) = \lim_{m \rightarrow \infty} 1/m \ln |U_{m+1}^+(E)/U_1^+(E)|,$$

$$\lim_{M' \rightarrow \infty} 1/(2\bar{m}_{(M')}(E)) = -\lim_{m \rightarrow \infty} 1/m \ln |U_{m+1}^-(E)/U_1^-(E)|,$$

exist with probability 1 (w. p. 1) on our statistically homogeneous ensemble.

In this case the two limits must coincide to conserve the Wronskian for difference system.

(B) When the limiting value  $1/(2\bar{m}(E))$  exists, it does not depend on the sample systems w. p. 1 and on the local initial base  $|1\rangle$ .

Assumptions (A) and (B) lead us to the existence and uniqueness of the Lyapunov exponent of  $\{U_n^\pm(E)\}$  w. p. 1 defined as

$$1/2\bar{m}(E) \equiv \lim_{M' \rightarrow \infty} 1/(2\bar{m}_{(M')}(E)) = \lim_{m \rightarrow \infty} 1/m \ln |U_{m+1}^+(E)/U_1^+(E)|,$$

$$= \lim_{M' \rightarrow \infty} 1/(2\bar{m}_{(M')}(E)) = -\lim_{m \rightarrow \infty} 1/m \ln |U_{m+1}^-(E)/U_1^-(E)|. \quad (2.5)$$

We have known that Lyapunov exponent exists, w. p. 1, in some class of disordered systems<sup>10-12)</sup> and the existence is expected in a wider class of disordered systems. Our linear chain represented by (1.2) does not correspond to a stationary process but seems to belong to a class of stochastic process in which  $|\alpha_n - \langle \alpha \rangle|$  and  $|\beta_n^+ - \langle \beta^+ \rangle|$  obey power law as functions of  $n$ .<sup>13)</sup>

Our numerical data of  $\bar{m}_{(M')}(E)$ , ( $M' < M$ ) of finite systems (which are shown in § 3) also suggest the existence of it.

We thus proceed in this section assuming the existence of the Lyapunov exponent and leave it as a conjecture for a future study.

Once the existence of  $\bar{m}(E)$  is guaranteed w. p. 1, we can derive the following characteristics of it.

(i) We can write down the following inequalities for infinite system w. p. 1

$$\left| \frac{U_{n+m}^+(E)}{U_n^+(E)} \right|^2 \geq \frac{(\gamma/\Gamma)}{m_f(E)} \exp\{m/\bar{m}(E)\},$$

$$\left| \frac{U_{n-m}^-(E)}{U_n^-(E)} \right|^2 \geq \frac{(\gamma/\Gamma)}{m_f(E)} \exp\{m/\bar{m}(E)\}, \quad (1 \leq n, n \pm m) \quad (2.6)$$



where the quantity  $m_f(E)$  ( $< \infty$  for  $\Gamma > 0$ ), named a measure of fluctuation, is defined as the inferimum which satisfies the inequalities (2.6) for any choice of  $n$ ,  $m$  and the initial base  $|1\rangle$ . This inequalities are (as are in I) essential to our conclusive results in this paper.

(ii) The following inequality is immediately derived by using the inequality (1.4) and the definition of  $\bar{m}(E)$  (2.5)

$$\bar{m}(E) \leq m_f(E). \quad (2.7)$$

(iii) Localization length  $l(\epsilon)$  is defined for any desired dimension as

$$1/l(\epsilon) \equiv 1/2\bar{m}(\epsilon) \equiv \lim_{\Gamma \rightarrow 0} 1/2\bar{m}(\epsilon + i\Gamma). \quad (2.8)$$

In 1-dimension(1-D) the quantity  $1/l(\epsilon)$  is the one Matsuda and Ishii,<sup>14),15)</sup> and Goda<sup>16)</sup> studied extensively by using Furstenberg's<sup>10)</sup> or Furstenberg-type<sup>16)</sup> theorem. Matsuda and Ishii<sup>14)</sup> assumed in their "if assumption", that the  $1/l(\epsilon)$  just described the exponent of the exponentially localized eigenfunctions of a very large but finite system. This has been justified by Avron and Simon<sup>17)</sup> and Kotani<sup>18)</sup> by proving Hurbert-Jones-Thouless-Avron-Simon-Kotani (HJTASK) formula<sup>17)-20)</sup> (see Ref. 15)). In this sense the  $l(\epsilon) = 2\bar{m}(\epsilon)$  is the localization length describing a rough extent of the localized eigenfunctions. Now we can claim that the  $l(\epsilon)$  in 2- and 3-D is the extension of the localization length of Matsuda and Ishii, because the  $l(\epsilon)$  just guarantees the exponential decay of the  $G_{l,l'}(\epsilon)$  with increasing  $m(l, l')$  and the exponential decay of the environment effect from outside of the two spheres centered by the sites  $l$  and  $l'$  with increasing the radii.

(iv) An essential feature of introducing  $\bar{m}(E)$  is that it remains finite for  $\Gamma > 0$  when  $l(\epsilon) < \infty$ .

(v) If the  $\bar{m}(E)$  is an analytic function of  $E$  on the upper half of the complex energy plane, the  $2\bar{m}(E)$  is just the analytic continuation of  $l(\epsilon)$ .

(vi) The measure of fluctuation  $m_f(E)$  is finite for  $\Gamma > 0$  (from (2.6)) and thus we get from (2.7)

$$\bar{m}(E) \leq m_f(E) < \infty \quad \text{for } \Gamma > 0. \quad (2.9)$$

The  $\bar{m}(E)$  would also be a monotonically decreasing function with increasing  $\Gamma$ , because the more coarse-grained a quantity is, the less information of the environment is necessary.

