Delocalization in One-Dimensional Tight-Binding Models with Fractal Disorder

Hiroaki S. Yamada

Yamada Physics Research Laboratory, Aoyama 5-7-14-205, Niigata 950-2002, Japan

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In the one-dimensional disordered systems, the correlation-induced localization-delocalization transition has been observed. In this study, we investigate the effect of the differentiability and/or correlation of the potential on the localization property in a tight-binding model with fractal disorder. We obtain a phase transition diagram from localized to extended states based on the renormalized localization length by controlling the correlation and the disorder strength of the potential. In addition, the transition of the diffusive property of wavepacket dynamics is shown around the transition point.

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I. INTRODUCTION

Mathematically rigorous results on the localization phenomena in one-dimensional Schrödinger operators are followings [1, 2]. G-M-P theorem states that one-dimensional tight-binding model with an ergodic and stationary random potential have a positive Lyapunov exponent of the wavefunction with probability 1 [3]. The positive Lyapunov exponent is necessary-sufficient condition for a pure point set spectrum of the operator and all the eigenfunctions decay exponentially in the thermodynamic limit. However, necessary-sufficient condition for the exponential localization has not been given yet. The Kotani’s theory state that if the potential sequence is nondeterministic under the conditions (i) stationarity, (ii) ergodicity, (iii) integrability, then there is no absolutely continuous (a.c.) spectrum of the operators [3]. These theorems can be proven true for continuous and discrete one-dimensional disordered systems [6, 8]. An interesting question to ask is whether it is possible to characterize the potentials with the metal-insulator transition in the one-dimensional tight-binding model.

There is a possibility that the correlation effect of the potential sequence breaks the strong exponential localization and can generate a localization-delocalization transition. Indeed, many authors numerically observed correlation-induced a localization-delocalization transition by using the some correlated potential sequence with correlation-induced a localization-delocalization transition. In this paper, we numerically study the correlation-induced localization-delocalization transition by using tight-binding model with Weierstrass potential which was used by Garcia and Guevas [21]. We can see a quite different feature between the cases for \( D \leq 3/2 \) and ones for \( D > 3/2 \) in the weak disorder strength. The finite-size scaling analysis for the renormalized localization length at band center numerically suggests the existence of the delocalized states around \( D \approx 3/2 \) in the case of the relatively weak potential strength. On the other hand, in the case with the relatively strong disorder strength, the transition point becomes smaller value than \( D = 3/2 \). Petercen and Sandler insisted that effect of the anticorrelation is also important to understand the transition due to the correlation of the sequence [23].

On the other hand, the localization-delocalization transition due to the differentiability of the potential function also exists without contradiction with the Kotani’s theory. Indeed, Garcia and Cuevas recently studied the transition based on the differentiability of the disorder potential as a necessary condition for the delocalization [20, 21]. They modeled an algebraic decaying power spectrum by some fractal functions with fractal dimension \( D \). A certain degree of differentiability assures that the potential in neighboring sites is strongly correlated. It has been numerically suggested that the transition takes place at \( D = 3/2 \), and the potentials with minimum degree of differentiability and sufficiently strong long-range correlations produce a band of metallic states by means of the distribution of the level-spacing.

In this paper, we numerically study the correlation-induced localization-delocalization transition by using tight-binding model with Weierstrass potential which was used by Garcia and Guevas [21]. We see a quite different feature between the cases for \( D \leq 3/2 \) and ones for \( D > 3/2 \) in the weak disorder strength. The finite-size scaling analysis for the renormalized localization length at band center numerically suggests the existence of the delocalized states around \( D \approx 3/2 \) in the case of the relatively weak potential strength. On the other hand, in the case with the relatively strong disorder strength, the transition point becomes smaller value than \( D = 3/2 \). Furthermore, we investigate the quantum diffusion of the initially localized wavepacket in the system. The transition from the localized state to ballistic states occurs around \( D \approx 3/2 \) without scale invariant subdiffusive behavior.

