Theory of quasiperiodic lattices. I. Scaling transformation for a quasiperiodic lattice

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A theory of quasiperiodic lattices that consist of only two types of atoms is introduced. If a ratio between the numbers of the two types of atoms in a chain is irrational, the lattice is quasiperiodic. First, we present the scaling transformation for the construction of any quasiperiodic lattice in terms of a continued-fraction expansion of the ratio. Second, we show that all the scaling transformations preserve an invariant surface, which was first discovered by Kohmoto, Kadanoff, and Tang.

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. However, even for one-dimensional problems, traditional methods based on the Bloch theorem are not applicable to solve quasiperiodic-lattice problems, each of which is specified by an irrational number:

$$\lambda=n_0+\frac{1}{n_1+(1/n_2+\cdots)}=[n_0,n_1,n_2,\ldots]\ , \quad (1)$$

where $n_0,n_1,n_2\ldots$ are positive integers, the set of which is called the tail of λ.

The first successes in understanding the physics of quasiperiodic lattices appeared in the studies of the one-dimensional Fibonacci lattice by Kohmoto, Kadanoff, and Tang[4] (KKT) and Ostlund, Pandit, Rand, Schellnhuber, and Siggia.[5] 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 band structures and critical wave functions of the electron on the lattice.[6,7] 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, Gumps and Ali[8] and Holzer[9] showed that there exist the same types of trace maps and the invariant surface, even for a series of irrational numbers which are obtained by taking all n_i as the same n (n any positive integer). Therefore, one fascinating question arises: whether or not there exist the same types of trace maps and the invariant surface for any irrational number. The answer is yes. This is the principal accomplishment of this paper.

The motivation for this research on quasiperiodic lattices came from a very different direction that the usual studies. We had been particularly stimulated by a mathematician's works on a famous problem, known as the Markov spectrum problem: how to classify all the irradiation numbers.[10–14] The great clue needed in order to tame quasiperiodic lattices lies in the concept of the substitution groups, which are subgroups of the free group constructed from the transfer matrices of lattice, M_A and M_B belonging to $SL(2,\underline{C})$.[15] We shall denote the two matrices M_A and M_B as A and B, respectively.

The purpose of this paper is to present the general aspects of a theory of quasiperiodic lattices that consist of only two types of atoms. What we are going to discuss is model independent as long as we are concerned with the discretized models such as the tight-binding model with two site potentials on the two types of atoms, respectively. For this reason we do not specify physical models. First, we introduce the concept of a *substitution group* in the mathematics for quasiperiodic physics. Second, we use it to construct scaling transformations in terms of the generators of the substitution group. Finally, we construct quasiperiodic lattices from those scaling transformations.

II. FUNDAMENTAL STRUCTURE OF A SUBSTITUTION GROUP (REFS. 11–14)

There exists a free group generated by A and B, which belongs to $SL(2,\underline{C})$, where A and B are the transfer matrices of a lattice problem, as discussed above. We define the matrix group $\underline{G}=SL(2,\underline{C})$, where A and B are elements of $\underline{G}$. Then we take a pair (A,B) as the seed of a lattice. This pair (A,B) is an element of the product group $\underline{G}\times\underline{G}$.

Now, taking g as an element of $\underline{G}$, then we transform the pair (A,B) to a new element; $g(A,B)g^{-1}=(A',B')$, which belongs to the same $\underline{G}\times\underline{G}$. We also assume that there is an element of $\underline{G}$, which we shall denote as U, that satisfies $UAU^{-1}=A^{-1}$ We can now define the following four transformations:

$$\begin{aligned} &g_I(A,B)g_I^{-1}=(A,B)\ ,\\ &g_x(A,B)g_x^{-1}=(B,A)\ ,\\ &g_q(A,B)g_q^{-1}=(B^{-1},A)\ , \end{aligned} \quad (2)$$

