Exact electronic ground state of a one-dimensional disordered lattice: Multifractal analysis

Kazumoto Iguchi
Computational Sciences Research Laboratory, Fujitsu Limited, Shinkamata, Ota-ku, Tokyo 144, Japan
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We discuss an exact electronic gound state of a one-dimensional disordered lattice, where the lattice disorder is introduced by a multiplicative random-walk process. The disorder fluctuation and the spatial fluctuation of the wave function are investigated. The theory proves that for the symmetric random walk there is multifractality for the former and non-self-similarity for the latter, using the multifractal analysis that has been developed recently. However, for the asymmetric case, we prove the multifractality for both. Also a connection betwen the ground state, the random walk, and statistical mechanics in one dimension is shown.

I. INTRODUCTION

The localization of electrons in disordered solids has been of theoretical and experimental interest for many years among condensed-matter physicists. Although Anderson[1] and Abrahams *et al.*[2] provided the fundamental theory of the disordered lattices, much of the problem is still unclear. The most important point is whether or not we can understand the nature of the exact wave function of an electron in certain physical models.

Recently, the concept of multifractals in the quasiperiodic lattices has been developed by Tang and Kohmoto,[3] Sutherland,[4] Kohmoto, Sutherland, and Tang,[5] and Sutherland.[6] In this problem a Fibonacci-lattice-type structure shows a power-law growth of the wave functions. Also, the Harper equation arising from the problem of an electron in a two-dimensional lattice under a uniform magnetic field shows a similar behavior of multifractality at the critical strength of the potential (i.e., $\lambda_c=2$). When the strength is smaller than λ_c, all the electronic states are extended, and when the strength is larger than λ_c, all the states are localized. Thus it is believed that at λ_c all the states are neither localized nor extended, namely, critical. Especially, for the golden-mean irrationality, it was shown that the multifractal analysis developed by Halsey *et al.*[7] played a crucially important role in order to determine both the energy band and wave functions of the quasiperiodic lattices.[3–6]

Following the same context of the multifractal nature of the wave function, electronic states of a disordered lattice have been studied by several authors,[8–11] using the idea of the multifractal analysis.[7] The most fascinating aspect of the problem is that even the one-dimensional disordered lattice model shows multifractality of the wave function. What is of interest is multifractality of both the disorder and spatial fluctuations of the wave functions of the disordered lattice. The former leads one to consider the generalized Lyapunov exponents $L(q)$ and the generalized localization lengths $\xi(q)$, where we have $1/\xi(q)=L(q)/q$, being defined by

$$L(q)\equiv\lim_{n\to\infty}\frac{1}{n}\ln(\langle|\psi_n|^q\rangle)\ . \quad (1)$$

Here the average for the wave function is taken over the disorder of lattice. This describes how the wave function fluctuates or disorders over the lattice with respect to the configurations of the disorder. The latter leads to consider how the single wave function is clustered in the space direction.

Pietronero *et al.*[11] studied the model that was proposed by Schneider *et al.*[12] In this model the lattice disorder is dominated by a random multiplicative process of a variable $\phi(n)$ and the disordered wave function is given as the "exponentiated random-walk" wave function [see Eq. (5)]. They considered only the case of the symmetric random walk [i.e., $p=\frac{1}{2}$ in Eq. (8)]. And they speculated that there is no self-similarity for the spatial fluctuation, while the disorder fluctuation of the wave function shows real multifractality based upon their numerical results.

In this paper we will reconsider the above problem and give an exact treatment of the multifractality for the electronic ground-state wave function in a one-dimensional disordered lattice. Fully using the multifractal analysis, we will prove the following with some nontrivial and exact results: In the symmetric random-walk case, we can prove the above conjecture, but otherwise the conjecture is no longer true, and we will prove contrarily that there appears multifractality for both the disorder and spatial fluctuations of the wave function. We will see that there is a mathematical connection between the expressions of the electronic ground state, the classical random walk, and statistical mechanics in one dimension.

The organization of the paper is the following. In Sec. II we present the model we are concerned with. In Sec. III the disorder fluctuation of the wave function is discussed. In Sec. IV the spatial fluctuation of the wave function is discussed. Finally, a summary is given in Sec. V.