### § 3. Numerical study of $\bar{m}_{(M)}^*(E)$ of simple binary alloys

A binary (AB) alloy ( $\epsilon_A = -\epsilon_B$ , 50%:50%, purely random) with only nearest-neighbour (N. N.) isotopic interaction ( $t=1$ ) on 1-D chain ( $N=L=1200$ ), 2-D square lattice ( $N=L^2$ ,  $L=100, 200$ ) and 3-D cubic lattice ( $N=L^3$ ,  $L=50$ ) are numerically examined as simple examples of (statistically) homogeneous (disordered) systems to show that  $\{U_m^+(E, N), m=1, 2, \dots, M+1=L/2\}(\{U_m^-(E, N)\})$  grows (decays) exponentially. By adopting the periodic boundary condition in the original ( $|l\rangle$ ) representation we can choose any  $|l\rangle$  as the initial base  $|1\rangle$  for which the boundary of the system does not affect the  $\{U_m^+(E, N), m=1, 2, \dots, M+1\}$ . The atomic energy  $\epsilon_A (= -\epsilon_B)$  is chosen 0 for ordered systems, or 1 for 1-D and 2 for 2- and 3-D in the unit of the isotopic N. N. transfer

energy.

To check the convergence of  $1/(2\bar{m}_{(M')}(E))$  as  $M'$  increases up to  $M$  we adopt real-space-renormalization technique which includes no approximation in our pseudo-one dimensional polar representation. First, we pick out two sequences of  $2^j$  ( $j$ ; integer) adjacent  $t$ -matrices  $\{t_{n'}, t_{n'+1}, \dots, t_{n'+2^j-1}\}$ , starting from two different sites (two  $n$ 's), so that none of  $(n'+2^j-1)$ 's exceed  $M$ , and calculate the sequence of  $2^j$  pairs of  $1/(2\bar{m}_{(1)}^\pm(E))$  and  $-1/(2\bar{m}_{(1)}^\pm(E))$  for each  $n'$  from the eigenvalues of the transfer matrices. Next we calculate the sequence of the  $2^{j-1}$  products of two adjacent transfer matrices  $\{t_{n'}t_{n'+1}, t_{n'+2}t_{n'+3}, \dots, t_{n'+2^j-2}t_{n'+2^j-1}\}$  and calculate the sequence of the corresponding  $2^{j-1}$  pairs of  $\pm 1/(2\bar{m}_{(2)}^\pm(E))$  for each  $n'$  from the eigenvalues of the new transfer matrices. In the same way we can, successively, calculate the corresponding sequence of  $2^{j-2}$  pairs of  $\pm 1/(2\bar{m}_{(4)}^\pm(E))$  for each  $n'$ , ..., the sequence of the 2 pairs of  $\pm 1/(2\bar{m}_{(2^{j-1})}^\pm(E))$  for each  $n'$  and the two single-pairs of  $\pm 1/(2\bar{m}_{(2^j)}^\pm(E))$ . More precisely we choose for 1-D ( $M+1=600$ )  $j=9$  and two sequences of  $2^9=512$  pairs of  $\pm 1/(2\bar{m}_{(1)}^\pm(E))$  starting from  $t_{20}(E)$  and  $t_{85}(E)$ , for 2-D ( $M+1=100$ )  $j=6$  and two sequences of  $2^6=64$  pairs of  $\pm 1/(2\bar{m}_{(1)}^\pm(E))$  starting from  $t_{15}$  and  $t_{35}$  ( $M+1=50$ ,  $j=5$  for regular system), and for 3-D ( $M+1=25$ )  $j=4$  and two sequences of  $2^4=16$  pairs of  $\pm 1/(2\bar{m}_{(1)}^\pm(E))$  starting from  $t_5$  and  $t_8$ . From the numerical point of view  $t_{m--m'}(E)$  is replaced by  $t_{m--m'}^*(E)$ , that is,  $\bar{m}_{(M')}(E) = \bar{m}_{(M')}^*(E)$  when  $M'=m+1-m' \geq 10$  in our case. The actual deviation from the symmetry is, for each pair, of the order of 0.01 for  $M'=8$  and these tend to cancel out when we take the average over the sequence. Thus to keep the symmetry for the help of our eyes the  $t_{m--m'}(E)$  is always replaced by  $t_{m--m'}^*(E)$  in this section even for small  $M'$ . The results are as follows.

### 3.1. 1-D chain

First, we calculate the Lyapunov exponent  $1/(2\bar{m}(E))$  of the regular chain where all  $\alpha_n(n=1, 2, \dots, M+1)=0$  and all  $\beta_n^+(n=2, \dots, M)=1$  except for  $\beta_1^+(=\sqrt{2})=\beta_2^-$ . This is the case where the exponent is guaranteed to exist. The analytic expression of  $\bar{m}(E)$  is obtained such that

$$1/(2\bar{m}(E)) = |\operatorname{Re}(\ln(E/2 \pm \sqrt{(E/2)^2 - 1}))|. \quad (3.1)$$

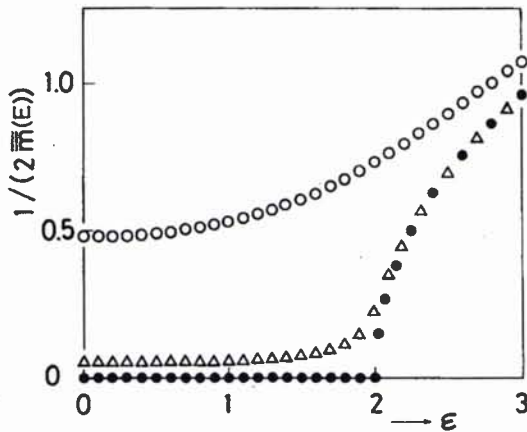


Fig. 1. Lyapunov exponent  $1/(2\bar{m}(E))$  of the ordered chain for (O)  $\Gamma=1$ , ( $\Delta$ )  $\Gamma=0.1$  and ( $\bullet$ )  $\Gamma=0$ , as functions of  $\epsilon$ .

