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Numerical Study of a Universal Distribution and Non-Universal Distributions of Resistance and Transmission Coefficient in 1-D Disordered Systems

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A universal probability distribution of resistance and transmission coefficient in a one dimensional disordered system proposed by Mello from a macroscopic point of view is examined numerically from a microscopic point of view for some tightly binding disordered systems. Some universal relations between the cumulants are well observed at the band center energy $E=0$ in a weakly disordered system, while these are modified at the other energies $E\neq 0$. They are modified even at $E=0$ in the strongly disordered system. It is further found that the universal relations are broken in a modified Bernoulli system with an inverse-power law structural correlation.

[universality, universal distribution, modified Bernoulli map, disordered system, resistance, macroscopic approach, transmission coefficient]

§1. Introduction

Universality in relation to a scaling property is an important concept in macroscopic physics. For example, it is well-known in the critical phenomena that the critical indexes are insensitive to microscopic details of Hamiltonian and they are decided only by the macroscopic informations; the dimensionality, the symmetry and so on.[1)]

A similar concept appears in electronic states and transport phenomena in some disordered electronic systems.[2-6)] A typical example is seen in a scaling theory for quantum conductance of a system with random elastic scatterers proposed by Abrahams *et al.*[7)] It has been proposed that the bata function of the conductance g ($\beta=\mathrm{d}\ln g/\mathrm{d}\ln L$) has only one parameter g and it's functional form is decided only by the dimensionality of the disordered system, in the absence of magnetic field or spin-orbit interaction. The scaling theory has been extensively studied theoretically and numerically.[8-11)]

Moreover it has been proposed by Mello in a one dimensional disordered system (1-DDS) that the distribution $P_L(\rho)$ of the dimensionless zero temperature resistance $\rho=1/g$ over an ensemble of samples of macroscopic size L scaled by the localization length has a universal functional form depending only on the size L.[12,13)] However, from a microscopic point of view, neither the exact distribution functions of the resistance or transmission coefficient of the microscopic 1-DDS's of finite systemsize nor the high-order moments of the distributions have been obtained.

On the other hand, in another 1-DDS (called a modified Bernoulli (MB) system) with an inverse-power low structural correlation, it has been found numerically that the distribution of the transmission coefficient in MB system deviates from the lognormal distribution and it's convergent property is more slow than that of the central-limit theorem (CLT).[14-16)]

Hence we are interested in the applicability of the universal distribution $P_L(\rho)$ of the resistance obtained from a macroscopic point of view to these microscopic disordered systems.

It is thus the purpose of the present paper to study numerically the applicability of the universal distribution $P_L(\rho)$ in the macroscopic theory (M-theory) to some cases of a one-electron tightly binding model (TB model). In addition to the case well described by the universal distribution $P_L(\rho)$, it is shown that there are some other situations in which the universal distribution $P_L(\rho)$ does not hold.

This paper is constructed as follows. In §2 we give a brief review of the macroscopic theory of resistance distribution in a 1-DDS. In §3 we numerically discuss the applicable and non-applicable regime of the M-theory in the tightly binding electronic system with random site energies. Section 4 is given to the arguments for the non-universal distribution of the transmission coefficient in the MB electronic system introduced in refs. 7–9. Section 5 is devoted to the summary and discussion.

§2. A Macroscopic Theory of Resistance and Transmission Coefficient

For the sake of the discussions in the later sections, a brief review is given here for the macroscopic theory of the resistance distribution on a random phase model (RP model), proposed by Mello.[12,13)]

According to the quantum scattering problem, a dimensionless zero temperature quantum resistance of the 1-DDS embeded in a infinite perfect lead is given by,[17,18)]

$$\rho=\frac{|r|^2}{|t|^2}, \tag{2.1}$$

where t and r are the transmission and reflection amplitude. The transfer matrix (T-matrix) characterizing this random system is given by

$$S=\begin{Bmatrix} 1/t^* & -r^*/t^* \\ -r/t & 1/t \end{Bmatrix}, \tag{2.2}$$

where we have used the current conservation and time reversal symmetry. Furthermore this matrix is parametrized as follow;[12)]

$$S=\begin{Bmatrix} e^{-i\mu} & 0 \\ 0 & e^{i\mu} \end{Bmatrix}\begin{Bmatrix} \sqrt{1+\rho} & \sqrt{\rho} \\ \sqrt{\rho} & \sqrt{1+\rho} \end{Bmatrix}\begin{Bmatrix} e^{-i\nu} & 0 \\ 0 & e^{i\nu} \end{Bmatrix}, \tag{2.2'}$$

where the parameters μ, ν and ρ vary in the regimes $-\pi\leqq\mu, \nu\leqq\pi$ and $0\leqq\rho\leqq\infty$. The eqs. (2.1) and (2.2) are valid even for microscopic system.