II. MODEL OF A ONE-DIMENSIONAL DISORDERED LATTICE

We start with a one-dimensional tight-binding model for an electron on a disordered lattice:[1]

$$-\psi_{n+1}-\psi_{n-1}+V_n\psi_n=E\psi_n \; . \tag{2}$$

We now assume a field $h(n)$ on each bond, such that a single-valued scalar function $\phi(n)$ on lattice sites is defined by

$$\phi(n)=\sum_{n'=0}^{n} h(n) \tag{3}$$

and

$$h(n)=\phi(n+1)-\phi(n) \; . \tag{4}$$

We try an ansatz for an exact unnormalized wave function of the following form as well as the form used by Peietronero *et al.*[11] and Schneider *et al.*:[12]

$$\psi_n=\psi(n|1)=\exp[-\phi(n)] \; . \tag{5}$$

This is the ground-state wave function because it is always positive definite on all sites, with $E=0$.[12] Since the eigenvalue equation [Eq. (2)] can be written as

$$\frac{\psi_{n+1}+\psi_{n-1}}{\psi_n}=V_n-E \; , \tag{6}$$

identically it becomes

$$\exp[-h(n+1)]+\exp[h(n-1)]=V_n-E \; , \tag{7}$$

which determines V_n as a local potential, depending upon the nature of local coordination of the lattice at site n. When we take the probability distribution of $h(n)$ characterized by

$$P(h(n))=p\delta(h(n)-h_0)+(1-p)\delta(h(n)+h_0) \; , \tag{8}$$

with $0\le p\le 1$, for the ground state ($E=0$), V_n takes only possible three values: $2\exp(h_0)$ with probability $p(1-p)$, $2\exp(-h_0)$ with $(1-p)p$, and $2\cosh(h_0)$ with p^2 or $(1-p)^2$.

The problem that we are going to understand here becomes equivalent to that of the random multiplicative processes as studied by Pietronero and Siebesma.[13] If we use the probability distribution given by Eq. (8), we have the recursive equation for the probability of $\phi(n)$ taking the value $(2r-n)h_0$ for $0\le r\le n$:

$$D(r|n+1)=pD(r+1|n)+(1-p)D(r-1|n) \; , \tag{9}$$

which describes a one-dimensional random walk of $\phi(n)$ on the sites (usually $p=\frac{1}{2}$ for a symmetrical random walk). Physically speaking, this distribution describes the possible ensemble of the wave function at the nth site. If we take continuum limit of Eq. (9), we get a diffusion equation biased with $2p-1$:

$$\frac{\partial}{\partial n}D(r|n)=\frac{\partial^2}{\partial r^2}D(r|n)+(2p-1)\frac{\partial}{\partial r}D(r|n) \; . \tag{10}$$

Hereafter we will follow the method for the critical electronic states of quasicrystals by Sutherland.[4,6] Let us define the Fourier transform of the probability distribution $D(r|n)$:

$$D(r|n)=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\omega\, e^{i\omega(r-n)}\mathcal{D}(\omega|n) \; . \tag{11}$$

Substituting Eq. (11) into Eq. (9), we get

$$\begin{aligned} D(\omega|n+1)&=(pe^{i2\omega}+1-p)D(\omega|n)\\ &=(pe^{i2\omega}+1-p)^n D(\omega|0) \; . \end{aligned} \tag{12}$$

Then substituting Eq. (12) into Eq. (11), again, we are able to get the following for the probability that $\phi(n)$ has the value of $(2r-n)h_0$ at the nth site:

$$\begin{aligned} D(r|n)&=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\omega\, e^{i\omega r}[pe^{i\omega}+(1-p)e^{-i\omega}]^n D(\omega|0)\\ &=\frac{n!}{(n-r)!r!}p^r(1-p)^{n-r} \; , \end{aligned} \tag{13}$$

where we have used $D(\omega|0)\equiv 1$ without losing generality.