An overall feature of  $1/(2\bar{m}(E))$  is shown in Fig. 1. It is worth to mention

$$\bar{m}(\epsilon + i\Gamma) \propto 1/\Gamma \quad \text{for } |\epsilon| < 2 \text{ except for band edges,} \quad (3.2a)$$

$$\bar{m}(\epsilon + i\Gamma) \propto 1/\sqrt{\Gamma} \quad \text{for } \epsilon \text{ at the band edges } (|\epsilon|=2), \quad (3.2b)$$

$$\bar{m}(\epsilon + i\Gamma) = \text{const}(\epsilon) \quad \text{outside the band } (|\epsilon| > 2), \quad (3.2c)$$

as  $\Gamma$  decreases to zero. As will be seen later, the types (3.2a) and (3.2c) appear also in 2- and 3-D regular systems and are understood as typical examples of  $\bar{m}(E)$  for

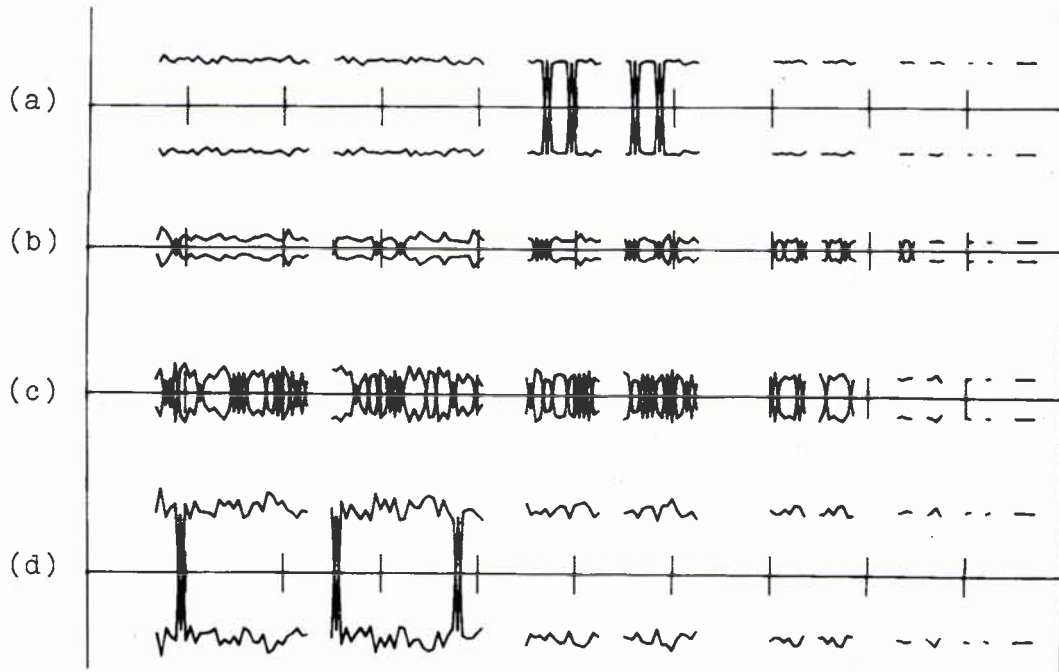


Fig. 2. From the left, two sequences of 32 pairs of  $1/(2\bar{m}^+_{(16)}(E))$  (upper half) and  $-1/(2\bar{m}^-_{(16)}(E))$  (lower half) stitched with straight lines, (starting from  $t_{20}$  and  $t_{85}$ ), the corresponding two sequences of 16 pairs of  $\pm 1/(2\bar{m}^{\pm}_{(32)}(E))$ ,  $8 \pm 1/(2\bar{m}^{\pm}_{(64)}(E))$ ,  $4 \pm 1/(2\bar{m}^{\pm}_{(128)}(E))$ ,  $2 \pm 1/(2\bar{m}^{\pm}_{(256)}(E))$  and the two single-pairs of  $\pm 1/(2\bar{m}^{\pm}_{(512)}(E))$ , of a 1200 disordered chain with  $\varepsilon_A = -\varepsilon_B = 1$  for (a)  $\Gamma = 1, \varepsilon = 0$ , (b)  $\Gamma = 0.1, \varepsilon = 0$ , (c)  $\Gamma = 0.1, \varepsilon = 2$ , and (d)  $\Gamma = 0.1, \varepsilon = 3$ . The last two single-pairs are connected with straight lines to see that the difference due to different starting points is small.

extended (transparent) energy region and localized (damping) energy region.

Next we consider a sample of  $\varepsilon_A = 1, N = 1200$  binary alloy. Numerical data of  $\{\alpha_n\}$  and  $\{\beta_n^+\}$  show that the processes look like stationary ones with

$$\langle \alpha \rangle \cong 0 \text{ and } \langle \beta^+ \rangle \cong 1.18. \quad (3.3)$$

Some examples ( $\Gamma = 1, \varepsilon = 0$  and  $\Gamma = 0.1, \varepsilon = 0, 2, 3$ ) of the two sequences of 32 pairs of  $1/(2\bar{m}^+_{(16)}(E))$  and  $-1/(2\bar{m}^-_{(16)}(E))$ , (starting from  $t_{20}$  and  $t_{85}$ ), the corresponding two sequences of 16 pairs of  $\pm 1/(2\bar{m}^{\pm}_{(32)}(E))$ ,  $8 \pm 1/(2\bar{m}^{\pm}_{(64)}(E))$ ,  $4 \pm 1/(2\bar{m}^{\pm}_{(128)}(E))$ ,  $2 \pm 1/(2\bar{m}^{\pm}_{(256)}(E))$  and the two single-pairs of  $\pm 1/(2\bar{m}^{\pm}_{(512)}(E))$  are shown in Fig. 2 to show that these quantities seem to be statistically homogeneous in the polar ( $\{|n\rangle\}$ ) representation and thus seem to converge.