Because macroscopically identical samples of a finite size have different resistances depending on the specific microscopic impurity arrangement in each sample, it is necessary to introduce a statistical ensemble of systems and to consider the resistance distribution $P_L(\rho)$ over the ensemble of systems of a macroscopic length L. The dimensionless length L is scaled by the localization length. The corresponding ensemble of all the T-matrix forms a noncompact group SU(1, 1). It's differential probability is given by $dP(S)=P(S)\,d\mu(S)$, where $d\mu(S)=(2\Pi)^{-2}\,d\mu\,d\nu\,d\rho$ is an invariant measure and $P(S)$ is a probability density.

Now, let's suppose that two samples of the macroscopic lengths L and δL, which have T-matrices S and δS and probability density $P_L(S)$ and $P_{\delta L}(\delta S)$, are put together into a combined sample having the transfer matrix $\tilde{S}=S\times\delta S$. (i) Assuming that S and δS are statistically independent each other (it is accomplished in the macroscopic scale much larger than the structural correlation length of the electronic system) then the following expression

$$P_{L+\delta L}(\tilde{S})=\int P_L(\tilde{S}\delta S^{-1})P_{\delta L}(\delta S)\,d\mu(\delta S), \tag{2.3}$$

is obtained by convolution. (ii) Suppose that the probability density $P_L(S)$ is isotropic, that is, it depends only on the parameter ρ. Moreover, (iii) M-theory proposes an ansatz that the distribution $P_{\delta L}(\delta S)$ has to maximize the following information entropy ε with a constraint of the Ohm's law,[19)] $\langle\rho\rangle_{\delta L}=\delta L$ for $\delta L\ll 1$, to determine uniquely the form of $P_{\delta L}(\rho)$.

$$\varepsilon[P_{\delta L}]\equiv-\int P_{\delta L}(\delta S)\ln P_{\delta L}(\delta S)\,d\mu(\delta S). \tag{2.4}$$

Under these requirements ((i)-(iii)), the probability density $P_L(\rho)$ satisfies the following Fokker-Planck equation,

$$\frac{\partial P_L(\rho)}{\partial L}=\frac{\partial}{\partial\rho}\left(\rho(\rho+1)\frac{\partial P_L(\rho)}{\partial\rho}\right). \tag{2.5}$$

This is the fundamental equation of the M-theory of resistance derived by Mello.[12)] The equation (2.5) is derived also by some different approaches.[20,21] The moments of the resistance can be obtained by solving the following equation

$$\frac{\partial}{\partial L}\langle \rho^n\rangle_L = n(n+1)\langle \rho^n\rangle_L + n^2\langle \rho^{n-1}\rangle_L. \quad (2.6)$$

On the other hand, the transmission coefficient $T(=|t|^2)$ obeys the following eqs.,

$$\frac{\partial}{\partial L}Q_L(T) = T^2\frac{\partial}{\partial T}\left((1-T)\frac{\partial}{\partial T}Q_L(T)\right), \quad (2.7)$$

$$\frac{\partial}{\partial L}\langle T^n\rangle_L = n\,\{(n-1)\langle T^n\rangle_L - n\langle T^{n+1}\rangle_L\}, \quad (2.8)$$

by using the relation $T=(1+\rho)^{-1}$, where $Q_L(T)$ and $\langle T^n\rangle_L$ are probability distribution and moment of the transmission coefficients.

We call the distributions $P_L(\rho)$ and $Q_L(T)$ following the eqs. (2.5) and (2.7) the universal distributions throughout this paper. The universal relation between these moments based on the M-theory is inspected numerically in some microscopic disordered systems in the following section.