II. MODEL AND METHOD

We consider the usual tight-binding model describing single-particle electronic wave function \( \{ u(n) \} \) in the
site representation as follows;
\begin{equation}
    u(n - 1) + u(n + 1) + WV(n)u(n) = Eu(n),
\end{equation}
where $E$ and $WV(n)$ are energy of the system and the on-site energy with the $W$ is the disorder strength, respectively. To model correlated and non-differential disorder potential, we use the following prescription for $V(n)(n \leq N)$ in Eq. (1):
\begin{equation}
    V(n) = C(D) \sum_{k=0}^{L} \frac{\sin(2\pi a^k n/N + \phi_k)}{a^{(2-D)k}},
\end{equation}
where $a$ is a constant value ($a > 1$), $D$ is a fractal dimension ($1 < D < 2$), and $\phi_k$ is random independent variable chosen in the interval $[0, 2\pi]$. $C(D)$ is the normalization constant which is determined by a normalization condition
\begin{equation}
    \sqrt{\langle V(n)^2 \rangle} - \langle V(n) \rangle^2 = 1,
\end{equation}
where $\langle \ldots \rangle$ indicates the average over realization of the phases in Eq. (2).

If we set $n/N = x$, $\phi_k = 0$, the potential becomes "Weierstrass function" with continuous and indifferentiable everywhere by taking a continuous limit $N \to \infty$ and $L \to \infty$. The potential will be shortly transferred to as "Weierstrass potential", and we set $a = 2$ and $L = 50$ thorough this paper without loss of the generality and numerical accuracy. The power spectrum $S(f)$ of the Weierstrass function is empirically characterized by the fractal dimension $D$ as follows;
\begin{equation}
    S(f) \sim \frac{1}{f^{\alpha - 2D}}.
\end{equation}
In compassion with the form $S(f) \sim 1/f^\alpha$,
\begin{equation}
    D = 1 + \frac{3 - \alpha}{2}.
\end{equation}
Accordingly, the condition $\alpha \geq 2$ corresponds to the condition for the fractal dimension $D \leq 3/2$ that suggests the presence of the metal-insulator transition. Increasing $\alpha$ corresponds to increasing correlations up to long-range correlated disorder. The analytical property of the autocorrelation function of the Weierstrass potential $V(n)$ is given in appendix A.

In addition to the long-range correlation, the fractal dimension $D$ also controls the degree of the differentiability of the potential part. The degree of the differentiability increases as the decrease of the fractal dimension $D$. The smoothness of the potential fluctuation can induce the delocalization of the quantum states, which property is directly related to analyticity of the potential function in the continuum limit, as pointed out by Garcia and Cuevas. They numerically showed possibility of the localization-delocalization transition at $D = 3/2$ as increasing the degree of the differentiability $D$ of the Weierstrass sine potential by using level-space distribution of the energy spectrum [20, 21]. The result is not contradict to Kotani’s theory because the Weierstrass potential become non-stationary for $1 \leq D \leq 3/2$. Moreover, we also investigate the potential strength $W$ dependence of the delocalization in the long-range correlated disordered potential.

In the following sections, we numerically investigate the localization-delocalization property for various parameter combinations ($E, W, D, N$).

## III. SOME PRELIMINARY

The finite size Lyapunov exponent $\gamma_N(N \gg 1)$ of the one-dimensional systems can be defined by
\begin{equation}
    \gamma_N = \frac{\langle \ln |u(N) - u(N + 1)|^2 \rangle}{2N},
\end{equation}
with initial state $u(0) = u(1) = 1$. Then the Lyapunov exponent $\gamma$ and the localization length $\xi$ are given by $\gamma = \lim_{N \to \infty} \gamma_N$ and by $\xi = 1/\gamma$, respectively. In addition, the normalized localization length,
\begin{equation}
    \Lambda_N \equiv \frac{\xi(N)}{N} = \frac{1}{\gamma_N N},
\end{equation}
is useful to study the localization-delocalization transition. It is known that $\Lambda_N$ decreases (increases) with the system size $N$ for localized (extended) states, and it becomes constant for the critical states.

