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LETTER TO THE EDITOR

Universalities in one-electron properties of limit quasiperiodic lattices

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Abstract

We investigate one-electron properties of one-dimensional self-similar structures called limit quasiperiodic lattices. The trace map of such a lattice is nonconservative in contrast to the quasiperiodic case, and we can determine the structure of its attractor. It allows us to obtain the three new features of the present system: (1) The multi-fractal characters of the energy spectra are *universal*. (2) The supports of the $f(\alpha)$-spectra extend over the whole unit interval, [0, 1]. (3) There exist marginal critical states.

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Since the discovery of a quasicrystal, deterministic and aperiodic systems have been attracting much attention [1]. They are classified into a third group in addition to periodic systems and random systems. Although they include a wide range of diverse structures, self-similar structures such as the Fibonacci lattice or the Penrose tiling are especially important because quasicrystals belong to materials of this type. In particular, a one-dimensional (1D) self-similar structure has the symmetry described by a semi-group, and the electronic state on it exhibits rich properties [2–5]. The presence of energy spectra and wavefunctions with multifractal characters is peculiar to such systems. Here we will consider the problem of *universality* among the structures of interest; in particular, we focus on an important class of self-similar structures called limit quasiperiodic lattices.

An aperiodic array of two types of letters (sites), A and B, is called a self-similar lattice (SSL) if it is invariant against a substitution rule (SR) [6]; an SR, σ, acts on the letters as $A \xrightarrow{\sigma} \sigma(A) := \sigma_A(A, B)$, $B \xrightarrow{\sigma} \sigma(B) := \sigma_B(A, B)$, where $\sigma_A(A, B)$ and $\sigma_B(A, B)$ are words of the two letters. σ can be specified by the pair $(\sigma_A(A, B), \sigma_B(A, B))$. With every SR, we can associate a Frobenius matrix, $M := \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ with a and c (resp. b and d) being the numbers of A and B in $\sigma_A(A, B)$ (resp. $\sigma_B(A, B)$); we shall call it the substitution matrix of the SR or of the relevant SSL. If there are several locally isomorphic classes of SSLs with a common substitution matrix, we may call them isomers. For example, two SSLs with SRs,

$(B, ABBA)$ and $(B, ABAB)$, are isomers of the mixed mean lattice being specified by the SR, $(B, BAAB)$ [7]. When an SSL has a global centre of the reflection symmetry, it can be called a symmetric SSL and the relevant SR a symmetric SR [8]. We may call an SR, (σ_A, σ_B), palindromic if both σ_A and σ_B are palindromes, while we may call it quasi-palindromic if it is written with a palindromic SR (σ'_A, σ'_B), as $(\sigma'_A B, \sigma'_B B)$ (or $(\sigma'_A A, \sigma'_B A)$). Palindromic SRs and quasi-palindromic ones produce symmetric SSLs. If a substitution matrix is specified, at least one of the relevant isomers is a symmetric SSL. The three SRs presented above produce all symmetric SSLs.

An important class of SSLs is formed of SSLs such that the structure factor consists only of Bragg peaks [9, 10]. We shall denote it by the symbol Π. An SSL in Π has its own Fourier module $\mathcal{M}$, which is a dense set on the real axis. On the basis of a property of $\mathcal{M}$, the class Π is divided, further, into the three subclasses (i) Π_{I}: quasiperiodic, (ii) Π_{II}: limit quasiperiodic and (iii) Π_{III}: limit periodic. The number of the generators of $\mathcal{M}$ is two for Π_{I} but infinite otherwise, while an SSL belongs to Π_{I} or Π_{II} iff the Frobenius eigenvalue τ of the relevant substitution matrix M is a Pisot number. The Frobenius eigenvector of M is given by the column vector ${}^{\mathrm{t}}(1, \omega)$ with $\omega := (\tau - a)/b = c/(\tau - d)$ being a positive number. The Fourier module $\mathcal{M}$ of an SSL in Π_{I} or Π_{II} is written as $\mathcal{M} = (1+\omega)^{-1}\mathbf{Z}\{\omega\}$ with $\mathbf{Z}\{\omega\} := \mathbf{Z}[\omega] \cup \tau^{-1}\mathbf{Z}[\omega] \cup \tau^{-2}\mathbf{Z}[\omega] \cup \cdots$, where $\mathbf{Z}[\omega] := \{x + y\omega \mid x, y \in \mathbf{Z}\}$. Since $\mathcal{M}$ is uniquely determined by M, it is common among different isomers. In particular, if M is unimodular, the relevant SSL belongs to Π_{I} and vice versa. We may write for this SSL $\mathcal{M} = (1+\omega)^{-1}\mathbf{Z}[\omega]$ because $\tau\mathbf{Z}[\omega] = \mathbf{Z}[\omega]$ and $\mathbf{Z}\{\omega\} = \mathbf{Z}[\omega]$ for this SSL.