III. DISORDER FLUCTUATION OF THE WAVE FUNCTION

First, we are concerned with multifractality of the disorder fluctuation of the wave function. What we would like to know is the ensemble average of the wave function at site n with respect to the configurations of the disorder, which is called the partition function. This allows us to understand the nature of the wave function. The growth of this quantity provides much information about the localization of the wave function. The partition function is defined by

$$Z_n(\beta)\equiv\langle|\psi_n|^\beta\rangle=\langle\psi(n|\beta)\rangle\propto e^{nF(\beta)} \; , \tag{14}$$

where we have used an identity $\psi^\beta(n|1)=\psi(n|\beta)$ and $F(\beta)$ for the index β is an exponent to see how fast the wave function grows (or decreases). By means of this identity, the wave function satisfies

$$\psi(n+1|\beta)=e^{-\beta h(n+1)}\psi(n|\beta) \; , \tag{15}$$

which allows us to calculate the exponents of the wave function, using the multiplicative nature of the random walk.[13]

Coming back to the expression of the partition function $Z_n(\beta)$, this can be converted to

$$Z_n(\beta)=\sum_{0\le r\le n}D(r|n)[A(r|n)]^\beta \; , \tag{16}$$

with

$$A(r|n)=e^{-(n-2r)h_0} \; , \tag{17}$$

which measures the order of the amplitude of the wave function. It is proven directly by the following idea. If we use the multiplicative random walk of $\phi(n)$, the ensemble average is taken over the distribution of r for the amplitude $A(r|n)$ of the wave function on site n. Thus we end up with the expression (16).

To obtain the asymptotic behavior of the partition function as $n\to\infty$, we first substitute Eq. (13) into Eq. (16). Then we obtain

$$Z_n(\beta)=\sum_{0\le r\le n}\frac{n!}{(n-r)!r!}p^r(1-p)^{n-r}e^{-(n-2r)\beta h_0}$$
$$=\sum_{0\le r\le n}\frac{n!}{(n-r)!r!}e^{r\ln p+(n-r)\ln(1-p)-(n-2r)\beta h_0}$$
$$=\sum_{0\le r\le n}\frac{n!}{(n-r)!r!}e^{n[(r/n)\ln p+(1-r/n)\ln(1-p)-(1-2r/n)\beta h_0]} . \tag{18}$$

And we use the Stirling formula $\ln(n!)=n\ln n-n$ as $n\to\infty$ for the first factor in the integrand of Eq. (18). Therefore we have

$$\frac{n!}{(n-r)!r!}=\exp[\{n\ln n-n\}-\{(n-r)\ln(n-r)-(n-r)\}-\{r\ln r-r\}]$$
$$=\exp[n\ln n-(n-r)\ln(n-r)-r\ln r]$$
$$=\exp[-n\{(1-r/n)\ln(1-r/n)+(r/n)\ln(r/n)\}] . \tag{19}$$

After substituting Eq. (19) into Eq. (18) and changing the variable $x=r/n$, we can express the partition function in terms of an integral:

$$Z_n(\beta)\xrightarrow{n\to\infty}\int_0^1 dx\, e^{nF(x)} , \tag{20}$$

where for an arbitrary $p\,(0\le p\le 1)$ we have

$$F(x)=-x\ln x-(1-x)\ln(1-x)+x\ln p+(1-x)\ln(1-p)-(1-2x)\beta h_0 , \tag{21}$$

with $x=r/n$. The expression of $F(x)$ for $p=\frac{1}{2}$ is exactly equivalent to that of the free energy of independent spins in a uniform magnetic field h_0, β being regarded as the inverse temperature, $\beta=1/k_BT$.

Using the steepest-descent method, we can estimate the most probable contribution of the integrand from the condition

$$F'(x)|_{x=x_0}=0 . \tag{22}$$

This determines x_0 as

$$x_0=1/[1+\exp(-2\beta h_0-\xi)] , \tag{23}$$

with $\xi=\ln[p/(1-p)]$. Substituting Eq. (23) into Eq. (21), finally we get the asymptotic behavior of the partition function:

$$Z_n(\beta)\approx e^{nF(\beta)} , \tag{24}$$

with

$$f(\beta)=\ln[p\exp(\beta h_0)+(1-p)\exp(-\beta h_0)] . \tag{25}$$

Here we can recognize that $F(\beta)$ is the free energy per spin in a uniform magnetic field h_0 for $p=\frac{1}{2}$. The result includes that of Pietronero and Siebesma[13] if we take

