Exact wave functions of an electron on a quasiperiodic lattice: Definition of an infinite-dimensional Riemann theta function

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A scheme for obtaining the exact wave functions of an electron on a quasiperiodic lattice is presented. It is shown that the trace map plays a very important role for construction of the infinite-dimensional Riemann theta function in terms of which the wave functions can be represented.

I. INTRODUCTION

Quasiperiodic lattices have fascinated both theoretical physicists and mathematicians for a long time.[1] Since the discovery of quasicrystals[2] and the manufacturing of quasiperiodic materials,[3] the study of quasiperiodic lattices has attracted experimental physicists and engineers.

A quasiperiodic lattice that we consider consists of only two types of atoms, A and B. It is characterized by the ratio of the total number of A's to that of B's in the chain, an irrational number λ, whose kth approximation is defined by a continued fraction expansion:

$$\lambda_k=n_0+\cfrac{1}{n_1+\cfrac{1}{n_2+\cdots+n_k}}=[n_0,n_1,n_2,...,n_k], \tag{1}$$

where $n_0,n_1,n_2,...,n_k$ are positive integers. This set of integers is called the *tail* of λ.

Traditional methods based on the Bloch theorem are not directly applicable to solving the above one-dimensional quasiperiodic-lattice problems. This is because, in a quasiperiodic lattice, there is no translational symmetry (i.e., no spatial translation). Instead of the translational symmetry, there appears a different kind of symmetry operation, the *scaling transformation*.[4–13] This challenges the concepts of the periodic lattices—crystals.[14]

The first successes in understanding the physics of the quasiperiodic lattices appeared in the studies of the one-dimensional Fibonacci lattice by Kohmoto, Kadanoff, and Tang (KKT) and Ostlund, Pandit, Rand, Schellnhuber, and Siggia.[4] This is because the Fibonacci number is in some sense the simplest out of all the irrational numbers. It should be especially noted that KKT were able to obtain both the *trace map* and an *invariant surface*, which played a crucial role in obtaining the *Cantor-set*-like energy bands and critical wave functions of the electron on the lattice.[5,6] Since there exists an infinite number of irrational numbers in a real interval [0, 1], almost all other irrational numbers have not been studied.

Recently, Ostlund and Kim,[7] Gumps and Ali,[8] Holzer,[9] and Wijnands[10] showed that there exist the same types of trace maps and the invariant surface, even for a series of irrational numbers that are obtained by taking all n_i as the same n (n an arbitrary positive integer).

Finally, this direction was completed by Kalugin, Kitaev, and Levitov,[11] Sutherland,[12] and Iguchi[13] This is summarized as follows.

According to the approximated irrational number λ_k, we can construct the scaling transformations in order to define a quasiperiodic lattice in terms of two symbols, A and B, in the following:

$$(L^{k+1}(A,B),L^k(A,B))=\mathbf{S}^{n_k}\mathbf{S}^{n_{k-1}}\cdots\mathbf{S}^{n_0}(A,B), \tag{2}$$

where we have started from the seed of a lattice (A, B) by using the scaling transformation $\mathbf{S}^{n_k}(A,B) = (BA^{n_k},A)$ at each step. Here $L^k(A,B)$ denotes the unit cell of the kth generation of the lattice, which consists of P_k A's and Q_k B's defining λ_k by P_k/Q_k, where $P_{k+1}=n_{k-1}P_k+P_{k-1}$, $Q_{k+1}=n_{k-1}Q_k+Q_{k-1}$ with the initial conditions $(P_0,Q_0)=(0,1)$ and $(P_1,Q_1)=(1,0)$. The size of the unit cell becomes $N_k\equiv P_k+Q_k$, having $N_1=N_0=1$. Then the one-dimensional lattice structure of this unit cell is explicitly given by

$$\begin{aligned} L^k(A,B) &\equiv L_{P_k,Q_k}(A,B) \\ &\equiv BA^{a_{Q_k}}BA^{a_{Q_k-1}}\cdots BA^{a_1} \\ &\equiv \prod_{n=1}^{Q_k} BA^{a_n}, \end{aligned} \tag{3}$$

with

$$a_n=[n\lambda_k]-[(n-1)\lambda_k], \tag{4}$$

where [ ] denotes the Gauss symbol. We remark here that if we define the ratio $\sigma_k\equiv N_{k+1}/N_k=[n_k,n_{k-1},n_{k-2},...,n_0+1]$, this measures how fast the unit cell grows up.

We would like to solve the discretized Schrödinger equation (the tight-binding model):[14]

$$T_n\psi_{n+1}+T_{n-1}\psi_{n-1}+V_n\psi_n=E\psi_n\,. \qquad (5)$$

In this case, it is convenient to map the Schrödinger equation into the transfer matrix form:

$$\Psi_n=M_{n,n-1}\Psi_{n-1} \qquad (6)$$

with

$$M_{n,n-1}=\begin{pmatrix}\frac{E-V_n}{T_n} & -\frac{T_{n-1}}{T_n}\\ 1 & 0\end{pmatrix} \text{ and } \Psi_{n-1}=\begin{pmatrix}\psi_n\\ \psi_{n-1}\end{pmatrix}. \qquad (7)$$

The above setup leads us to the generic trace map induced by the scaling transformations. Let the initial triple be $(x_0,y_0,z_0)\equiv(\frac{1}{2}\operatorname{Tr}(B),\frac{1}{2}\operatorname{Tr}(A),\frac{1}{2}\operatorname{Tr}(AB))$, where A and B stand for the two transfer matrices associated with the two types of neighboring coordinations of the lattice.[4] We then have the following trace map according to the scaling transformations:[11–13]

$$(x_k,y_k,z_k)=\mathbf{T}_{n_{k-1}}\mathbf{T}_{n_{k-2}}\cdots T_{n_0}(x_0,y_0,z_0), \qquad (8)$$

$$\mathbf{T}_n(x,y,z)\equiv(y,C_{n-1}(y)z-C_{n-2}(y)x,C_n(y)z-C_{n-1}(y)x), \qquad (9)$$

where $C_n(y)$ is the nth Chebyshev polynomial of the second kind, being defined by the recursion relation $C_{n+1}(y)=2yC_n(y)-C_{n-1}(y)$ with $C_{-1}(y)=0$, $C_0(y)=1$. We remark that, according to the scaling transformations, the trace map at each step preserves an invariant surface defined by

$$\mathbf{I}=x^2+y^2+z^2-2xyz-1. \qquad (10)$$

This invariant surface is completely equivalent to that first found by KKT.[4] The role of the invariant surface for the spectrum was first studied by Kohmoto and Oono.[5] It was also studied by Casdagli,[15] and by many authors.[6,13,16–18]

Thanks to the generic trace map, we can calculate the energy bands for an electron on a quasiperiodic lattice: If $|x_k|<1$, then the energy is allowed, and if $|x_k|>1$, then the energy is forbidden. Following this algorithm, the energy bands for an electron on a quasiperiodic lattice was first demonstrated by the author.[13,16,17] In the Appendix, following this scheme we give a simple program that provides the energy bands.