§3. Numerical Results for Purely Disordered System

3.1 Models

The following tightly binding one electron Hamiltonian,

$$H=\sum_{n=0}^{N}|n\rangle\,\varepsilon_n\,\langle n| + \sum_{n=0}^{N}(|n\rangle\, t_{n,n+1}\,\langle n+1| + |n+1\rangle\, t_{n+1,n}\,\langle n|), \quad (3.1)$$

is considered in order to investigate the applicability of the universal distributions $P_L(\rho)$ and $Q_L(T)$ of macroscopic systems to microscopic 1-DDS's. We consider two kinds of diagonally disordered systems. The first is the Anderson model (A-model), in which site energy ε_n is randomly and uniformly distributed in the range $[-W, W]$. The second model, which we will refer to as the discrete model (D-model), is the one in which the site energy takes only the value $-W$ or W.

The numerically obtained distributions of the transmission coefficient T and resistance ρ for a case of the system (3.1) are given in Fig. 1. Long tails are observed in these distributions, because these are expected to be the lognormal distributions for large enough systemsize L.

Now, we will investigate the moments or cumulants of the distribution instead of the distribution itself, because it is rather difficult to judge whether or not the numerically obtained histgrams itself of the distribution coincides with the universal one. Note that the larger the systemsize is, the more significantly the long tail appears in the distribution. As the contribution to the higher moments are dominated by the tail of the distribution for large systemsize, we will calculate numerically only the moments $\langle\rho\rangle_L$ and $\langle\rho^2\rangle_L$ of the nesistances, and the first-, second-, third- and the forth-order cumulants of the transmission coefficients.

3.2 *Numerical results of a universal distribution*

We consider only the case of the band center energy $E=0$ in this subsection. Figure 2 shows the numerical results of the relation between the variance $\langle(\Delta\rho)^2\rangle = \langle\rho^2\rangle - \langle\rho^2\rangle^2$ and the mean value $\langle\rho\rangle$ for a weakly disordered case, $W\leqq 0.3$, in A-model and D-model to decimate the unknown parameter; the localization length. A broken curve in Fig. 2 shows the following relation between the mean value and the variance derived by solving the eq. (2.6) ($\langle\rho\rangle_L = 1/2(e^{2L}-1)$, $\langle\rho^2\rangle_L = 1/6(e^{6L}-3e^{2L}+2)$),

$$\langle\rho^2\rangle - \langle\rho\rangle^2 = \langle\rho\rangle^2\,(4/3\,\langle\rho\rangle + 2). \quad (3.2)$$

The mean value $\langle\rho\rangle_L = 1/2(e^{2L}-1)$ coincides with the well-known exponential increase of the resistance with increasing the length L, obtained by a microscopic approach by Landauer[17] and Abrahams and Stephen[22] in RP model and by Stone *et al.*[23] in the weak scattering limit of TB model.