$$p=\exp(\beta h_0)/[\exp(\beta h_0)+\exp(-\beta h_0)] .$$

We summarize the behavior of the free energy $F(\beta)$ varying the value of p as follows. If $p=\frac{1}{2}$, then $F(\beta)$ is symmetrical round $\beta=0$, at which $F(\beta)=0$. This coincides with the results by Pietronero *et al.*[11] Unless $p=\frac{1}{2}$, the free-energy curves deviate from one for $p=\frac{1}{2}$, having another zero of the free energy such that $F(\beta_c)=0$, where $\beta_c=(1/h_0)\ln[p/(1-p)]$ (see Fig. 1). Thus this leads to a totally different scaling behavior from that of $p=\frac{1}{2}$ and also to a different localization nature. This interesting situation has not been mentioned from the numerical efforts.[11] This singular behavior is related to a metal-insulator transition of the averaged wave function at a special value of $p=p_c$ for β being fixed. Because, if $F(\beta)=0$ at $\beta=\beta_c$, then $Z_n\approx e^{nF(\beta)}\to 1$, which means that the wave function is neither fluctuating nor localized.

We now note the following. It has been recognized that there is a strong mathematical connection between the partition functions of the multifractal analysis developed by Halsey *et al.*[7] and that of statistical mechanics. Several authors[14–19] have noted that this connection is realized when we use the comparison of notations $\beta\Longleftrightarrow q$, $\varepsilon\Longleftrightarrow\alpha$, $F(\beta)\Longleftrightarrow\tau(q)$, and $S(\varepsilon)\Longleftrightarrow f(\alpha)$, where the set of the notations $\{\alpha,\tau(q),f(\alpha)\}$ was introduced by Halsey *et al.*[7] Given the partition function $Z_n(\beta)$, we can define the free energy $F(\beta)$ and entropy function $S(\varepsilon)$ in the following:

$$F(\beta)\equiv\lim_{n\to\infty}\frac{1}{n}\ln Z_n(\beta) , \quad S(\varepsilon)=\beta\varepsilon-F(\beta) , \tag{26}$$

with $\varepsilon=\partial F(\beta)/\partial\beta$. This is the reason why we have used the notations of $Z_n(\beta)$ and $F(\beta)$ for its partition function

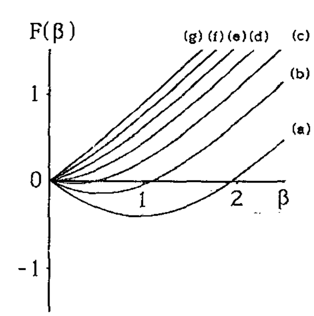

FIG. 1. $F(\beta)$ is shown, varying the values of p: (a) $p=0.125$, (b) $p=0.25$, (c) $p=0.375$, (d) $p=0.5$, (e) $p=0.625$, (f) $p=0.75$, and (g) $p=0.875$.

and for its exponent in Eq. (14), respectively. If we compare $F(\beta)$ with the generalized Lyapunov exponents $L(q)$, using the above correspondence, exactly, $F(\beta)$ is equivalent to $L(q)$ and $F(\beta)/\beta$ to $1/\xi_q = L(q)/q$.

IV. SPATIAL FLUCTUATION OF THE WAVE FUNCTION

Second, we are concerned with the spatial fluctuation of the single wave function. As shown numerically and as speculated by Pietronero *et al.*,[11] it was conjectured that the spatial fluctuation of the single wave function seems not to have multifractal nature. We will prove their claim rigorously for the symmetric random-walk case. But for other cases, we will prove that there appears multifractality of the spatial fluctuation of the wave function. This is contrary to their conjecture.

Before doing that we remark the following. There is a quite confusing point when we use the partition functions. Indeed, they used the same definitions of the partition functions in order to get the exponents for both the disorder and spatial fluctuations of the wave function. To escape from this confusion in using the expressions of the partition functions, we have chosen the free energy $F(\beta)$ for the disorder fluctuation. And we will use for the spatial fluctuation the conventional expression of the partition function $\chi_n(q)$ with the index q as Pietronero *et al.*[11] define that in the following:

$$\chi_n(q) \equiv \lim_{s\to 0} \sum_{j=1}^{n/s} \left[\sum_{sj<k<s(j+1)} |\psi_k|^2 \right]^q \approx s^{\tau(q)} , \quad (27)$$

with $n = sk$. Here we have divided the entire spatial region with length of n into k segments with length of s.