However, it has been extremely difficult to obtain the electronic wave functions for a quasiperiodic lattice, even for a Fibonacci lattice.[6] In this paper we would like to present for attacking this problem a scheme that enables us to obtain the exact wave functions for an electron on a quasiperiodic lattice.

The organization of the paper is the following. In Sec. II, we will discuss the electronic band structure for a quasiperiodic lattice. In Sec. III, we will study the Bloch wave function for an electron on a periodic lattice as a rational approximation of a quasiperiodic lattice. In Sec. IV, the wave functions for a quasiperiodic lattice will be constructed as a limit from the rational approximation. In Sec. V, we will summarize what we have done.

II. THE ENERGY BAND STRUCTURE

First, let us try to solve the energy band problem of a periodic lattice whose unit cell consists of N types of atoms as introduced in Sec. I. From Eq. (5), we have basically two independent solutions for the Schrödinger equation: One solution is obtained by the initial condition $\Psi_0{}^{(1)}=(0,1)$ and the other by $\Psi_0{}^{(2)}=(1,0)$. Let us call them $\Psi_{n-1}{}^{(1)}=(\phi_1(n),\phi_1(n-1))$ and $\Psi_{n-1}{}^{(2)}=(\phi_2(n),\phi_2(n-1))$, where $\phi_1(n)$ is an $(n-2)$th-order polynomial of E and $\phi_2(n)$ is an $(n-1)$th-order polynomial of E. Thus we are able to represent the matrix product $M(N|0)$ in terms of $\phi_1(n)$ and $\phi_2(n)$ in the following:

$$\begin{aligned}M(N|0)&\equiv M_{N,N-1}M_{N-1,N-2}\cdots M_{1,0}\\&\equiv\begin{pmatrix}m_{11} & m_{12}\\ m_{21} & m_{22}\end{pmatrix}\\&\equiv\begin{pmatrix}\phi_2(N+1) & \phi_1(N+1)\\ \phi_2(N) & \phi_1(N)\end{pmatrix},\end{aligned} \qquad (11)$$

where we have used

$$\begin{aligned}\Psi_{n+N}&=M_{n+N,n+N-1}M_{n+N-1,n+N-2}\cdots M_{n+1,n}\Psi_n\\&\equiv M(N|n)\Psi_n\,.\end{aligned}$$

We notice that $\operatorname{Tr} M(N|0)=\phi_1(N)+\phi_2(N+1)$, which is an nth-order polynomial of E and

$$\begin{aligned}\operatorname{Det} M(N|0)&=\phi_1(N)\phi_2(N+1)-\phi_2(N)\phi_1(N+1)\\&=1.\end{aligned} \qquad (12)$$

This matrix plays a very crucial role to obtain the energy bands. Let us define $x_N(E)=\frac{1}{2}\operatorname{Tr} M(N|0)$. As already mentioned before, if $|x_N(E)|\leqslant 1$, then the energy lies in a band, and if $|x_N(E)|>1$, then the energy lies in a band gap. From the Bloch theorem for ψ_n, we obtain the Bloch theorem for Ψ_n such that $\Psi_{n+N}=e^{ikN}\Psi_n$. Therefore we can rewrite the trace as $x_N(E)=\cos(Nk)$ when an energy lies in a band, where $-\pi/N\leqslant k\leqslant\pi/N$, the *Brillouin zone*. Let us define a function $\Delta_N(E)=x_N(E)-\cos(Nk)=0$. Obviously $\Delta_N(E)$ has N roots as $E_j(k)$ for $j=1,\ldots,N$, each of which satisfies $E_j(k)=E_j(k+2\pi/N)$. So we can rewrite it as

$$\Delta_N(E)=\prod_{j=1}^{N}(E-E_j(k)). \tag{13}$$

Since

$$\frac{dE}{dk}=-\frac{\partial\Delta}{\partial k}\bigg/\frac{\partial\Delta}{\partial E},$$

if we set E as $E_j(k)$ in it, then it leads to a set of equations:

$$\frac{dE_j(k)}{dk}=-\frac{\pm N\sqrt{1-[x_N(E_j(k))]^2}}{\prod_{i(\neq j)=1}^{N}(E_j(k)-E_i(k))}\quad (j=1,\ldots,N). \tag{14}$$

If we solve the above equations for $E_j(k)$ $(j=1,\ldots,N)$, we can determine the entire band structure with respect to k.

The above argument is quite general and we did not use the generic trace map for obtaining the band structure for a quasiperiodic lattice.

We are now going to consider the energy bands of a quasiperiodic lattice. For this purpose, N in the above discussion is replaced by N_k for the kth generation of a quasiperiodic lattice. We only discuss the off-diagonal model of the tight-binding Schrödinger equation, where $V_n=0$. Using the results of Sec. I, we have to take the initial triple as

$$x_0=\frac{1}{2}\,\mathrm{Tr}\,B\equiv\frac{1}{2}\frac{E}{T_b},$$

$$y_0=\frac{1}{2}\,\mathrm{Tr}\,A\equiv\frac{1}{2}\frac{E}{T_a}, \tag{15}$$

$$z_0=\frac{1}{2}\,\mathrm{Tr}\,AB\equiv\frac{1}{2}\left(\frac{E^2}{T_aT_b}-\frac{T_b}{T_a}-\frac{T_a}{T_b}\right),$$

where T_a, T_b are the two types of hopping matrices. Since the invariant surface is preserved under the scaling transformations, it is evaluated by the initial triple such that

$$\mathbf{I}=\frac{1}{4}\left(\frac{T_b}{T_a}-\frac{T_a}{T_b}\right)^2>0. \tag{16}$$

If $T_a/T_b=1$, then $\mathbf{I}=0$, and the solution is trivial. If $E/T_b=E/T_a=2\cos\theta_0$ with θ_0 real, we are in an allowed region of the spectrum since $x_k=\cos(N_k\theta_0)$. However, if $|E/T_a|>2$, i.e., if $E/T_a=2\cosh u_0$ with u_0 real, then $x_k=\cosh(N_ku_0)$ grows exponentially and this energy is forbidden.