When we decrease  $\Gamma$  from 0.1 to 0, the feature almost does not change probably because the  $2\bar{m}^{\pm}_{(M')}(E)$  in this (small  $\Gamma$ ) case is essentially determined by the localization length  $l(\varepsilon)$ .

When  $\Gamma$  is large ( $> 0.5$ ), the damping effect due to it predominates over that from localization and remarkably smoothed almost constant lines are obtained. In Fig. 3 an overall feature of  $1/(2\bar{m}^{\pm}_{(512)}(E))$  is shown with the density of state (DOS) of the sample to show that the details of  $1/(2\bar{m}^{\pm}_{(512)}(\varepsilon + i0))$  indicate a sharp reflection of the details of the DOS of the sample system known as the HJTASK relation.<sup>17)-20)</sup> Some typical

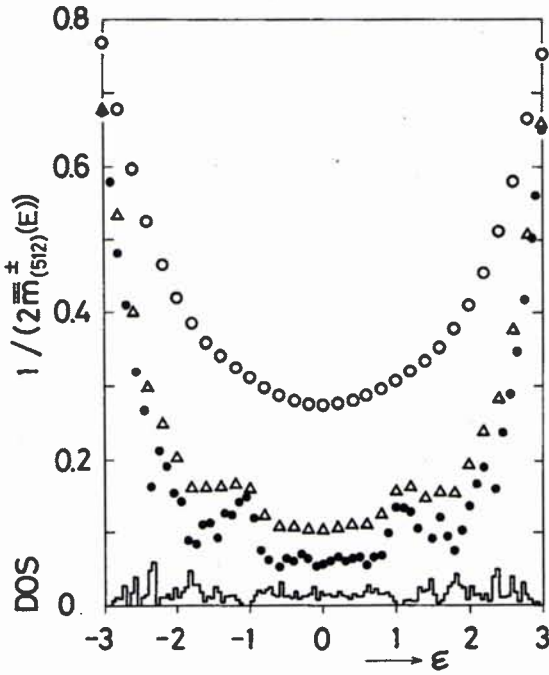


Fig. 3. Lyapunov exponent  $1/(2\bar{m}_{(512)}^\pm(E))$  of a 1200 disordered chain with  $\varepsilon_A = -\varepsilon_B = 1$  for (○)  $\Gamma=1$ , (△)  $\Gamma=0.1$  and (●)  $\Gamma=0$ , as functions of  $\varepsilon$ . The histogram is the DOS of the system in arbitrary unit by the negative factor counting method.

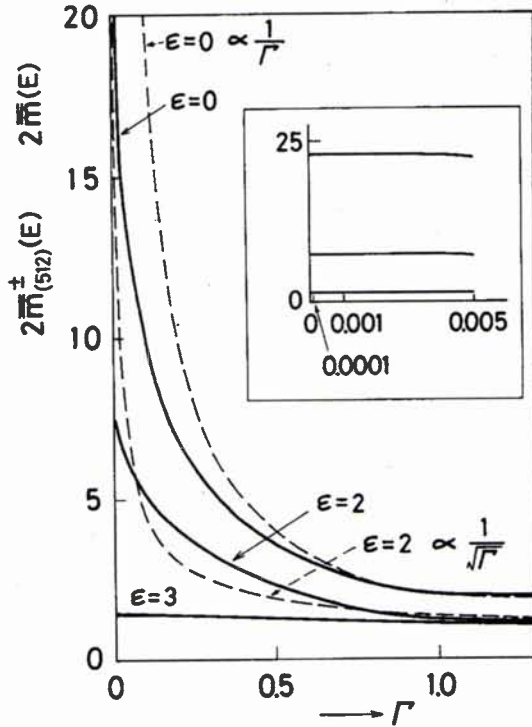


Fig. 4. Effective "distance"  $2\bar{m}_{(512)}^\pm(E)$  (real line) of a 1200 disordered chain with  $\varepsilon_A = 1$  as functions of  $\Gamma$ , with an inset for  $\Gamma \rightarrow 0$  region. The  $2\bar{m}(E)$  (broken line) of the ordered system are shown for reference.

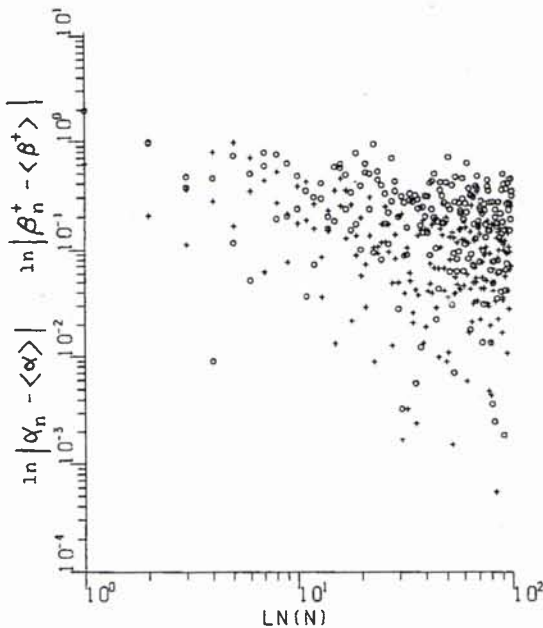


Fig. 5. (○)  $\ln|\alpha_n - \langle \alpha \rangle|$  and (+)  $\ln|\beta_n^+ - \langle \beta^+ \rangle|$  of two samples of a  $200 \times 200$  disordered square lattice with  $\varepsilon_A = -\varepsilon_B = 2$  as functions of  $n$ .

examples of  $2\bar{m}_{(512)}^\pm(E)$  are shown in Fig. 4 with an inset for  $\Gamma \rightarrow 0$  region.