Figure 1(a) shows the energy dependence of the Lyapunov exponent $\gamma_N$ for some values of the fractal dimension $D$. The Lyapunov exponent $\gamma_N$ at the band center $E = 0$ decreases as the value of the $D$ decreases. It suggests the possibility of the delocalized states (extended states) at the band center $E = 0$ for small values of $D(\leq 3/2)$. Figure 1(b) and (c) show the potential strength dependence of the Lyapunov exponent $\gamma_N$ and the renormalized localization length $\Lambda_N$ at the band center $E = 0$ for some parameter sets. In the weak disorder case $W < < 1$, the numerical data lead to
\begin{equation}
    \gamma_N \propto W,
\end{equation}
despite of the system size, which is equivalent to case of the uncorrelated potential case. In the strong disorder cases, the Lyapunov exponent do not depend on the system size $N$. Figure 1(c) shows the $W-$dependence of the normalized localization length $\Lambda_N$. It is found that the localization length is larger than system size in the week disorder limit.

The results suggest that for the strongly correlated limit, there is a possibility of the states with $\gamma_N \to 0$ and/or $\Lambda_N > 1$ in the thermodynamic limit $N \to \infty$, which correspond to a delocalized phase of the extended states in week disorder limit $W < < 1$.

In the next section, we investigate the localization-delocalization transition in more detail.
The result suggests that in the relatively weak potential regime $W < 1$, the quantum states can be classified by the exponent $\delta$. Generally, if the system size dependence of the normalized localization length $\Lambda_N$ algebraically behaves as,

$$\Lambda_N \sim N^{\delta},$$

the quantum states can be classified by the exponent $\delta$, i.e., $\delta < 0$ for the localized states, $\delta > 0$ for the extended states, $\delta = 0$ for the critical states.

IV. LOCALIZATION-DELOCALIZATION TRANSITION

This is the main section of the present paper. Generally, if the system size dependence of the normalized localization length $\Lambda_N$ algebraically behaves as,

$$\Lambda_N \sim N^{\delta},$$

the quantum states can be classified by the exponent $\delta$, i.e., $\delta < 0$ for the localized states, $\delta > 0$ for the extended states, $\delta = 0$ for the critical states.

Figure 2 shows the system size dependence of the normalized localization length at the band center for $W = 0.98$ and $W = 0.4$. It clearly found that the wavefunction goes to localized states in the thermodynamic limit as $\Lambda_N \sim N^{-1}$ independent of the fractal dimension when the potential strength is relatively large ($W = 0.98$). On the other hand, there is a possibility of a localization-delocalization transition for small values of the disorder strength ($W = 0.4$) depending on the fractal dimension. It seems that in the $N$-dependence of the normalized localization length the sign of the index $\delta$ changes from negative to positive at the point $D = 3/2$. The result suggests that in the relatively weak $W$ the quantum states are localized for $D > 3/2$ and are delocalized for $D < 3/2$. The exponents $\delta$ obtained by the least-square method are shown in Fig. 3. The exponent $\delta$ decreases with respect to the fractal dimension $D$ as

$$\delta \sim (3/2 - D)^{-1.88}.$$ (10)

In what follows, we investigate the renormalized localization length $\Lambda_N$ as a function of the system size $N$ for the potential strength (a) $W = 0.98$ and (b) $W = 0.4$ at the potential with several values of the fractal dimensions.

FIG. 1: (Color online) (a) The Lyapunov exponent $\gamma_N$ as a function of energy $E$ for some values of the fractal dimension $D$ at a weak disorder case, $W = 0.2$. The system and ensemble sizes are $N = 2^{12}$ and $2^{10}$, respectively. (b) The Lyapunov exponent $\gamma_N$ and (c) renormalized localization length $\Lambda_N$ at the band center $E = 0$ as a function of the potential strength $W$ for the several values of the $D$. This system and ensemble sizes are $N = 2^{14}$ and $2^{10}$, respectively.