If T_a/T_b is close to one, the invariant $\mathbf{I}$ is close to zero. This limit corresponds to the case where a perturbative approach is applicable. The position of gaps in the energy bands is fitted by $\pm 2\cos(\pi n/d)$, where d is the average spacing between B's $(d\equiv 1+\lambda)$ and n is an integer greater than one, giving the order of the band gaps (Fig. 1).

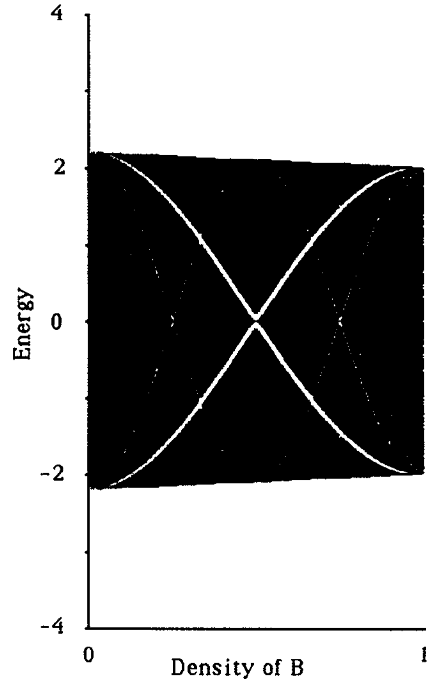

FIG. 1. The energy spectrum of quasiperiodic lattices for $T_a/T_b=1.1$. The horizontal line indicates the density ρ, which varies from 0 to 1. The vertical line indicates energy E.

It is worthwhile noting that the global features of the energy bands for small values of the invariant are preserved through any positive value of the invariant $\mathbf{I}$. This is one of the main results of our research[13,16,17] (Figs. 2 and 3).

We were able to understand this important result from the point of view of the topology of the invariant surface as follows.[13,16,17] The invariant surface has a certain topology as a manifold: There are the four horns which are directed to $P(1,1,1)$, $Q(1,-1,-1)$, $R(-1,1,-1)$, and $S(-1,-1,1)$ respectively.[4–6,16,17] When the value of $\mathbf{I}$ is a very small positive number, the necks of the horns narrow to almost points. The escape of the trace is then very slow. This produces the very small gaps in the bands. Even if the value of $\mathbf{I}$ becomes large, the topology of the invariant surface, such as the number of connected parts, never changes because only the surface is deformed. Since we have much bigger necks of the horns, the escape becomes much faster, and so the gaps of the spectrum become much bigger, but qualitatively the global features of the energy bands are preserved.

If we investigate the escape problem of the trace using four colors, then we are able to paint the whole invariant surface by the four colors; the four colors show to

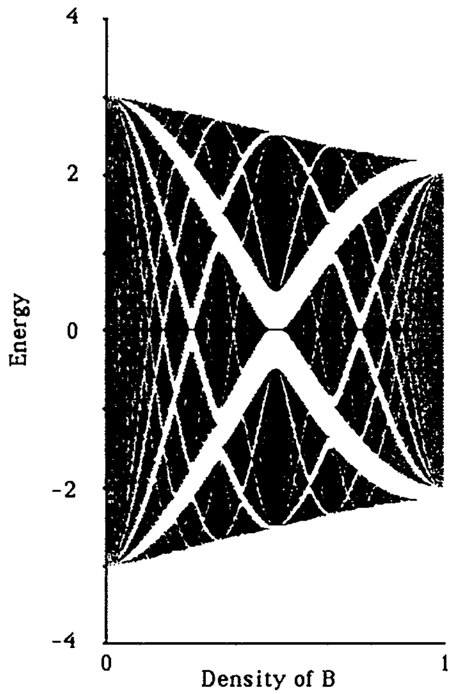

FIG. 2. The energy spectrum of quasiperiodic lattices for $T_a/T_b=1.5$. The horizontal line indicates the density ρ, which varies from 0 to 1. The vertical line indicates energy E.

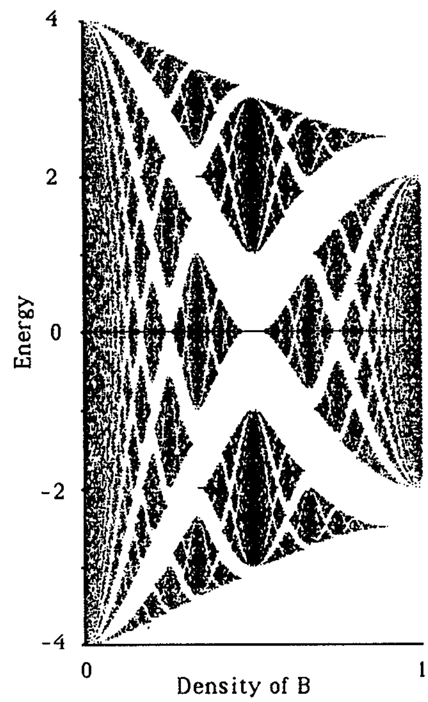

FIG. 3. The energy spectrum of quasiperiodic lattices for $T_a/T_b=2.0$. The horizontal line indicates the density ρ, which varies from 0 to 1. The vertical line indicates energy E.

which horn a point on the surface escapes.[13,16,17] A region of the surface painted by one of the colors represents the location of escaping points to a particular horn, which then corresponds to a band gap. Thus we can label all the band gaps by using the four colors. So the boundaries between colored regions remain as the nonescaping points. They seem to be essentially the *Julia set*[19] of the trace map or the *strange repeller*, but this point is open. Since a boundary has measure zero on the surface, the corresponding band also has measure zero, because the initial triple sweeps a line on the surface as the energy is changed. This view point explains why we must have a Cantor-set-type of energy bands for any quasiperiodic lattice.

The above result seems to be related to the gap labeling theorem,[18,20] but at this moment the connection is still unclear to us.