### 3.2. 2-D square lattice

Regular system is examined first numerically as we do not know the exact expression of  $\{\beta_n^+\}$  and get that  $\beta_n^+ - 2$  obeys the following power law with respect to  $n$

$$\beta_n^+ - 2 = c(-1)^n/n^\xi, \quad 1.10 < \xi < 1.18,$$

$$0.2 < c < 0.3, \quad (1 \leq n \leq 49)$$

$$\text{while } \alpha_n = 0. \quad (1 \leq n \leq 50) \quad (3.4)$$

The overall feature of  $1/(2\bar{m}_{(32)}^\pm(E))$  is quite similar to that in Fig. 1 with remarkably fine convergent property and with the characteristics (3.2a) and (3.2c).

When we introduce disorder ( $\varepsilon_A = -\varepsilon_B$



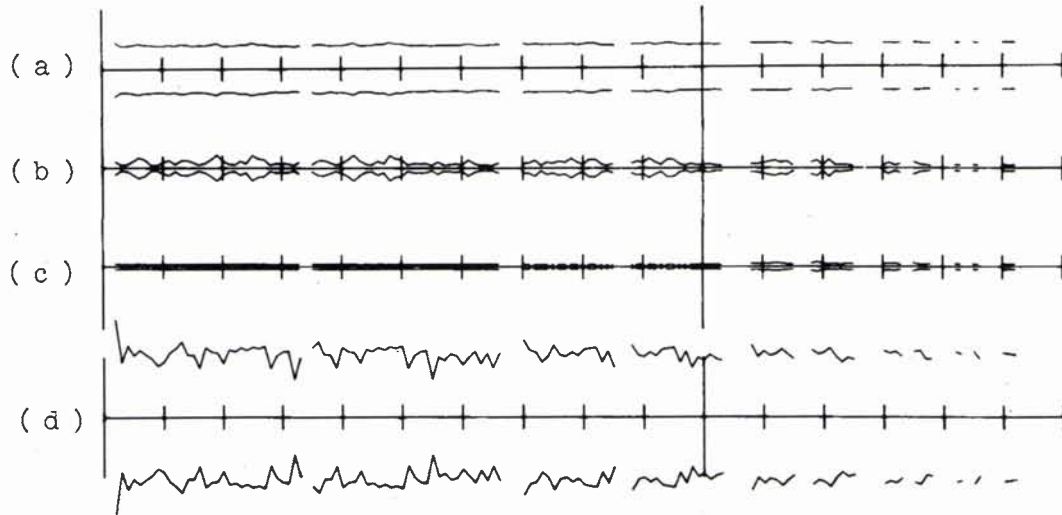


Fig. 6. From the left, two sequences of 32 pairs of  $1/(2\bar{m}_{(2)}^+(E))$  (upper half) and  $-1/(2\bar{m}_{(2)}^-(E))$  (lower half) stitched with straight lines (starting from  $t_{15}$  and  $t_{35}$ ), the corresponding two sequences of 16 pairs of  $\pm 1/(2\bar{m}_{(4)}^+(E))$ ,  $8 \pm 1/(2\bar{m}_{(6)}^+(E))$ ,  $4 \pm 1/(2\bar{m}_{(16)}^+(E))$ ,  $2 \pm 1/(2\bar{m}_{(32)}^+(E))$  and the two single-pairs of  $\pm 1/(2\bar{m}_{(64)}^+(E))$ , of a  $200 \times 200$  disordered square lattice with  $\epsilon_A = -\epsilon_B = 2$  for (a)  $\Gamma=1$ ,  $\epsilon=0$  (b)  $\Gamma=0.1$ ,  $\epsilon=0$ , (c)  $\Gamma=0.1$ ,  $\epsilon=2$ , and (d)  $\Gamma=0.1$ ,  $\epsilon=6$ . The last two single-pairs are connected with straight lines.

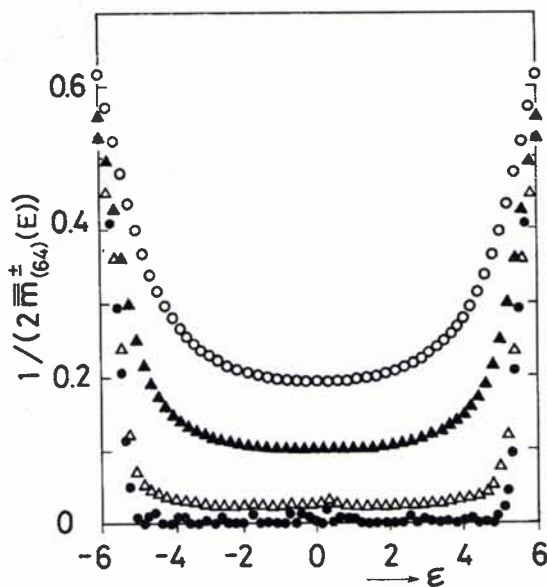


Fig. 7. Lyapunov exponent  $1/(2\bar{m}_{(64)}^+(E))$  of a  $200 \times 200$  disordered square lattice with  $\epsilon_A=2$  for (○)  $\Gamma=1$ , (▲)  $\Gamma=0.5$ , (△)  $\Gamma=0.1$  and (●)  $\Gamma=0$ , as functions of  $\epsilon$ .