Even in the microscopic regime, $L \ll 1$ ($\langle\rho\rangle_L$

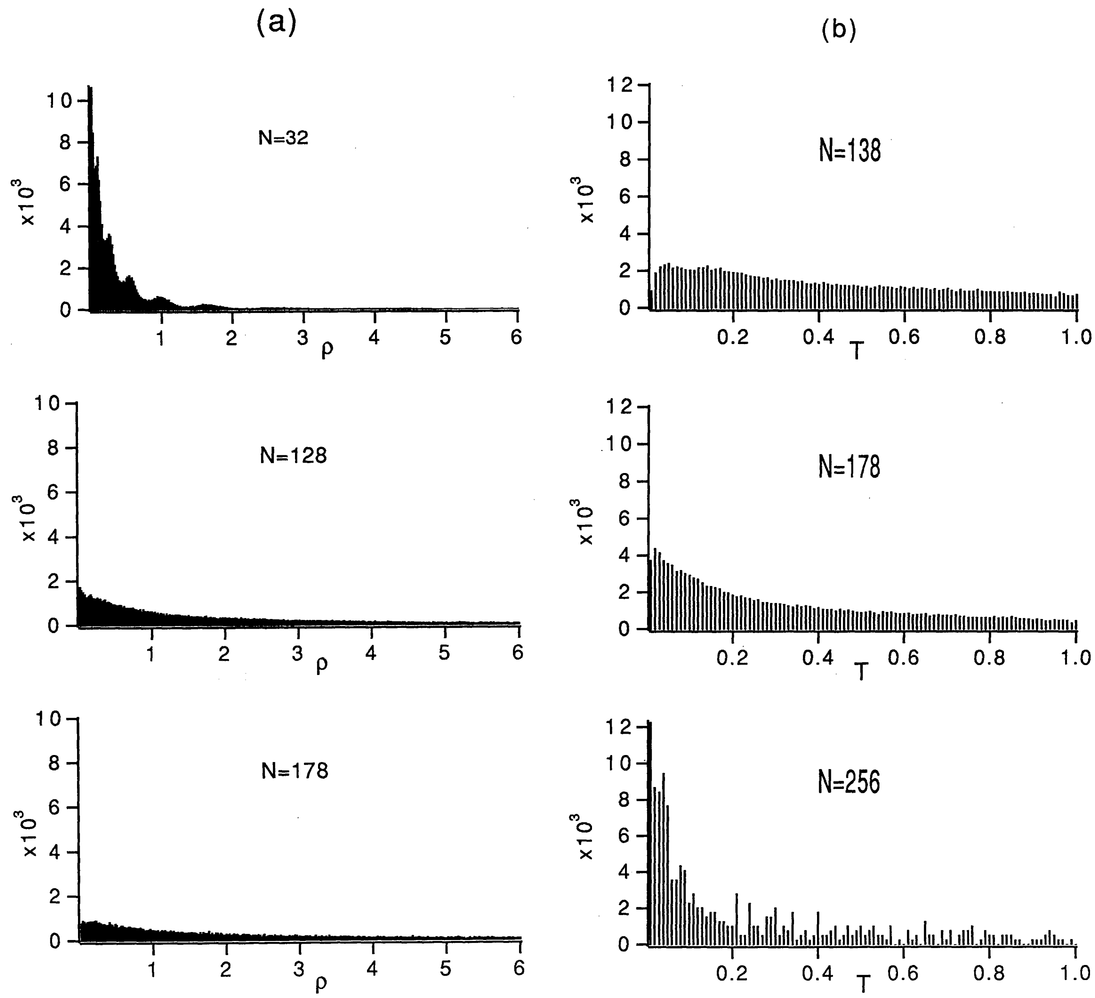


Fig. 1. Histograms of the distribution of the (a) resistance ρ and (b) transmission coefficient T at $E=0$ for D-model with $E=0$, $W=0.3$. The size of the ensemble is 2^{17}.

$\ll 1$), our numerical result obeys the relation (3.2) derived from M-theory within some uncertainties. The lognormal distribution observed in Fig. 1 causes the discord in a large scale, $L \gg 1$, as has been stated in §3.1, because a shortage of the number of samples becomes a serious problem in the numerical calculation when the scaled length L increases.

The relation between the values of several low-order cumulants of the transmission coefficient are given in Fig. 3, in which C_n indicates the n-th order cumulant. Each relation between the values of C_n and C_1 ($n=2, 3, 4$) looks like being on a common curve. Although we cannot draw the corresponding curves based on M-theory, because eq. (2.8) is unsolvable in the sense that the higher order moment $\langle T^{n+1}\rangle_L$ is necessary in order to obtain the moment $\langle T^n\rangle_L$, we can check whether or not our numerical results satisfy the following relations derived from eq. (2.8).

$$\frac{\partial}{\partial L}\langle T\rangle_L = -\langle T^2\rangle_L, \tag{3.3a}$$

$$\frac{\partial}{\partial L}\langle T^2\rangle_L = 2\langle T^2\rangle_L - 4\langle T^3\rangle_L, \tag{3.3b}$$

$$\frac{\partial}{\partial L}\langle T^3\rangle_L = 6\langle T^3\rangle_L - 9\langle T^4\rangle_L. \tag{3.3c}$$