and

$$g_t(A,B)g_t^{-1}=(B,C) ,$$

where g_I, g_x, g_q, and g_t are the elements of $\underline{G}$ and C is defined by $ABC=\underline{1}$. We represent these four transformations as $\underline{I}$, $\underline{X}$, $\underline{Q}$, and $\underline{T}$, respectively. We can then rewrite them as

$$\begin{aligned} &\underline{I}(A,B)=(A,B) ,\\ &\underline{X}(A,B)=(B,A) ,\\ &\underline{Q}(A,B)=(B^{-1},A) , \end{aligned} \tag{3}$$

and

$$\underline{T}(A,B)=(B,C) .$$

We call the group generated by $\underline{I}$, $\underline{X}$, $\underline{Q}$, and $\underline{T}$, the *substitution group* $\underline{F}$. It is easy to verify the following properties: $\underline{X}^2=\underline{Q}^4=\underline{T}^3=\underline{I}$. These are the defining relationships of the substitution group. The dimension of the substitution group $\underline{F}$ is infinite since $\underline{X}$ and $\underline{T}$ do not commute with each other. There is a representation of the substitution group by a finite dimensional group that is generated as follows.

We will denote a string of words (i.e., matrices), which consists of p A's and q B's, as string $L_{p,q}(A,B)$. Then we can define a pair of strings as

$$W(A,B)\equiv(L_{p,q}(A,B),L_{r,s}(A,B)) .$$

If we define the canonical projection of the string

$$\pi(L_{p,q}(A,B))=pA+qB ,$$

then

$$\pi(W(A,B))\equiv\begin{bmatrix} p & q \\ r & s \end{bmatrix} . \tag{4}$$

The group structure becomes equivalent to that of the hexagonal dihedral group. (See Fig. 1.) According to the hexagonal dihedral group, we have the 12 transformations in terms of the generators of $\underline{F}$, which are simply written $\underline{H}_{d,u,v}\equiv\underline{X}^d\underline{Q}^{2u}\underline{T}^v$ where d,u (mod2), v (mod3), belonging to a subgroup of $\underline{F}$, say $\underline{F}_1$.

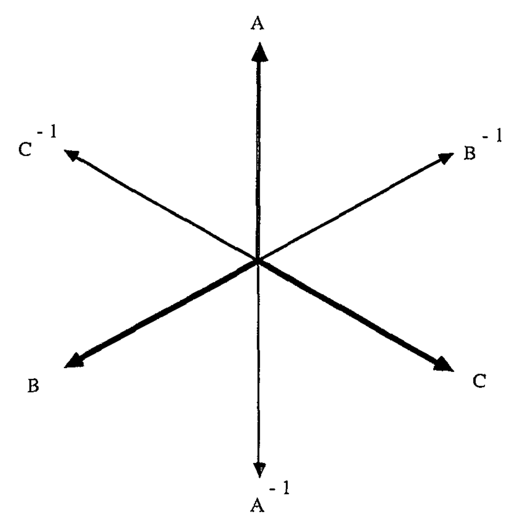

FIG. 1. The structure of a hexagonal dihedral group.

When the subgroup $\underline{F}_1$ acts on the canonical projection of the strings, it induces a subgroup $\underline{F}_2$ of a group $\underline{G}_2=\underline{SL}(2,\underline{Z})$. Elements of the subgroup are the following 12 matrices:

$$\begin{aligned} &\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \pm\begin{bmatrix} 0 & 1 \\ -1 & -1 \end{bmatrix}, \pm\begin{bmatrix} -1 & -1 \\ 1 & 0 \end{bmatrix},\\ &\pm\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \pm\begin{bmatrix} -1 & -1 \\ 0 & 1 \end{bmatrix}, \pm\begin{bmatrix} 1 & 0 \\ -1 & -1 \end{bmatrix}. \end{aligned} \tag{5}$$