III. THE BLOCH WAVE FUNCTIONS

Let us go back to the original Schrödinger equation (5). We now shift all suffices n by a constant r; we obtain the *shifted Schrödinger equation*:[21]

$$T_{n+r}\psi_{n+1}(r)+T_{n-1+r}\psi_{n-1}(r)+V_{n+r}\psi_n(r)=E\psi_n(r). \tag{17}$$

Then it requires us to impose the initial conditions for $\psi_n(r)$ such that $\Psi_0^{(1)}(r)=(0,1)$ and $\Psi_0^{(2)}(r)=(1,0)$. Following the argument for the original Schrödinger equation, we obtain the matrix product $M(N|r)$:

$$\begin{aligned}M(N|r)&\equiv M_{N+r,N+r-1}M_{N+r-1,N+r-2}\cdots M_{r+1,r}\\&\equiv\begin{pmatrix}m_{11}(r)&m_{12}(r)\\m_{21}(r)&m_{22}(r)\end{pmatrix}\\&\equiv\begin{pmatrix}\phi_2(N+1|r)&\phi_1(N+1|r)\\\phi_2(N|r)&\phi_1(N|r)\end{pmatrix}.\end{aligned} \tag{18}$$

Here we have $\mathrm{Tr}\,M(N|r)=\phi_1(N|r)+\phi_2(N+1|r)$, which is an nth-order polynomial of E, and $\mathrm{Det}\,M(N|r)=\phi_1(N|r)\phi_2(N+1|r)-\phi_2(N|r)\phi_1(N+1|r)=1$. Since we only shift the origin for the initial position, $\phi_1(n|r)$ and $\phi_2(n|r)$ are related to $\phi_1(n)$ and $\phi_2(n)$ by

$$\begin{aligned}\phi_1(n|r)&=(T_r/T_0)[\phi_1(r+n)\phi_2(r+1)\\&\quad-\phi_1(r+1)\phi_2(r+n)],\\\phi_2(n|r)&=(T_r/T_0)[\phi_2(r+n)\phi_1(r)-\phi_2(r)\phi_1(r+n)].\end{aligned} \tag{19}$$

From these relations we can prove that $\mathrm{Tr}\, M(N|r) = \mathrm{Tr}\, M(N|0)$, which means that *the energy bands never change by the shift of the origin.*

We are now ready to consider the so-called *auxiliary spectrum problem.* Physicists first encountered this problem in the theory of solitons as a *periodic Toda lattice,*[21] or a *periodic KdV equation,*[22] which requires the idea of the *inverse scattering method.*[21,22] As we shall show later, we find that the theoretical framework is still applicable and becomes a very powerful tool to study the usual periodic and quasiperiodic lattices as well.

Let us impose a particular condition for $\phi_1(N+1)$ and $\phi_1(N+1|r)$ such that $\phi_1(N+1)=0$ and $\phi_1(N+1|r)=0$, which provides us the *auxiliary spectra.* Since $\phi_1(N+1)$ and $\phi_1(N+1|r)$ are $(N-1)$th-order polynomials of E, we can determine the $N-1$ roots, say $\mu_j(0)$ and $\mu_j(r)$ $(j=1,...,N)$, as the zeros of $\phi_1(N+1)=0$ and $\phi_1(N+1|r)=0$, respectively. We then have $\mathrm{Tr}\, M(N|0) = \phi_1(N)+1/\phi_1(N)$ and $\mathrm{Tr}\, M(N|r)=\phi_1(N|r)+1/\phi_1(N|r)$, providing that $|M(N|0)|>2$ and $|M(N|r)|>2$. This means that $\mu_j(0)$ and $\mu_j(r)$ $[\neq\mu_j(0)]$ always lie in a band gap $[\lambda_{2j},\lambda_{2j+1}]$ for $j=1,...,N-1$, where λ_n $(n=1,...,2N)$ are the band edges given as the $2N$ roots of $[x_N(E)]^2-1=0$. Thus *$\mu_j(0)$ and $\mu_j(r)$ $(j=1,...,N-1)$ label all the band gaps.* (See Sec. II.)

Let us follow the argument of the inverse scattering method.[21] We know that for an arbitrary Bloch condition we have

$$c_1\phi_1(N)+c_2\phi_2(N)=\rho c_1,$$

$$c_1\phi_1(N+1)+c_2\phi_2(N+1)=\rho c_2, \tag{20}$$

$$\frac{c_1}{c_2}=\frac{\phi_2(N)}{\phi_1(N)-\rho}=\frac{\rho-\phi_2(N+1)}{\phi_1(N+1)},$$

$$\rho=e^{ikN}=x_N(E)\pm\sqrt{[x_N(E)]^2-1}. \tag{21}$$

For the sake of convenience, we set the Bloch function as

$$\psi_n^{\pm}(E)=(c_1/c_2)_{\pm}\phi_1(n)+\phi_2(n). \tag{22}$$

Here $\pm$ indicates the two independent values of c_1/c_2 due to the two independent values of ρ.

We can then prove the following very important expression:

$$\psi_n^{+}(E)\psi_n^{-}(E)=\frac{T_0}{T_n}\frac{\phi_1(N+1|n-1)}{\phi_1(N+1)}. \tag{23}$$

Since $\phi_1(N+1)$ and $\phi_1(N+1|n-1)$ have the $N-1$ zeros, $\mu_j(0)$ and $\mu_j(n-1)$ $(j=1,...,N-1)$, respectively, Eq. (23) turns out to be

$$\psi_n^{+}(E)\psi_n^{-}(E)=\prod_{j=1}^{N-1}\frac{E-\mu_j(n-1)}{E-\mu_j(0)}. \tag{24}$$

The above expression has a crucial importance in order to relate the zeros and poles of the wave function with the *rotation number*[20] of the wave function through the *Thouless formula.*[23] When E is thought of as a real number, in other words, when E lies in the real axis, $\psi_n^{+}(E)\psi_n^{-}(E)$ coincides with the usual $|\psi_n(E)|^2\geqslant 0$ and from the Bloch theorem it is equivalent to $U_n^{+}(E)U_n^{-}(E)$. So if we write $\psi_n^{+}(E)\times\psi_n^{-}(E)\equiv\exp\{(N-1)\gamma_n(E)\}$, then we can prove the following expressions:

$$\gamma_n(E)=\int_{-\infty}^{\infty}dE'\,\log(E-E')\,\frac{dk_n(E')}{dE'}, \tag{25}$$

$$\frac{dk_n(E)}{dE}=\frac{1}{N-1}\sum_{j=1}^{N-1}\{\delta(E-\mu_j(n-1))-\delta(E-\mu_j(0))\}, \tag{26}$$

where $\gamma_n(E)$ is called the rotation number.[20] Here δ is the Dirac delta function, $k_n(E)$ is the *integrated density of states* at site n, and Eq. (25) is called the Thouless formula.[23]