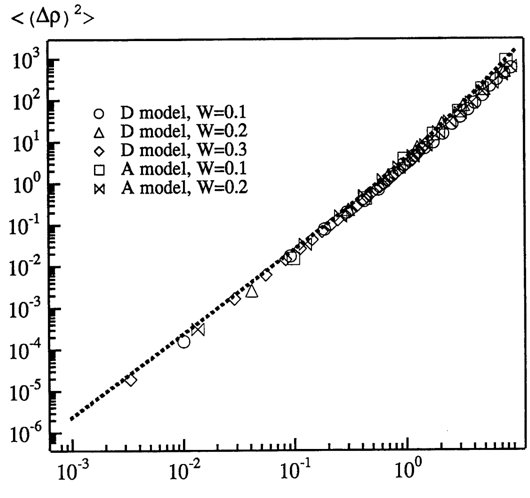
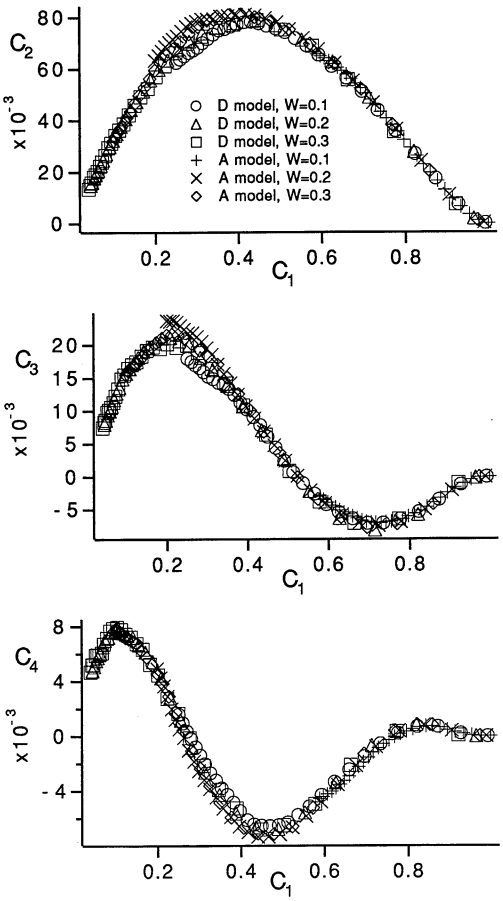


Fig. 2. Numerical results of the second-order cumulant $\langle(\Delta\rho)^2\rangle=\langle\rho^2\rangle-\langle\rho\rangle^2$ of the distribution of the resistance as a function of the mean value $\langle\rho\rangle$ for the case of $E=0$. The broken line shows the eq. (3.2).



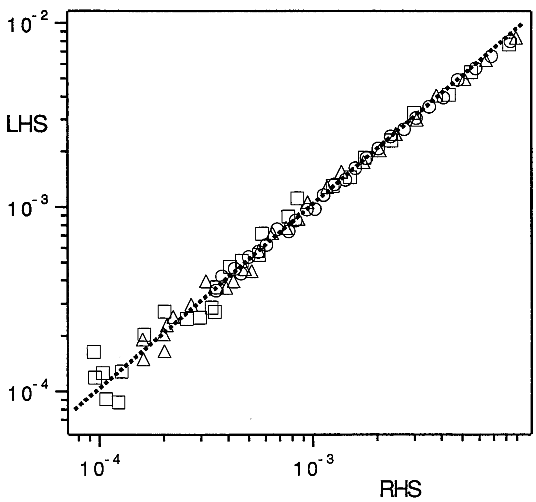


Fig. 4. Numerical results for the relations (3.3a) (○), (3.3b) (△), and (3.3c) (□) at $E=0$ by the numerical finite difference for D-model with $W=0.3$.

Figure 4 shows the numerical plots of the left hand side (lhs) versus rhs in eqs. (3.3a)–(3.3c) by means of the finite difference based on the numerical results. These data are plotted around the broken line describing lhs=rhs. Accordingly, we can say that at least the relations between these several low-order moments of the distributions of the transmission coefficient and resistance agree well with those based on the M-theory, irrespective of the potential strengths of the site energy in the weakly disordered regime and the model (A-model or D-model) in the case $E=0$.

Moreover, as the lower-order moments of the transmission coefficient include the information of the higher-order moments of the resistance, we can suggest that the resistance has a universal distribution $P_L(\rho)$, regardless of the potential strength and of A-model or D-model in a weakly disordered regime at the middle energy $E=0$.

◀ Fig. 3. Numerical results of the second-, third-, and the fourth-order cumulants of the distribution of the transmission coefficient T at $E=0$ as a function of the first-order cumulant. The C_n shows the n-th order cumulant of the distribution of the transmission coefficient.

3.3 Numerical results of non-universal distributions

In this subsection we propose the case violating the universal distribution $P_L(\rho)$. For this purpose, we indicate the deviation of a few cumulants of the distribution of the transmission coefficient from that of the D-model with $E=0$ and $W=0.3$ (we call it the standard distribution) discussed in the previous subsection and expected to have the universal distributions $P_L(\rho)$, $Q_L(T)$.