We now consider the spatial fluctuation of the single wave function. We will prove that this behavior is governed by the geometrical nature of the random walk. In other words, the scaling nature comes from only the geometrical part of the probability distribution $D(r|n)$. In this context we can redefine $\chi_n(q)$ as

$$\chi_n(q) \equiv \sum_{0\le r\le n} \left[\frac{n!}{(n-r)!r!} \right]^q p^r (1-p)^{n-r} [A(r|n)]^2 . \quad (28)$$

This is a generalization of Eq. (16). And $\tau(q)$ is defined through the ratio between $\chi_{2n}(q)$ and $\chi_n(q)$ such that

$$\chi_{2n}(q)/\chi_n(q) \approx (R_n)^{\tau(q)} , \quad (29)$$

with $R_n = 2^n$.

Treating q as β in Eq. (16), we can follow the similar argument mentioned earlier using the Stirling formula. We can express the partition function in terms of an integral:

$$\chi_n(q) \xrightarrow{n\to\infty} \int_0^1 dx\, e^{nG(x)} \quad (30)$$

where for an arbitrary p $(0 \le p \le 1)$, we have

$$G(x) = -q\{x \ln x + (1-x)\ln(1-x)\} + x \ln p + (1-x)\ln(1-p) - (1-2x)(2h_0) , \quad (31)$$

with $x = r/n$. Using the steepest-descent method, we can estimate the most probable contribution of the integrand from the condition

$$G'(x)|_{x=y_0} = 0 . \quad (32)$$

This determines y_0 as

$$y_0 = 1/(1+\exp[(-2(2h_0)-\xi)/q]) , \quad (33)$$

with $\xi = \ln[p/(1-p)]$. Substituting Eq. (33) into Eq. (31), finally we get the asymptotic behavior of the partition function:

$$\chi_n(q) \xrightarrow{n\to\infty} e^{nG(q)} , \quad (34)$$

with

$$G(q) = q \ln[p^{1/q} e^{2h_0} + (1-p)^{1/q} e^{-2h_0}] . \quad (35)$$

Let us obtain the fractal dimension $f(\alpha)$, which is defined by $f(\alpha) = \alpha q - \tau(q)$, with $\alpha = d\tau/dq$. For $p = \frac{1}{2}$ we have

$$G(q) = \left[q \left[1 + \frac{\ln[\cosh(2h_0)]}{\ln 2} \right] - 1 \right] \ln 2 . \quad (36)$$

Using this with Eqs. (29) and (34), we obtain

$$\tau(q) = q \left[1 + \frac{\ln[\cosh(2h_0)]}{\ln 2} \right] - 1 . \quad (37)$$

To obtain the relationship between α and q, first we differentiate $\tau(q)$ with respect to q. This gives $\alpha = 1 + \ln[\cosh(2h_0)]/\ln 2$. Next, we substitute this into Eq. (37). We then have $\tau(q) = q\alpha - 1$. From the definition of $f(\alpha)$, this provides the exact result $f(\alpha) = \alpha = 1$. This result supports the numerical result by Pietronero and Siebesma.[13] However, unless $p = \frac{1}{2}$, Eq. (35) provides the fractal dimension. This is contrary to their numerical result.

We remark on a possible generalization of the above partition function. In the sense of Kohmoto,[16] we are able to embed the two cases discussed above into the following form of the generalized partition function:

$$\Gamma_n(q,\beta) \equiv \sum_{0\le r\le n} \left[\frac{n!}{(n-r)!r!} \right]^q p^r (1-p)^{n-r} [A(r|n)]^\beta . \quad (38)$$

Following the similar argument mentioned earlier using the Stirling formula, we can express the partition function in terms of an integral:

$$\Gamma_n(q,\beta) \xrightarrow{n\to\infty} \int_0^1 dx\, e^{nH(x)} , \quad (39)$$

where for an arbitrary p $(0 \le p \le 1)$ we have

$$H(x) = -q\{x \ln x + (1-x)\ln(1-x)\} + x \ln p + (1-x)\ln(1-p) - (1-2x)(\beta h_0) , \quad (40)$$

with $x = r/n$. Using the steepest-descent method, we can estimate the most probable contribution of the integrand from the condition