We are now going to express the Bloch wave function by means of the *multidimensional Riemann theta (θ)-function.*[21,22,24] This point is the heart of the periodic lattice problem, namely it corresponds to the finite zone potential problem in the soliton theory.[21,22]

A multidimensional Riemann θ-function is defined by[21,22,24]

$$\theta_g(\mathbf{z};\underline{\Omega})\equiv\sum_{\{\mathbf{m}\}\in\mathbb{Z}^g}\exp\{\pi i\,{}^t\mathbf{m}\underline{\Omega}\mathbf{m}+2\pi i\,{}^t\mathbf{m}\cdot\mathbf{z}\}. \tag{27}$$

Here $\mathbf{m}$, $\mathbf{z}$ are thought of as column vectors so that ${}^t\mathbf{m}=(m_1,m_2,...,m_g)\in\mathbb{Z}^g$ and ${}^t\mathbf{z}=(z_1,z_2,...,z_g)\in\mathbb{C}^g$, and $\underline{\Omega}$ is a symmetric $g\times g$ complex matrix, the *Riemann matrix.* Here $\theta_g(\mathbf{z};\Omega)$ enjoys the so-called *quasiperiodicity conditions:*[21,22,24]

$$\theta_g(\mathbf{z}+\mathbf{m};\underline{\Omega})=\theta_g(\mathbf{z};\underline{\Omega}), \tag{28a}$$

$$\theta_g(\mathbf{z}+\underline{\Omega}\mathbf{m};\underline{\Omega})=\exp\{-\pi i\,{}^t\mathbf{m}\underline{\Omega}\mathbf{m}-2\pi i\,{}^t\mathbf{m}\cdot\mathbf{z}\}\theta_g(\mathbf{z};\underline{\Omega}). \tag{28b}$$

Here the argument of $\theta_g(\mathbf{z};\Omega)$ forms a lattice, $\mathbb{Z}^g+\Omega\mathbb{Z}^g$ in the space of $\mathbb{R}^{2g}$. We note the following. Although we use the same word "quasiperiodicity" for the above conditions, it does not mean the lattice quasiperiodicity in the real spatial direction. It is just terminological convention in mathematics. Rather, it means quasiperiodicity in the argument space of the theta function as we will see below.

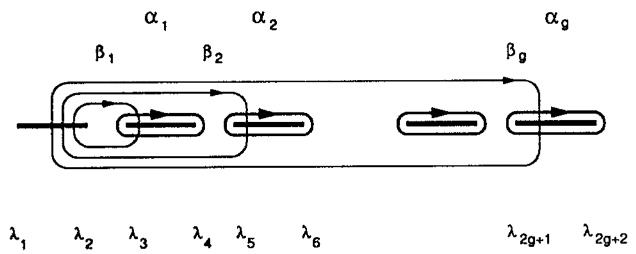

FIG. 4. The Riemann surface.

Let us set $g \equiv N-1$ equal to the *total number of band gaps*, for the later purpose. The key idea in order to express the Bloch function in terms of the multidimensional Riemann θ-function lies on the fact that the g zeros and g poles of the wave function can be regarded as g zeros of the multidimensional Riemann θ-function. To realize this idea, $\psi_n^+(E)\psi_n^-(E)$ needs to be thought of as a complex function of a complex variable E.

Let us go back to the energy bands problem. The band edges are determined by $[x_{g+1}(E)]^2=1$ as λ_n $(n=1,\ldots,2g+2)$. When we see Eq. (21), ρ has two values by whether or not $|x_{g+1}(E)|<1$ according to the value of E. In other words, when E lies in a band region, $\sqrt{R_{g+1}(E)} \equiv \sqrt{[x_{g+1}(E)]^2-1}$ becomes a two-valued function, where $R_{g+1}(E)$ is a $(2g+2)$th-order polynomial of E. Thus it is necessary to make *branch cuts* over all the energy bands that define a *Riemann surface* over the energy E (Fig. 4).[21,22,25] Here the Bloch function becomes an analytic function defined on the Riemann surface—the *hyperelliptic function*.[25]

The theory of Riemann surface tells us that there are only three types of differentials over the Riemann surface: the first, second, and third kinds.[25] The differentials of the first kind are defined by[21,22]

$$\omega_{(s)}=\frac{E^{s-1}\,dE}{\sqrt{R_{g+1}(E)}}, \quad s=1,\ldots,g. \tag{29}$$

Then we define the base $\{\omega_j\}$ such that

$$\omega_j=\sum_{s=1}^{g} c_{js}\omega_{(s)}, \quad j=1,\ldots,g, \tag{30}$$

where c_{js} are unknown constants determined by the following conditions:

$$\int_{\alpha_i}\omega_j=\delta_{ij}, \quad i,j=1,\ldots,g. \tag{31}$$

We define a vector $\mathbf{z}$ (these elements are called the *Abelian integrals*)[21,22] and the Riemann matrix $\underline{\Omega}$ such that

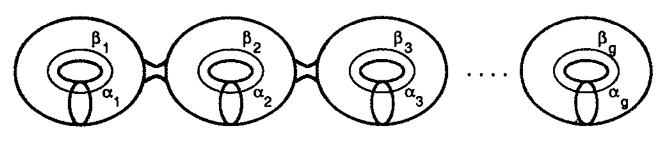

FIG. 5. A torus of genus g.

$$z_j(P)=\int_{P_0}^{P}\omega_j, \quad j=1,\ldots,g,$$

$$\int_{\beta_i}\omega_j=\Omega_{ij}, \quad i,j=1,\ldots,g. \tag{32}$$

Here α_i is a closed contour that surrounds the cut $(\lambda_{2j+1},\lambda_{2j+2})$ on the upper sheet, while β_j is a closed contour that starts at λ_2, goes on the lower sheet as far as λ_{2j+1}, crosses to the upper sheet, and ends at λ_2 (Fig. 4). Here α_i, β_i $(i=1,\ldots,g)$ define a torus of genus g (Fig. 5). Therefore *the number of band gaps in the spectrum defines the genus of the torus.*

We can thus define the multidimensional Riemann θ-function such that $\mu_j(n-1)$ $(j=1,\ldots,g)$ become g zeros of $\theta_g(\mathbf{z}(\mu_j(n\text{-}1)) - \mathbf{X}(n-1) - \mathbf{K};\underline{\Omega})=0$. Here $\mathbf{K}$ is a g-dimensional constant vector,

$$\begin{aligned} X_i(n-1) &= \sum_{j=1}^{g}\int_{\mu_0}^{\mu_j(n-1)}\omega_i \\ &= (n-1)\int_{\infty'}^{\infty}\omega_i+\sum_{j=1}^{g}\int_{\mu_0}^{\mu_j(0)}\omega_i \\ &\quad -\sum_{j=1}^{g} n_j W_{ij}+m_i \end{aligned} \tag{33}$$

(for $i=1,\ldots,g$), where n_j, m_i are integers. Here ∞ (∞') denotes infinity of the lower (upper) sheet.