Again, when the subgroup $\underline{F}_2$ acts on numbers p and q of the strings, it induces a subgroup $\underline{F}_3$ of the group $\underline{G}_3=\underline{Z}\times\underline{Z}$. Now we have the following 12 pairs (t_i,u_i):

$$\begin{aligned} &\pm(p,q),\ \ \pm(-q,p-q),\ \ \pm(-p+q,-p) ,\\ &\pm(q,p),\ \ \pm(-p,q-p),\ \ \pm(-q+p,-q) . \end{aligned} \tag{6}$$

We can assert that exactly one of these 12 pairs satisfies $t_i\geq 2u_i\geq 0$ unless $(p,q)=\pm(1,0)$, $\pm(0,1)$, $\pm(1,1)$ in one case, or $\pm(1,2)$, $\pm(2,1)$, $\pm(1,-1)$ in the other. Because, otherwise, those expressions in (6) degenerate without making sense. From this assertion, if we define a ratio between p and q as $\lambda=p/q$, we get the following six functions:

$$\lambda,\ \frac{1}{1-\lambda},\ \frac{\lambda-1}{\lambda},\ \frac{1}{\lambda},\ 1-\lambda,\ \frac{1}{\lambda-1}, \tag{7}$$

which forms the group S_6.

The most important property of the substitution group $\underline{F}$ is that, when we define the commutator $K\equiv B^{-1}A^{-1}BA$, any generator of the substitution group preserves the trace of K, which can be written in terms of traces of A, B, and C:

$$\begin{aligned} \Lambda\equiv\mathrm{Tr}(K)=&[\mathrm{Tr}(A)]^2+[\mathrm{Tr}(B)]^2+[\mathrm{Tr}(C)]^2\\ &-\mathrm{Tr}(A)\mathrm{Tr}(B)\mathrm{Tr}(C)-2 , \end{aligned} \tag{8}$$

where $\mathrm{Tr}(C)=\mathrm{Tr}(AB)$ and we have used the identity, called the Fricke identity, in mathematics:

$$\mathrm{Tr}(A^{-1}B)=\mathrm{Tr}(A)\mathrm{Tr}(B)-\mathrm{Tr}(AB) . \tag{9}$$

If we define three parameters $x=\frac{1}{2}\mathrm{Tr}(B)$, $y=\frac{1}{2}\mathrm{Tr}(A)$, $z=\frac{1}{2}\mathrm{Tr}(AB)$, we can define an invariant surface $\underline{I}$, in terms of x,y,z:

$$\underline{I}=\frac{\Lambda-2}{4}=x^2+y^2+z^2-2xyz-1 . \tag{10}$$

This invariant surface is completely equivalent to that studied by KKT,[4] Gumps and Ali,[8] and Holzer.[9] The Fricke identity and the presence of the invariant surface play an important role in understanding qusiperiodic lattices. This point is discussed in the following paper.[16]

III. HOW TO CONSTRUCT A QUASIPERIODIC LATTICE: THE CONCEPT OF THE SCALING TRANSFORMATIONS

Now we are going to construct a quasiperiodic lattice. To construct a quasiperiodic lattice characterized by an irrational number, in terms of generators of the subgroup $\underline{F}_1$, we define an approximation of the irrational number $\lambda_k = P_k / Q_k$ by recursion relations for P_k and Q_k:

$$P_{k+1} = n_k P_k + Q_{k-1}, \quad Q_{k+1} = P_k \tag{11}$$

or

$$P_{k+1} = n_k P_k + P_{k-1}, \quad Q_{k+1} = n_k Q_k + Q_{k-1} \tag{12}$$

with the initial conditions $(P_{-1}, Q_{-1}) = (0,1)$, $(P_0, Q_0) = (1,0)$. This corresponds to a continued fraction expansion truncated at the kth step:

$$\lambda_k \equiv \frac{P_k}{Q_k} = n_0 + \frac{1}{n_1 + [1/n_2 + \cdots + (1/n_k)]} = [n_0, n_1, n_2, \ldots, n_k] . \tag{13}$$

Since we know $P_{k+1}Q_k - P_k Q_{k+1} = (-1)^k$, the next approximation λ_{k+1} lies between $[\lambda_{k-1}, \lambda_k]$ (or $[\lambda_k, \lambda_{k-1}]$) with λ_k converging to λ as k increases.