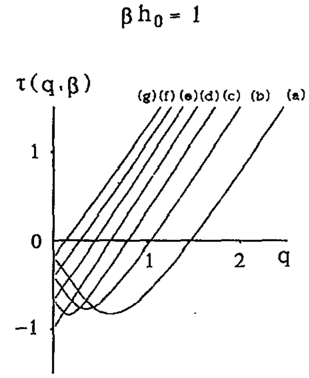

FIG. 2. $\tau(q,\beta)$ is shown, varying the values of p at $\beta h_0=1$: (a) $p=0.125$, (b) $p=0.25$, (c) $p=0.375$, (d) $p=0.5$, (e) $p=0.625$, (f) $p=0.75$, and (g) $p=0.875$.

$$H'(x)|_{x=z_0}=0\ . \tag{41}$$

This determines z_0 as

$$z_0=1/(1+\exp\{[-2(\beta h_0)-\xi]/q\})\ , \tag{42}$$

with $\xi=\ln[p/(1-p)]$. Substituting Eq. (42) into Eq. (40), finally we get the asymptotic behavior of the partition function:

$$\Gamma_n(q,\beta)\xrightarrow{n\to\infty}e^{nG(q,\beta)}\ , \tag{43}$$

where $G(q,\beta)$ means that the generalized free energy

$$G(q,\beta)=q\ \ln[p^{1/q}e^{\beta h_0}+(1-p)^{1/q}e^{-\beta h_0}]\ . \tag{44}$$

In this way we were able to embed all information of the electronic ground-state wave function into one expression.

We note that the above generalized free energy gives the same result for the spatial fluctuation when $p=\frac{1}{2}$. Following the similar argument, for $p=\frac{1}{2}$, we obtain

$$G(q,\beta)=\left[q\left[1+\frac{\ln[\cosh(\beta h_0)]}{\ln 2}\right]-1\right]\ln 2\ , \tag{45}$$

with

$$\tau(q)=q\left[1+\frac{\ln[\cosh(\beta h_0)]}{\ln 2}\right]-1\ . \tag{46}$$

Then this gives the exact result $f(\alpha)=\alpha=1$ no matter what β we have.

On the other hand, unless $p=\frac{1}{2}$, we have the multifractality of the spatial fluctuation of the single wave function. Following the similar argument as we obtained Eqs. (36) and (37), we define $\tau(q,\beta)$ as

$$\Gamma_{2n}(q,\beta)/\Gamma_n(q,\beta)\approx(R_n)^{\tau(q,\beta)}\ , \tag{47}$$

with $R_n=2^n$. From using Eq. (44), we then obtain

$$\tau(q,\beta)=q\frac{\ln[p^{1/q}e^{\beta h_0}+(1-p)^{1/q}e^{-\beta h_0}]}{\ln 2}\ . \tag{48}$$

The behavior of this is shown in Fig. 2, varying the value of p for $\beta h_0=1$.

V. CONCLUSION

In conclusion, we have discussed the scaling behavior of the exact electronic ground state of a one-dimensional disordered lattice, where the lattice disorder was introduced by the multiplicative random walk of $\phi(n)$. We obtained the exact scaling exponents of both the disorder and spatial fluctuations of the wave function. We have proved that for the symmetric random-walk case ($p=\frac{1}{2}$) the spatial fluctuation of the single wave function does not have multifractality, while the disordered wave function has multifractality. However, unless $p=\frac{1}{2}$, we have multifractality for both. This is contrary to the result by Pietronero *et al.*[11]

We mention some possible generalization of the present theory. Although we have assumed that the randomness comes from the multiplicative random walk, we may generalize this point to a much more strongly correlated one. This situation may lead us to a phase transition of the scaling behavior when we change the scaling index β (or q) from the point of view of the free energy. Finally, we are tempted to mention that this type of theory is also applicable to the electronic ground state of both various types of one-dimensional aperiodic lattices and the higher-dimensional disordered lattices. The results would strongly depend upon the dimensionality of lattices.

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