Finally, if we take the logarithm of $\psi_n^+(E)\psi_n^-(E)$, then

$$\log(\psi_n^+(E)\psi_n^-(E))=\sum_{j=1}^{g}\log\left(\frac{E-\mu_j(n-1)}{E-\mu_j(0)}\right). \tag{34}$$

Since the Cauchy theorem:

$$\frac{1}{2\pi i}\int_C f(z)\,\frac{\phi'(z)}{\phi(z)}\,dz=\sum_i r_i f(a_i)-\sum_i s_i f(b_i), \tag{35}$$

where a_i's (b_i's) are the zeros (poles) of a function $f(z)$ and r_i's (s_i's) the residues. The wave function is represented in the following:

$$\psi_n{}^{+}(E)\psi_n{}^{-}(E)=\frac{\theta_g(\mathbf{z}(E)-\mathbf{X}(n-1)-\mathbf{K};\underline{\Omega})}{\theta_g(\mathbf{z}(E)-\mathbf{X}(0)-\mathbf{K};\underline{\Omega})}, \quad (36)$$

where

$$z_j(E)=\int_{\mu_0}^{E}\omega_j, \quad j=1,\ldots,g.$$

Or, equivalently, we derive

$$\psi_n{}^{\pm}(E)=\exp(\pm ink(E))U_n{}^{\pm}(E). \quad (37)$$

Here

$$k(E)\equiv\int_{\mu_0}^{E}\omega(\infty',\infty),$$

$\omega(P,Q)$ is called the *normal differential of the third kind*, with the residue 1 and -1 at P and Q, respectively. Here we have the Bloch theorem as expected, since if $n=N+1$, then $\mathbf{X}(n-1)=\mathbf{X}(0)$ so that the wave function obviously has the lattice periodicity. This type of function is sometimes called the *Baker–Akhiezer function*. The scheme discussed above is called the *Jacobi inversion problem*.[21,22,25]

IV. THE QUASIPERIODIC WAVE FUNCTIONS

We now consider the binary quasiperiodic lattice problem. The point here is the following: *Until reaching the quasiperiodicity, a quasiperiodic lattice is always approximated to be periodic and the unit cell of the* k*th generation of the lattice consists of* N_k *atoms including* P_k *A-atoms and* Q_k *B-atoms*. Therefore, for any generation of the lattice we can use the idea of the inverse scattering method discussed in Sec. III. We thus are able to set the number $g_k\equiv N_k-1$ equal to the *total number of band gaps in the spectrum of the kth generation of the quasiperiodic lattice*.

We know that the traces x_k, y_k, z_k are written as

$$x_k(E)\equiv\tfrac{1}{2}\,\mathrm{Tr}\,M(g_k+1\,|\,0)\equiv\tfrac{1}{2}\,\mathrm{Tr}\,M_k,$$

$$y_k(E)\equiv\tfrac{1}{2}\,\mathrm{Tr}\{[M_k]^{n_{k-1}}M_{k-1}\}\equiv x_{k+1}(E),$$

and

$$z_k(E)\equiv\tfrac{1}{2}\,\mathrm{Tr}\{[M_k]^{n_{k-1}+1}M_{k-1}\}$$

$$\equiv\tfrac{1}{2}\,\mathrm{Tr}\,M(g'_{k+1}+1\,|\,0),$$

respectively. Here g'_k is given by $g'_k+1=N'_k\equiv N_k+N_{k-1}$. This gives the scaling transformations [see Eq. (2)] which induce the generic trace map [see Eqs. (8) and (9)]:

$$x_{k+1}=y_k,$$

$$y_{k+1}=C_{n_{k-1}-1}(y_k)z_k-C_{n_{k-1}-2}(y_k)x_k, \quad (38)$$

$$z_{k+1}=C_{n_{k-1}}(y_k)z_k-C_{n_{k-1}-1}(y_k)x_k.$$

Since $x_k(E)$ is a (g_k+1)th-degree polynomial in E, this is expanded with respect to E such as

$$x_k(E)=\tfrac{1}{2}D_k{}^{-1}[E^{g_k+1}+U_1^{(k)}E^{g_k}+U_2^{(k)}E^{g_k-1}+\cdots$$
$$+U_{g_k+1}^{(k)}], \quad (39)$$

$$y_k(E)=x_{k+1}(E) \quad (40)$$

with

$$D_k\equiv\sum_{j=1}^{g_k+1}T_j. \quad (41)$$

We expand z_k in the same way,

$$z_k(E)=\tfrac{1}{2}D'_{k+1}{}^{-1}[E^{g'_{k+1}+1}+V_1^{(k+1)}E^{g'_{k+1}}$$
$$+V_2^{(k+1)}E^{g'_{k+1}-1}+\cdots+V_{g'_{k+1}+1}^{(k+1)}], \quad (42)$$

with

$$D'_{k+1}\equiv\sum_{j=1}^{g'_{k+1}+1}T_j. \quad (43)$$

Hereafter we shall call the set $\{U_j^{(k)}\ (j=1,\ldots,g_k+1),\ U_j^{(k+1)}\ (j=1,\ldots,g_{k+1}+1),\ V_j^{(k+1)}\ (j=1,\ldots,g'_{k+1}+1)\}$ the kth set of the *invariants*, because in the soliton theory such as the periodic Toda lattice or KdV equation, they are exactly invariant under the time development—the *constants of motion*.[21,22] The kth invariants depend upon the hopping parameters T_n and the on-site potentials V_n, which are constants, T_a and T_b with $V_n=0$ for a quasiperiodic lattice and time-dependent variables, $T_n\equiv\exp\{-(X_{n+1}-X_n)/2\}$, and $V_n\equiv dX_n/dt$ for the Toda lattice[21] where X_n is the position of the nth atom.