We denote by the number P_k (Q_k) the total number of A's (B's) in the lattice. The total number of sites in the lattice is $N_k = P_k + Q_k$, where N_k / Q_k defines the average spacing between B's. Then we have a recursion relation for N_k such that $N_{k+1} = n_k N_k + N_{k-1}$ with $N_{-1} = 1$ and $N_0 = 1$. We can then write the lattice in the following form, called the primitive lattice:

$$L^k(A,B) \equiv L_{P_k, Q_k}(A,B) \equiv BA^{a_{Q_k}} BA^{a_{Q_k - 1}} \cdots BA^{a_1} \equiv \prod_{n=1}^{Q_k} BA^{a_n} , \tag{14}$$

where

$$a_n = [n\lambda_k] - [(n-1)\lambda_k] . \tag{15}$$

The symbol [ ] denotes the largest integer part of the number in the square bracket. Thus, once we have an approximation to an irrational number λ_k, we can construct the corresponding lattice at the kth generation. A representation of the quasiperiodic lattice structures for all the irrational numbers is shown in Fig. 2. This picture can be compared with one for the disordered lattice structures in Fig. 3. Here the horizontal axis is the lattice sites from the 0th site to the 400th site, and the vertical axis is the density of B s in the lattice.

Now we consider the role of $\underline{F}_1$ in the lattices. Building an idea from Cohn's work,[11-14] we have the following transformations of the seeds:

$$\mathcal{L}(A,B) = (AB, B)$$

and (16)

$$\mathcal{R}(A,B) = (A, AB) ,$$

where we have renamed $\underline{QT}$ as $\mathcal{L}$ meaning left multiplication, and $(\underline{TQ})^{-1}$ as $\mathcal{R}$, meaning right multiplication. We call the group generated by $\underline{X}$ and $\mathcal{L}$ or $\mathcal{R}$ the *scaling group* $\underline{S}$.

We are then able to construct transformations of primitive lattices in terms of $\mathcal{L}$ and $\mathcal{R}$:

$$\mathcal{L}(L_{r,s}, L_{t,u}) = (L_{r,s}L_{t,u}, L_{t,u}) ,$$

for left multiplication, and

$$\mathcal{R}(R_{r,s}, R_{t,u}) = (R_{r,s}, R_{r,s}R_{t,u}) , \tag{17}$$

for right multiplication, where we require

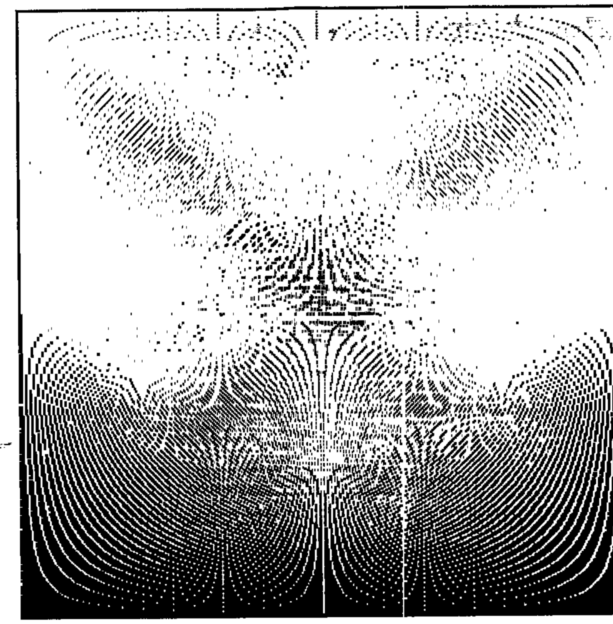

FIG. 2. Quasiperiodic lattices. The vertical line indicates density of B atom (solid circle) to A atom (open circle), which is varied between 0 and 1. The horizontal line indices the lattice sites from 0 to 400.