(A) Figure 5 shows some internal relations between the cumulants for the case of $E=0.5$ and $W\leqq 0.3$ of the A-model and D-model. Each relation between the values of C_n and C_1 ($n=2$, 3, 4) looks like being on a common curve as in the case of Fig. 3. The curves in Fig. 5 (for the case of $E=0.5$), however, are different from those in Fig. 3 (for the case of $E=0$) in the microscopic regime, $\langle T\rangle>0.5$ ($\langle\rho\rangle_L<1$). Figure 6 indicates the relation between the cumulants for several energies in D-model with $W=0.3$. The case of $E\neq 0$ is equivalent to a non-symmetric distribution of the site energy ε_n. Accordingly, we can say that the effect of it's microscopic non-symmetric property survives in the small scale, $\langle T\rangle>0.5$, and it disappears in the large scale limit.

(B) Moreover, when we consider the relations between the cumulants in a strongly disordered case (at $E=0$ and $W\geqq 1.0$), different functional forms from those of a standard distribution, which are partly shown in Fig. 6, are observed. This difference is partially suggested by a difference between the functional forms of the mean value $\langle\rho\rangle_L$ obtained by M-theory and by Stone *et al.* in the strongly disordered case.[23)]

In the above two cases, (A) and (B), we can guess that the assumptions (ii) or (iii) of the M-theory in §2 are violated.

In addition, it is easy to image that there is a different distribution from the universal one $P_L(\rho)$ for the off-diagonal disorder model ($\varepsilon_n=0$), because the requirement (i) is not accomplished on account of the correlation between the nearest neighbour sites.[24,25)]

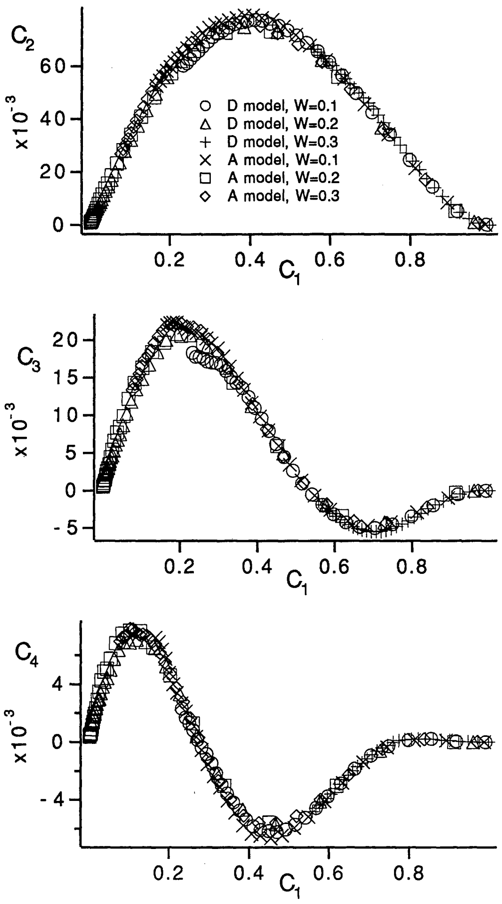


Fig. 5. Numerical results of the second-, third-, and the fourth-order cumulants of the distribution of the transmission coefficient T at $E=0.5$ as a function of the first-order cumulant.

§4. Modified Bernoulli Electronic System

We study in this section the distribution of the transmission coefficient in a disordered system with a long-range structural correlation.

These systems are described by a sequence $\{X_n\}$ generated by the following deterministic rule,

$$X^*_{n+1}=f(X^*_n)=X^*_n+2^{B-1}X^{*B}_n \quad (0<X^*_n\leqq 1/2)$$
$$\qquad\qquad X^*_n-2^{B-1}(1-x^*_n)^B \quad (1/2<X^*_n\leqq 1),$$
$$X_n=(2X^*_n-1)W, \tag{4.1}$$