FIG. 2: (Color online) The normalized localization length $\Lambda_N$ as a function of the system size $N$ for the potential strength (a) $W = 0.98$ and (b) $W = 0.4$ at the potential with several values of the fractal dimensions. The typical basis size $N$ and ensemble size used here are $N = 2^{12} \sim 2^{17}$ and $2^{10}$, respectively and the robustness of the numerical calculations with respect to the systems size is confirmed in each case. Figure 2 shows $W$-dependence of the renormalized localization length at band center $E = 0$ by changing the systems size for some typical parameter sets ($W, D$). The $W, D$ dependence regime $W > 1$, and the $W$-dependence relatively smoothly drops down around $W \sim 1$ in the same way even for all cases with different systems size.
for $D < 1$ becomes very weak and the $W-$dependence sharply decreases at certain value of $W$. Apparently, we can expect that for $D \leq 3/2$ the $W-$dependence of the renormalized localization length shows an universal jump in the thermodynamic limit $N \rightarrow \infty$. This feature suggests the existence of a transition to delocalized states in the limit $N \rightarrow \infty$. In the Fig. we show the $D-$dependence of the normalized localization length for some values of $W$ in order to find out the critical value $D_c$ that all curves of different system size intersect at the value . The intersection corresponding to a transition point can be observed around $D = 3/2$ in the relatively weak potential strength $W \leq 0.7$.

Figure shows the phase diagram in the $D-W$ space separating the localized and delocalized states, which is obtained by the $D-$dependence of the renormalized localization length, as shown in the Fig. In the relatively weak potential strength ($W \leq 0.7$), the result coincides with the renormalized localization length shows an universal jump in the thermodynamic limit $N \rightarrow \infty$. This feature suggests the existence of a transition to delocalized states in the limit $N \rightarrow \infty$. In the Fig. we show the $D-$dependence of the normalized localization length for some values of $W$ in order to find out the critical value $D_c$ that all curves of different system size intersect at the value . The intersection corresponding to a transition point can be observed around $D = 3/2$ in the relatively weak potential strength $W \leq 0.7$.
with the result obtained by Garcia and Cuevas. On the other hand, the result suggest that in the relatively large potential strength \( W \), the critical value of the fractal dimension becomes the smaller value than \( 3/2 \).

V. QUANTUM DIFFUSION

It can be expected that for sufficiently differentiable potentials a band of delocalized states occurs due to destruction of the interference effects in the reflected components of the wavepacket.

In this section, we examine the quantum diffusion of the initially localized wave packet by changing the parameter \( D \). Then we monitor the mean square displacement (MSD) of the wavepacket,

\[
m_2(t) = \sum_n (n - n_0)^2 |u(n, t)|^2,
\]

where \( n_0 \) is an initially localized site. The quantum time-evolution is given by,

\[
\frac{\text{i} \hbar}{\partial t} u(n, t) = u(n + 1, t) + u(n - 1, t) + W V(n) u(n, t),
\]

where \( n = 1, 2, ..., N \) with initial state \( u(n, t = 0) = \delta_{n,n_0} \) and \( \hbar = 1 \).

Figure 7 shows the time-dependence of the MSD for a fixed potential strength \( W = 0.8 \) for some values of \( D \). The parameter sets we used are denoted in Fig.6. Apparently, the \( m_2 \) ballistically grows for the relatively small values of \( D \) and it is suppressed and localized for the cases with \( D > 3/2 \).

Next, Fig.8 shows the diffusive properties for some values of the potential strength at fractal dimension, \( D = 1.4, D = 1.6 \), are shown in Fig.6. It follows that the ballistic motion \( (m_2 \sim t^\beta, \beta > 1) \) can be obtained for all cases with \( D = 1.4 \), while it is well-localized for the relatively larger value of \( W \) in the cases with \( D = 1.6 \). The all of the cases of \( D = 1.6 \) are localized for the long-time calculation. (It is not shown here.)

As a result, it seems that in the quantum diffusion the critical value also exists around \( D \approx 3/2 \) which is consistent with the result by the renormalized localization length in the last section.

However, clear subdiffusive behavior have not been observed around the critical point \( D = 3/2 \), which is different from the localization-delocalization transition in three-dimensional disordered systems and polychromatically perturbed systems as \( m_2 \sim t^{2/3} \), predicted by the one-parameter scaling theory at the critical point [24–26].

VI. SUMMARY AND DISCUSSION

In this work we numerically investigated the combined effects of the disorder strength \( W \) and the order of the
long-range correlation characterized by fractal dimension $D$ in the one-dimensional tight-binding model with the Weierstrass potential. The result strongly suggests that quantum states are localized for $D > 3/2$, whereas we have obtained critical disorder strength $W_c$ which separates extended and localized regimes for values $D \leq 3/2$. The localization-delocalization transition point $D = 3/2$ is consistent with one predicted by the other correlated potential with the power spectrum $S(f) \sim 1/f^\alpha$ , $\alpha = 2$.