$=2$ ), both  $\{\alpha_n\}$  and  $\{\beta_n^+\}$  fluctuate around the average values

$$\langle \alpha \rangle \cong 0, \quad \langle \beta^+ \rangle \cong 2.63. \quad (3.5)$$

It has been reported that a power law exists in  $|\alpha_n - \langle \alpha \rangle|$  and  $|\beta_n^+ - \langle \beta^+ \rangle|$  of the disordered system.<sup>13)</sup> The trend is shown in Fig. 5. Some examples ( $\Gamma=1$ ,  $\epsilon=0$ , and  $\Gamma=0.1$ ,  $\epsilon=0, 2, 6$ ) of the two sequences of 32 pairs of  $1/(2\bar{m}_{(2)}^+(E))$  and  $-1/(2\bar{m}_{(2)}^-(E))$ , starting from  $t_{15}$  and  $t_{35}$ , the corresponding two sequences of 16 pairs of  $\pm 1/(2\bar{m}_{(4)}^+(E))$ ,  $8 \pm 1/(2\bar{m}_{(6)}^+(E))$ ,  $4 \pm 1/(2\bar{m}_{(16)}^+(E))$ ,  $2 \pm 1/(2\bar{m}_{(32)}^+(E))$ , and the two single-pairs of  $\pm 1/(2\bar{m}_{(64)}^+(E))$  are shown in Fig. 6 to represent the convergent property of  $1/(2\bar{m}_{(M')}^+(E))$  for not so small  $\Gamma$ . When we increase  $\Gamma$ , the convergent property becomes much more distinguishable. When we decrease  $\Gamma$  down to 0, we also obtain rather good convergent property for strongly localized region ( $5.3 \leq |\epsilon| \leq 6$ ). However, contrary to the above we get a wrong convergent property of  $1/(2\bar{m}_{(M')}^+(E))$  for weakly localized region ( $|\epsilon| \leq 5.2$ ). In this case  $1/(2\bar{m}_{(M')}^+(E))$  strongly depends on the  $M' \sim 64$  when  $\Gamma \rightarrow 0$ ,

contrary to the above we get a wrong convergent property of  $1/(2\bar{m}_{(M')}^+(E))$  for weakly localized region ( $|\epsilon| \leq 5.2$ ). In this case  $1/(2\bar{m}_{(M')}^+(E))$  strongly depends on the  $M' \sim 64$  when  $\Gamma \rightarrow 0$ ,

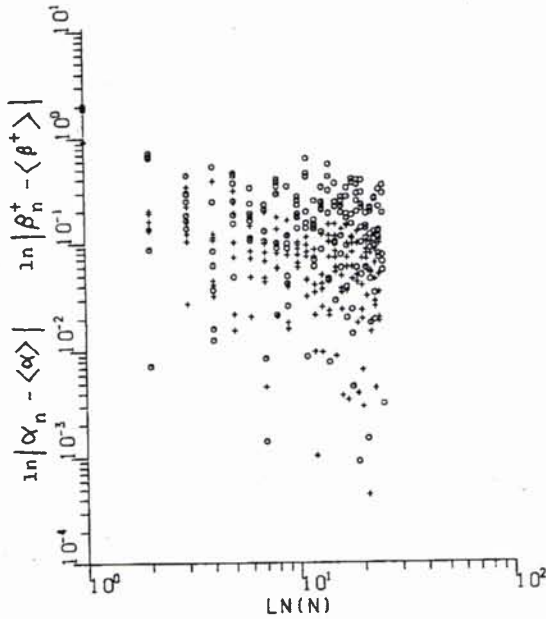


Fig. 8. (O)  $\ln|\alpha_n - \langle\alpha\rangle|$  and (+)  $\ln|\beta_n^+ - \langle\beta^+\rangle|$  of seven samples of a  $50 \times 50 \times 50$  disordered cubic lattice with  $\epsilon_A = -\epsilon_B = 2$  as functions of  $n$ .

reflecting a (weak but) wide range of local fluctuation of  $\{U_n^\pm\}$  in the polar space or of the eigenfunctions in the original space. We judge that in this case the size of the system we adopt ( $L=200, M+1=100$ ) is not large enough to get  $\bar{m}$ . An overall feature of  $1/(2\bar{m}_{(64)}^\pm(E))$  is shown in Fig. 7 with a reference of bad data of the case  $\Gamma=0, |\epsilon| \leq 5.2$  of wrong convergence.

### 3.3. 3-D cubic lattice

The quantity  $|\beta_n^+ - 3|$  of the regular system vibrates below an asymptotic form

$$\cong 0.597 \, 1/n^\xi, \quad \xi \cong 1.59, \quad (n=1, \dots, 24)$$

$$\text{while } \alpha_n = 0. \quad (n=1, 2, \dots, 25) \quad (3.6)$$

An overall feature of the  $1/(2\bar{m}_{(64)}^\pm(E))$  is quite similar to that in Fig. 1 with remarkably fine convergent property and with the