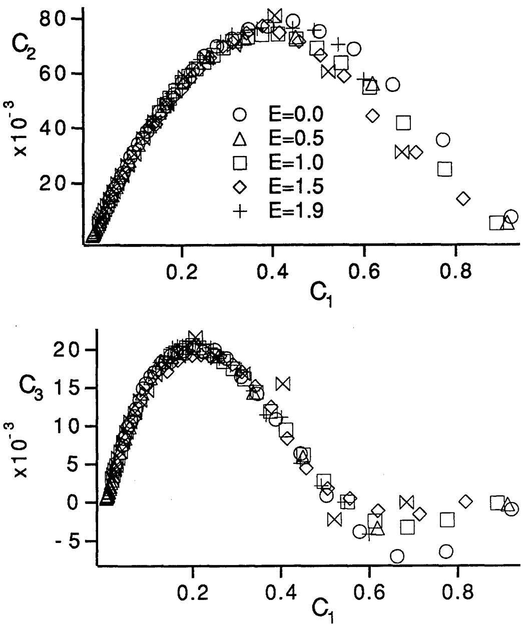


Fig. 6. Numerical results of the second- and the third-order cumulant of the distribution of the transmission coefficient T for various enrgies of D-model with $W=0.3$. The symbol(⋈) denotes a strongly disordered case of D-model at $E=0$ with $W=1.0$.

where B is a non-negative bifurcation parameter controlling the structural correlation.

We also use the symbolic sequence $\{Y_n\}$ coarse grained by the rule; $Y_n=-W$ for $0<X_n\leqq 1/2$ and $Y_n=W$ for $1/2<X_n\leqq 1$. We call these systems $\{X_n\}$ and $\{Y_n\}$ modified Bernoulli system (MB system) when the sequence $\{X_n\}$ or $\{Y_n\}$ is regarded as the site energy sequence $\{\varepsilon_n\}$ in eq. (3.1).

The properties of the MB system has been studied in detail ref. 26. It has turned out that the correlation functions $\langle X_i X_{i+n}\rangle$, $\langle Y_i Y_{i+n}\rangle$ decrease, obeying an inverse-power law with respect to the distance n for $1<B<2$.

Some typical distributions of the transmission coefficient are given in Fig. 7. We study the relation between the cumulants of transmission coefficient, as has been done in §3.3. Some typical relations between the cumulants are shown in Fig. 8 and Fig. 9. Remarkable deviations are observed in the relations when compared with those of the standard distribution. We can say that the distribution of the transmission coefficient in

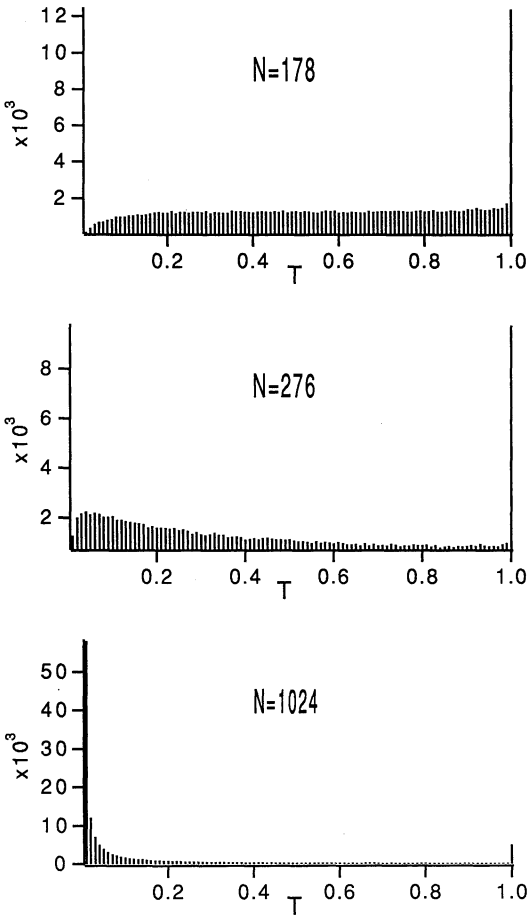


Fig. 7. Histograms of the distribution of the transmission coefficient T at $E=0$ of the Modified Bernoulli system with $B=1.7$ for some systemsize N.

MB system does depend on the bifurcation parameter B controlling the structural correlation, on the potential strength W, and also on the case of $\{X_n\}$ or $\{Y_n\}$.

Although the quantitative theoretical explanations for these behaviours has not been given, we can say qualitatively that the assumption (i) in §2 is broken in MB system, that is, the inverse-power law correlation in the microscopic sequences $\{X_n\}$ and $\{Y_n\}$ survives even in the macroscopic regime.