Moreover, there are the other types of long-range correlated potential with discrete values, such as binary and ternary sequences [28, 29]. One of the common point between the discrete and continuous models is nonstationary of the potentials caused by the long-range correlation. Accordingly, the indifferentiable everywhere condition may be unified into the nonstationary condition ($\alpha \geq 2$) for the delocalization in the one-dimensional disorder system.

It has been shown that in some sparse random potentials and binary systems the violation of the stationarity bring about the delocalized states. However, studying the effect of the disorder strength in a long-range correlated disorder chain is still open problem [3, 27]. The nonstationarity-induced delocalization and presence of the mobility edge are also interesting problems in the correlated disordered systems [10, 28, 30, 31].

In practice, real DNA chains can be described by the four symbolized sequence as "A", "C","G","T". It is well-known that the coding and/or non-coding regions exhibit the long-range correlation with the power spectrum $S(f) \sim 1/f^\alpha$ (1 < $\alpha$ < 2) [32, 33]. Accordingly, it is expected that the localization-delocalization problem is strongly related to electronic conduction in DNA chain. In the cases, the effect of the finite size will work on the conductive properties although the DNA chains with the exponent $\alpha < 2$ have the localized states in the thermodynamic limit.

Appendix A: Correlation function

The normalized autocorrelation function $C(a, n, m)$ of the Weierstrass potential sequence $V(n)$ can be analytically calculated, as given for the FFM-potential by Petersen and Sandler [23]. The explicit form becomes,

$$C(a, n, m) = \frac{< V(n)V(m) >}{< V(n)^2 >},$$

$$= \frac{\sum_{k=0}^{L/2} a^{-2(2-D)k} \cos \left[ 2\pi a^k |n - m| \right]}{\sum_{k=0}^{L/2} a^{-2(2-D)k}}$$

where $< ... >$ denotes the ensemble average over the independent phases $\{\phi_k\}$. We set the distance between positions $\ell = n - m$, and impose the periodic boundary conditions on the correlation function defined in $\ell \in [0, L/2]$. In addition, we set $r = 2\ell/L$ and $r \in [0, 1]$ for the thermodynamic limit $L \rightarrow \infty$. Then the autocorrelation function is

$$C(a, r) = \frac{\sum_{k=0}^{\infty} a^{-2(2-D)k} \cos(\pi a^k r)}{\sum_{k=0}^{\infty} a^{-2(2-D)k}},$$

In the critical case, $D = 3/2$, it becomes

$$C(a, r) = \frac{\sum_{k=0}^{\infty} a^{-k} \cos(\pi a^k r)}{\sum_{k=0}^{\infty} a^{-k}}.$$

Figure 9 shows the autocorrelation function $C(a = 2, r)$ for various values of the fractal dimension $D$ given by Eq. (A3). It follows that the correlation function becomes concave for $D < 3/2$ and it linearly decreases near $r \approx 0$ for the critical value of $D$. The smaller the fractal dimension $D$ becomes, the correlation becomes more

![Figure 8](https://example.com/figure8.png)

**FIG. 8**: (Color online) The second moment $m_2$ as a function of time for some values of $W$ ($W = 0.6, 0.7, 0.8, 0.9$) at (a) $D = 1.6$ and (b) $D = 1.4$. We set $\hbar = 1$ and $\delta t = 0.05$. The system size and sample sizes are $N = 2^{16}$ and 10, respectively. The inset shows the log-log plots.
negative. The inset of the Fig. 9 shows the values of the correlation function at $r = 1$ as a function of the fractal dimension. It is noted that the correlation function goes negative value at the thermodynamic limit $r = 1$ for $D < 3/2$. Such a property has been pointed out by Petersen and Sandler in the case of the FFM-potential [23].

![Fig. 9](image)

**FIG. 9:** (Color online) The autocorrelation function $C(r)$ as a function of the distance $r$ for various fractal dimension $D$ given by Eq. (A3). The parameters are $a = 2, N = 2^{15}$. The inset shows the correlation function between the two most distant points.

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