Since the trace $x_k(E)$ is factorized in the following:

$$x_k(E)=\tfrac{1}{2}D_k{}^{-1}(E-\gamma_1^{(k)})(E-\gamma_2^{(k)})\cdots(E-\gamma_{g_k+1}^{(k)})$$
$$\equiv\frac{1}{2}D_k{}^{-1}\prod_{j=1}^{g_k+1}(E-\gamma_j^{(k)}), \quad (44)$$

where the zeros of $x_k(E)$ are just *band centers*, say $\gamma_j^{(k)}$ $(j=1,\ldots,g_k+1)$, then the invariants $U_j^{(k)}$ prove to be symmetric functions of the band centers:

$$U_1^{(k)}=\gamma_1^{(k)}+\gamma_2^{(k)}+\cdots+\gamma_{g_k+1}^{(k)},$$

$$U_2^{(k)}=-(\gamma_1^{(k)}\gamma_2^{(k)}+\gamma_2^{(k)}\gamma_3^{(k)}+\cdots+\gamma_{g_k}^{(k)}\gamma_{g_k+1}^{(k)}),$$

$$\vdots \tag{45}$$

$$U_{g_k+1}^{(k)}=(-)^{g_k+1}\gamma_1^{(k)}\gamma_2^{(k)}\cdots\gamma_{g_k}^{(k)}\gamma_{g_k+1}^{(k)}.$$

The above setup enables us to understand the role of the generic trace map. From the initial triple for the off-diagonal model [Eq. (15)], we obtain the initial condition for the invariants:

$$U_1^{(0)}=U_1^{(1)}=0$$

and

$$V_1^{(0)}=0,\quad V_2^{(0)}=-(T_a^{\,2}+T_b^{\,2}). \tag{46}$$

Therefore, this provides a mapping on the invariants as follows. Starting from Eq. (46), we can calculate the values of the invariants for the next generation of the quasiperiodic lattice. Recursively, the successive three sets of the invariants $\{U_j^{(k-1)}\ (j=1,...,g_{k-1}+1)\}$, $\{U_j^{(k)}\ (j=1,...,g_k+1)\}$, and $\{V_j^{(k)}\ (j=1,...,g'_k+1)\}$ determine the new sets of the invariants $\{U_j^{(k)}\ (j=1,...,g_k+1)\}$, $\{U_j^{(k+1)}\ (j=1,...,g_{k+1}+1)\}$, and $\{V_j^{(k+1)}\ (j=1,...,g'_{k+1}+1)\}$ for the next generation of the lattice, where

$$D_{k+1}\equiv D_k^{\,n_{k-1}}D_{k-1} \quad \text{and} \quad D'_k\equiv D_k^{\,n_{k-1}+1}D_{k-1}$$

with

$$D_0\equiv T_b,\quad D_1\equiv T_a,\quad D'_0=T_aT_b\,. \tag{47}$$

In this way, the invariants are always polynomials of T_a and T_b, even though the expressions for the mapping on the invariants look very complicated. Since the generic trace map preserves the invariant surface, the three sets of the invariants are constrained to satisfy Eq. (10). If we start with the triple (x_k,y_k,z_k), then there are $2g'_{k+1}+2$ *constraints*, because the leading terms with respect to E in the expression I come from both $z_k^{\,2}$ and $x_ky_kz_k$, whose degree in E are $g'_{k+1}=g_{k+1}+g_k+1$. The expressions are, again, very complicated, even for the Fibonacci lattice. These expressions can be extracted from expanding the traces in Eq. (10) with respect to E such that all coefficients of powers of E must vanish. The newer the generation of the lattice, the more constraints appear. In this way, the generic trace map provides an *infinite-dimensional algebra* for the invariants as k goes to infinity.

The above mapping on the invariants includes a particular case of $E=0$. If $E=0$, we have the mapping of

$$x_k(E=0)=\tfrac{1}{2}D_k^{-1}U_{g_k+1}^{(k)}. \tag{48}$$

Starting from the initial triple $(0, 0, -a)$ where

$$a\equiv-\frac{V_2^{(1)}}{2D'_1}=\frac{T_a^{\,2}+T_b^{\,2}}{2T_aT_b}=\frac{1}{2}\left(\frac{T_a}{T_b}+\frac{T_b}{T_a}\right),$$

it never hops out about the particular set of points on the invariant surface: $(\pm a, 0, 0)$, $(0, \pm a, 0)$, $(0, 0, \pm a)$, called the *invariant six-cycle*.[5,13,14,16,17]

Similarly, for the function $R_{2g_k+2}(E)\equiv[x_k(E)]^2-1$ we expand it with respect to E as follows:

$$R_{2g_k+2}(E)\equiv\tfrac{1}{4}D_k^{-2}[E^{2g_k+2}-R_1^{(k)}E^{2g_k}+R_2^{(k)}E^{2g_k-1}+\cdots$$

$$+(-)^{2g_k+2}R_{2g_k+2}^{(k)}]$$

$$\equiv\frac{1}{4}D_k^{-2}\prod_{j=1}^{2g_k+2}(E-\lambda_j^{(k)}). \tag{49}$$

Therefore, we have another set of the invariants $R_j^{(k)}$ (for $j=1,...,2g_k+2$), which are rational functions of T_a and T_b:

$$R_1^{(k)}=\lambda_1^{(k)}+\lambda_2^{(k)}+\cdots+\lambda_{2g_k+2}^{(k)},$$

$$R_2^{(k)}=\lambda_1^{(k)}\lambda_2^{(k)}+\lambda_2^{(k)}\lambda_3^{(k)}+\cdots+\lambda_{2g_k+2}^{(k)}\lambda_{2g_k+1}^{(k)},$$

$$\vdots \tag{50}$$

$$R_{g_k+1}^{(k)}=\lambda_1^{(k)}\lambda_2^{(k)}\cdots\lambda_{2g_k+1}^{(k)}\lambda_{2g_k+2}^{(k)},$$

where $\lambda_j^{(k)}$ $(j=1,...,2g_k+2)$ are the band edges at the kth generation of the quasiperiodic lattice.

Now we have come to the heart of this section. The above algebra guarantees the *irreducibility of the trace* for any generation of the quasiperiodic lattice. In other words, the trace at any generation of the lattice is never factorized in terms of the traces for the previous generations of the lattice. Therefore, we have no degeneracy in energy bands at each generation of the lattice. In this way the band centers determine the band edges so that *the gaps always open and never degenerate for the parameters T_a and T_b*, unless $T_a=T_b$. As was discussed in Sec. II, this point was demonstrated and proved from the topology of the invariant surface.[13,16,17] Therefore, for a quasiperiodic lattice the *total number of bands always coincides with that of sites in the unit cell*, while for the Toda lattice[21] some of band gaps disappear. Thus, the situation presented here is quite different from that in the soliton theories.