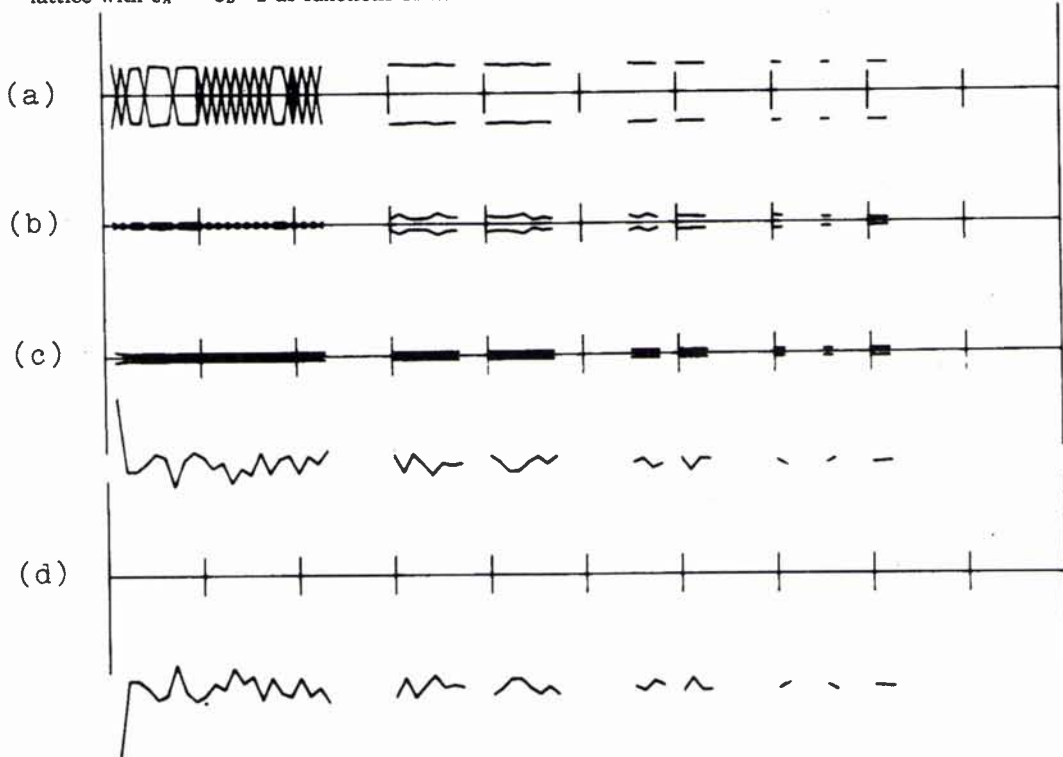


Fig. 9. From the left, the sequence of 24 pairs of  $1/(2\bar{m}_{(1)}^\pm(E))$  (upper half) and  $-1/(2\bar{m}_{(1)}^\mp(E))$  (lower half) stitched with straight lines, starting from  $t_1$  and the two sequences of 8 pairs of the  $1/(2\bar{m}_{(2)}^\pm(E))$  and  $-1/(2\bar{m}_{(2)}^\mp(E))$  starting from  $t_2$  and  $t_3$ , the corresponding two sequences of 4 pairs of  $\pm 1/(2\bar{m}_{(4)}^\pm(E))$ ,  $2 \pm 1/(2\bar{m}_{(8)}^\pm(E))$ , and the two single-pairs of  $\pm 1/(2\bar{m}_{(16)}^\pm(E))$ , for (a)  $\Gamma=1, \epsilon=0$ , (b)  $\Gamma=0.1, \epsilon=0$ , (c)  $\Gamma=0.1, \epsilon=4$ , and (d)  $\Gamma=0.1, \epsilon=8$ . The last two single-pairs are connected with straight lines.

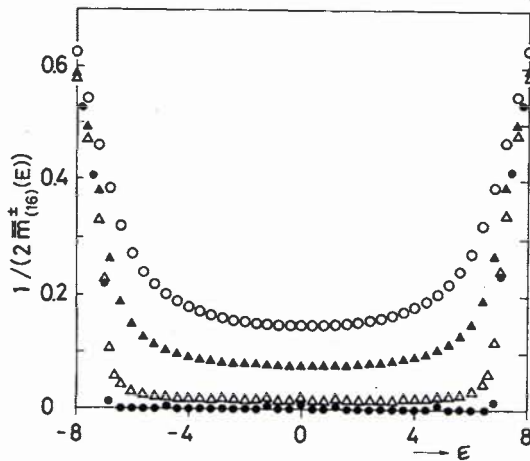


Fig. 10. Lyapunov exponent  $1/(2\bar{m}_{(16)}^\pm(E))$  of a  $50 \times 50 \times 50$  disordered cubic lattice with  $\epsilon_A=2$  for (○)  $\Gamma=1$ , (▲)  $\Gamma=0.5$ , (△)  $\Gamma=0.1$  and (●)  $\Gamma=0$ , as functions of  $\epsilon$ .

even though the sequence in the polar ( $\{|n\rangle\}$ ) representation is short ( $M+1=25$ ). An overall feature of  $1/(2\bar{m}_{(16)}^\pm(E))$  is shown in Fig. 10, with a reference of bad data for the case  $\Gamma=0$ ,  $|\epsilon| \leq 6.6$  of wrong convergence.

#### § 4. Concluding remarks

The existence of a refined effective "distance"  $\bar{m}(E)$  w. p. 1 in infinite systems was conjectured to measure the contribution of local environment around the sites  $l$  and  $l'$  to the Green function  $G_{l,l'}(E)$ .

Numerical investigation of  $\bar{m}_{(M')}^\pm(E)$  for some simple finite systems (1-D chain with  $N_0=L=1200$ , 2-D square lattice with  $N_0=L^2$ ,  $L=100, 200$  and 3-D cubic lattice with  $N_0=L^3$ ,  $L=50$ ) suggested its existence.