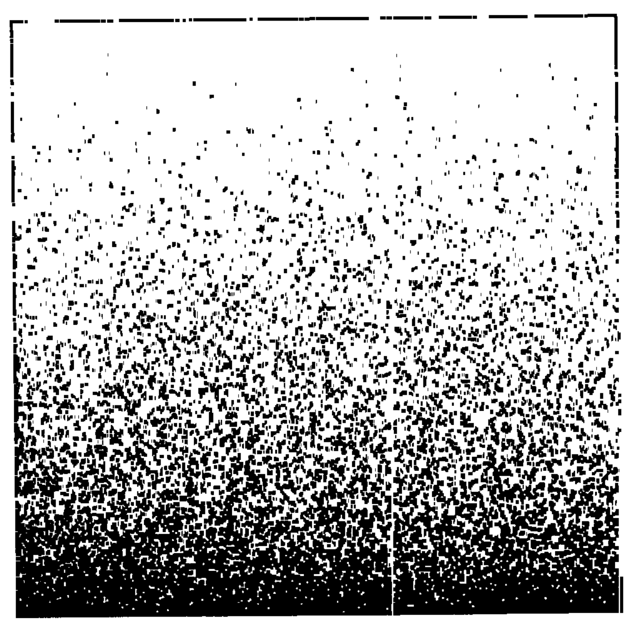

FIG. 3. Disordered lattices. The vertical line indicates density of B atom (solid circle) to A atom (open circle), which is varied between 0 and 1. The horizontal line indicates the lattice sites from 0 to 400.

$L_{r,s}L_{t,u}\equiv L_{r+t,s+u}(R_{r,s}R_{t,u}\equiv R_{r+t,s+u})$ with $ru-st=1$. This is all we need to define the scaling transformations in terms of generators of $\underline{S}$. We then construct scaling transformations such that

$$\underline{X}\mathcal{L}^{n_k}(L^{k-1},L^k)=(L^k,L^{k+1}) ,$$
$$\underline{X}\mathcal{R}^{n_k}(R^k,R^{k-1})=(R^{k+1},R^k) , \tag{18}$$

where we have used $L^k\equiv L^k(A,B)$ and $R^k\equiv R^k(A,B)$, whose lengths are constrained to be N_k. These exactly correspond to the scaling transformations which are the inflation rules for the lattice

$$B\to A,\quad A\to BA^{n_k} ,$$
$$B\to A,\quad A\to A^{n_k}B . \tag{19}$$

Therefore, by successive transformations of the generators, we can rewrite the scaling transformations as

$$(L^k,L^{k+1})=\underline{X}\mathcal{L}^{n_k}\underline{X}\mathcal{L}^{n_{k-1}}\cdots\underline{X}\mathcal{L}^{n_0}(B,A) ,$$
$$(R^{k+1},R^k)=\underline{X}\mathcal{R}^{n_k}\underline{X}\mathcal{R}^{n_{k-1}}\cdots\underline{X}\mathcal{R}^{n_0}(A,B) , \tag{20}$$

which correspond to the continued fraction expansion (1). We note that when we use the continued fraction approximation of the irrational number we regard the lattice as being an infinite repetition of L^k or R^k as the unit cell. In this way we obtain the scaling transformations in terms of the generators of the substitution group. The scaling transformations (20) play a crucially important role in the application of the theory to physical systems. This point is discussed in the following paper.[16]

In conclusion, we have presented the scaling transformation for constructing any quasiperiodic lattice. We also showed that the scaling transformation for any quasiperiodic lattice preserves an invariant surface first discovered by KKT.

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