§5. Summary and Discussion

We have studied numerically the moments and cumulants of the distribution of the transmission coefficient and resistance in some tightly binding 1-DDS's, and we have ob-

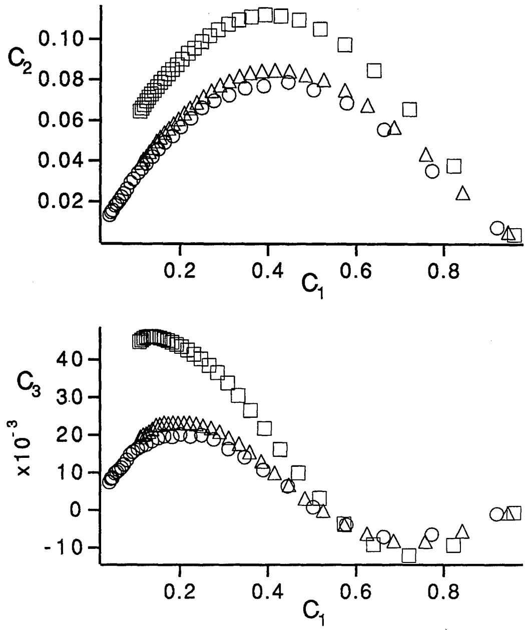


Fig. 8. Numerical results of the second- and the third-order cumulant of the distribution of the transmission coefficient T at $E=0$ as a function of the first-order cumulant for MB system $\{Y_n\}$ with $W=0.3$ and with the bifurcation parameter $B=1.5$(△) and 1.7(□). The circle (○) shows the case of the D-model as a reference.

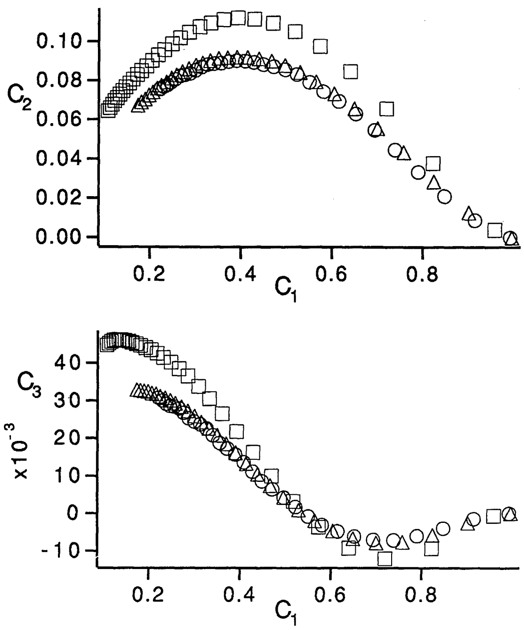


Fig. 9. Numerical results of the second- and the third-order cumulant of the distribution of the transmission coefficient T as a function of the first order cumulant for MB system $\{Y_n\}$ ($E=0, B=1.7$) with the potential strength $W=0.1$ (△), 0.3 (□), and those for MB system $\{X_n\}$ for the potential strength $W=0.3$ (○).

tained the following results.

(1) It is confirmed that the universal distribution $P_L(\rho)$ or $Q_L(T)$ derived in the M-theory is well realized at the middle energy $E=0$ of the A-model and D-model in the weakly disordered case, regardless of the detail of the potential strength. The above universality holds even in the microscopic regime characterized by an atomic length scale.

(2) On the contrary, in the case of non vanishing energy $E\neq 0$, the distributions are different from the universal ones $P_L(\rho)$, $Q_L(T)$ in the microscopic regime $\langle T\rangle > 0.5$. Also in the strongly disordered case at $E=0$, the distributions are different from the universal ones. It is suggested that the requirement (ii) or (iii) in §2 is not satisfied in these cases.

(3) In addition, in the MB system with an inverse-power law structural correlation the distributions are extremely different from the universal ones $P_L(\rho)$ and $Q_L(T)$. It is suggested qualitatively by a simple physical consideration that at least requirement (i) is not satisfied in MB system.

Finally, let's discuss on the relation between the conductance fluctuation numerically studied by Giordano[27] and our numerical results. He proposed that the cumulants of the conductance are universal functions of the average $\langle g\rangle$ in both one and two dimensions. However, we can say from the results in §3.3 and MB system that this universality comes true only for limited cases of 1-DDS's.

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