We can classify the upper half of the complex energy plane into three regimes. Regime (a), where  $\Gamma$  is large and the forced damping due to it predominates for  $G_{l,l'}(E)$  as  $m(l, l')$  increases. Regime (b) is constituted of the energy  $\epsilon$  (and small  $\Gamma$ ) on which the eigenfunctions are strongly localized or of the energy in the energy gap where the damping of  $G_{l,l'}(E)$  due to the localization or due to the energy gap predominates, and regime (c) with small  $\Gamma$  and with  $\epsilon$  at which the eigenfunctions are weakly localized ( $l(\epsilon) > M$ ) or extended. In regimes (a) and (b) the  $\bar{m}_{(M')}^\pm(E)$  has good convergent property which suggests the existence of the  $\bar{m}(E)$  in infinite systems and also suggests that the  $2\bar{m}(\epsilon + i0) = l(\epsilon)$  remains finite in regime (b), while in regime (c) the  $\bar{m}_{(M')}^\pm(E)$  depends on the size  $M'$  suggesting the not large enough size of the system.

It is our guess that the size dependence of  $\bar{m}_{(M')}^\pm(E)$  will disappear when the size increases because some trend toward convergence has been observed in our numerical data and also because we have no good reason to believe that only (c) is the exceptional case of the convergence. Actually, for regular systems in 1-, 2- and 3-D we have obtained convergent  $1/(2\bar{m}_{(M')}^\pm(E))$  on all over the upper half of the complex energy plain (regimes

characteristics (3.2a) and (3.2c).

As for the disordered system ( $\epsilon_A = -\epsilon_B = 2$ ) the matrix elements  $\{a_n\}$  ( $n=1$  to 25) and  $\{\beta_n^+\}$  ( $n=1$  to 24) are shown in Fig. 8 with

$$\langle a \rangle \cong 0, \quad \langle \beta^+ \rangle \cong 3.4. \quad (3.7)$$

Some examples ( $\Gamma=1$ ,  $\epsilon=0$  and  $\Gamma=0.1$ ,  $\epsilon=0, 4, 8$ ) of the sequence of 24 pairs of  $1/(2\bar{m}_{(1)}^\pm(E))$  and  $-1/2\bar{m}_{(1)}^\pm(E)$  starting from  $t_1$ , the two sequences of 8 pairs of  $\pm 1/(2\bar{m}_{(2)}^\pm(E))$ , (starting from  $t_5$  and  $t_8$ ), the corresponding two sequences of 4 pairs of  $\pm 1/(2\bar{m}_{(4)}^\pm(E))$ , 2  $\pm 1/(2\bar{m}_{(8)}^\pm(E))$  and the two single-pairs of  $\pm 1/(2\bar{m}_{(16)}^\pm(E))$  are shown in Fig. 9. Except for weakly localized region and extended region for small  $\Gamma$  ( $<0.1$ ) the convergent property is remarkably good

(a), (b) and (c)). The exponent  $1/(2\bar{m}_{(M)}^\pm(E))$  converges to zero (within the double precision we adopted) for  $\Gamma=0$  and for  $\epsilon$  in the energy band (regime (c)). The wrong convergent property presumably comes from the fact that the localization length  $l(\epsilon)$  exceeds far over the sample size  $L$  we investigated. When the disorder  $\epsilon_A(=-\epsilon_B)$  increases regime (c) would shrink. In 2-D at least  $L=600$ ,  $M+1=300$  may be necessary to check the convergent property in the regime (c) of the case in this paper. In 3-D our computational power may be far from checking it. Some other technique such as finite size scaling<sup>21),22)</sup> is necessary to overcome the difficulty in regime (c).

One of the theoretical backgrounds of yielding the Lyapunov exponent may be a kind of quasi-stationality in which  $|\alpha_n - \langle \alpha \rangle|$  and  $|\beta_n^+ - \langle \beta^+ \rangle|$  obey power law as functions of  $n$ . In 2- and 3-D ordered systems the trend is clearly found while in disordered systems the trend contains an increasing variance of  $\ln|\alpha_n - \langle \alpha \rangle|$  ( $\ln|\beta_n^+ - \langle \beta^+ \rangle|$ ) with increasing  $n$ . In 1-D the  $\{\alpha_n\}$  and  $\{\beta_n^+\}$  behave like stationally processes.

Once the inequalities (2.6) are established for the  $\bar{m}(E)$  and the optimal  $m_f(E)$ , the following results are derived just like in I,

$$\begin{aligned} \text{[I]} \quad |G_{l,l'}(E)| &\leq \min\{|G_{l,l}(E)|, |G_{l',l'}(E)|\} \\ &\quad \times (m_f(E)/(1 - \exp\{-1/\bar{m}(E)\}))^{1/2} \\ &\quad \times \exp\{-m(l, l')/2\bar{m}(E)\}, \text{ w. p. 1.} \end{aligned}$$

II] The Green function  $G_{l,l'}(E)$  is essentially determined by the local situation within the refined effective "distance"  $\bar{m}(E)$  from the sites  $l$  and  $l'$  in the sense that the dependence of  $G_{l,l'}(E)$  on the matrix elements  $\{\epsilon_{l''}\}$  and  $\{t_{l'',l'''}\}$  in the region  $m(l'', l), m(l'', l') > m$  decreases with increasing  $m$  by a factor of  $\exp\{-m/\bar{m}(E)\}$ , w. p. 1.

$$\text{[III]} \quad 0 < \bar{m}(E) \leq \bar{m}(E) < m_0 \equiv (1 + (\|H\|/\Gamma)^2) \quad \text{for } \Gamma > 0.$$

$$\text{[IV]} \quad \bar{m}(E) \leq m_f(E) < \infty \quad \text{for } \Gamma > 0.$$

An essential feature of defining  $\bar{m}(E)$  is that the  $\bar{m}(\epsilon + i0)$  remains finite for finite  $l(\epsilon)$  though the  $\bar{m}(\epsilon + i0)$  diverges. If  $2\bar{m}(E)$  is analytic this is expected to be the analytic continuation of  $l(\epsilon)$  on the upper half of the complex energy plane.

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