The situation discussed above seems relevant to prove the *irreducibility of the Riemann matrix* $\underline{\Omega}^{(k)}$ by which

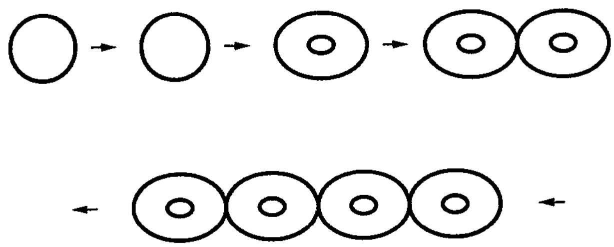

FIG. 6. A scheme to reach a torus of genus infinity. The figure is drawn for a Fibonacci lattice.

the multidimensional Riemann θ-function is defined, although the strict proof has yet been made. Thus, we are able to express the wave function for the kth generation of the quasiperiodic lattice in the same manner as Eq. (36). Finally, we end up with the following expression of the quasiperiodic wave function:

$$\psi_n^+(E)\psi_n^-(E)$$

$$\equiv \lim_{k\to\infty} \prod_{j=1}^{g_k} \frac{E-\mu_j^{(k)}(n-1)}{E-\mu_j^{(k)}(0)}, \tag{51}$$

$$= \lim_{k\to\infty} \frac{\theta_{g_k}(\mathbf{z}^{(k)}(E)-\mathbf{X}^{(k)}(n-1)-\mathbf{K}^{(k)};\underline{\underline{\Omega}}^{(k)})}{\theta_{g_k}(\mathbf{z}^{(k)}(E)-\mathbf{X}^{(k)}(0)-\mathbf{K}^{(k)};\underline{\underline{\Omega}}^{(k)})}. \tag{52}$$

Here $\mu_j^{(k)}(0)$ and $\mu_j^{(k)}(n-1)$ $(j=1,...,g_k)$ lie within the jth band gap $[\lambda_{2j},\lambda_{2j+1}]$ in the spectrum. Also, $\mathbf{z}^{(k)}$, $\mathbf{X}^{(k)}$, and $\mathbf{K}^{(k)}$ are g_k-dimensional vectors and $\underline{\underline{\Omega}}^{(k)}$ a symmetric $g_k \times g_k$ complex matrix, replaced with $\bar{g}$ by g_k in Sec. III. This means that a torus of genus g_{k+1} is defined by the tori of the lower genera g_k, g_{k-1}, and g_{k-2}, with an apparent relation (see Fig. 6):

$$g_{k+1}=n_{k-1}g_k+g_{k-1}+n_{k-1}. \tag{53}$$

We note the following: Since there is no rigorous proof on whether or not the limit exists, the above assertion is a *conjecture* at this moment. However, we may expect that this conjecture is likely to be valid because if we take $E=0$, it provides the invariant six-cycle of the wave function for a quasiperiodic lattice case, as is discussed in Ref. 13.

To close this section we remark the following. The irreducibility of the Riemann matrix is very important to represent the wave functions by means of the multidimensional Riemann θ-functions because if the matrix is reducible, the Riemann θ-functions become a multiple of the lower-dimensional θ-functions. Especially, for the off-diagonal model discussed above, we prove

$$U_j^{(k)}=0, \quad V_j^{(k)}=0, \quad \text{and} \quad R_j^{(k)}=0 \quad \text{for} \quad j=\text{odd}. \tag{54}$$

This is because the wave function has symmetry $\psi_n(-E) = (-)^n\psi_n(E)$ and the energy spectrum is symmetric arround $E=0$.[13,17] Therefore, the dimension of the Riemann matrix must be reduced from g_k to $g_k/2[(g_k-1)/2]$ for g_k=even (odd).

V. CONCLUSIONS

In summary, we have presented a scheme for obtaining the exact wave functions of an electron on a quasiperiodic lattice. Also, we shed light on the new aspects of the quasiperiodic physics for the first time.

If the size of the unit cell $N_k=g_k+1$ is finite, the exact wave functions have both g_k zeros and g_k poles that can be regarded as the g_k zeros of the g_k-dimensional Riemann θ-function. It is proved that they are related to the rotation number of the wave functions through the Thouless formula and they label all the band gaps, where energy gaps are obtained by the trace map.

It is shown that as k goes to infinity the generic trace map induced by the scaling transformations for construction of a quasiperiodic lattice provide us with an infinite-dimensional algebra on the invariants that are recursively given to be polynomials of T_a and T_b. Those invariants define the infinite-dimensional Riemann θ-function by which the wave functions can be exactly represented in a closed manner.

Finally we remark the following. The scheme that we are proposing and we have studied in this paper is very important because this enables us to treat an infinite series of manifolds—tori as a family (Fig. 6). One series of such manifolds is related, by the generic trace map, with another series of those through the algebra of its invariants. From this point of view, the scheme presented here seems closely related to the "schemes" studied by Grothendieck.[26] This type of theory promises great future in its own right.

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APPENDIX: PROGRAM FOR THE CALCULATION OF ENERGY BANDS

We give a simple program by which the readers are able to generate and calculate the energy bands in the following.

(A) If $0<\rho<\frac{1}{2}$, then do the following.

(1) Define the initial triple (x_0,y_0,z_0), fixing the parameters E, T_a, and T_b.

(2) Define the density of B in a quasiperiodic lattice, ρ. Here ρ is related to λ by $\rho=1/(1+\lambda)$.

(3) Make a continued fraction of λ such that $\lambda =[n_0,n_1,...,n_{k-1}]$.

(4) Generate a string R such that $R = XL^{n_{k-1}}XL^{n_{k-2}}\cdots XL^{n_1}XL^{n_0}$, where $L^n=L\cdots L$.

(5) Read the above string from the right to the left. Each time we read L, go to Subroutine MAPL; otherwise, go to Subroutine MAPX.

(6) Make the judgment: If $|x_k|\leqslant 1$, then E is allowed; otherwise, E is forbidden.

(7) Plot E with respect to ρ.

(B) Otherwise (i.e., $\frac{1}{2}<\rho<1$), the roles of A and B are switched. Then do the same thing.

Subroutine MAPL:

$$(x_1,y_1,z_1)=(z_0,y_0,2y_0z_0-x_0),\quad (x_0,y_0,z_0)=(x_1,y_1,z_1).$$

Subroutine MAPX:

$$(x_1,y_1,z_1)=(y_0,x_0,z_0),\quad (x_0,y_0,z_0)=(x_1,y_1,z_1).$$

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