We shall denote by Π^{s} the subset composed only of the symmetric members in Π. Π^{s} is divided, further, into the three subsets, $\Pi^{\mathrm{s}}_{\mathrm{I}}$, $\Pi^{\mathrm{s}}_{\mathrm{II}}$ and $\Pi^{\mathrm{s}}_{\mathrm{III}}$. Self-similarity of an SSL allows us to use the trace map (TM) for researches of the electronic states on it [2, 3]. The character of the TM as a nonlinear map depends crucially on whether it is conservative or not [7, 11–13]. It is known that SSLs with conservative TMs form a special subset, $\Pi^{\mathrm{c}}_{\mathrm{I}}$, of $\Pi^{\mathrm{s}}_{\mathrm{I}}$ [8, 13]. Previous researches on the one-electron states of SSLs have focused exclusively on Π^{s}. More precisely, $\Pi^{\mathrm{c}}_{\mathrm{I}}$ is investigated thoroughly [5] but $\Pi^{\mathrm{s}}_{\mathrm{II}}$ and $\Pi^{\mathrm{n}}_{\mathrm{I}} := \Pi^{\mathrm{s}}_{\mathrm{I}} - \Pi^{\mathrm{c}}_{\mathrm{I}}$ have never been investigated, while there are a considerable number of papers on the subclass $\Pi^{\mathrm{s}}_{\mathrm{III}}$ but they are still at a rudimentary stage (see, for example, [7, 11]). The authors, therefore, investigated in detail the case of the subclass $\Pi^{\mathrm{s}}_{\mathrm{II}}$. Though $\Pi^{\mathrm{s}}_{\mathrm{II}}$ appears a simple extension of $\Pi^{\mathrm{s}}_{\mathrm{I}}$, it turns out as shown later that its one-electron states exhibit a remarkably different character from the case of the latter. We shall call hereafter an SSL in $\Pi^{\mathrm{s}}_{\mathrm{II}}$ a limit quasiperiodic lattice (LQL), while the one in $\Pi^{\mathrm{c}}_{\mathrm{I}}$ is called a conservative SSL. Note that an LQL is never conservative [13]. The Fibonacci lattice is a representative of $\Pi^{\mathrm{c}}_{\mathrm{I}}$ but the mixed mean lattice is a case of $\Pi^{\mathrm{s}}_{\mathrm{II}}$.

Generic characters of one-electron states of an SSL can be investigated using the tight-binding Hamiltonian $\mathcal{H}$, each site-energy of which takes V_A or V_B depending on the type of site [5]. The unit of energy can be so chosen that the transfer integral assumes -1. It was shown generally that the energy spectrum $\sigma = \sigma(\mathcal{H})$ is singular continuous [14]. This means that the integrated state density $H(E)$ per one site is a devil's staircase. The set, G_σ, of the heights of all the steps of the staircase is a discrete subset of the unit interval [0, 1], and is determined by the gap labelling theorem [15]. Since σ is a multifractal, the distribution of its singularity α in σ is characterized by the $f(\alpha)$-spectrum, whose support is a closed interval, $[\alpha_{\min}, \alpha_{\max}] \subset [0, 1]$ [5]. A remarkable feature of an SSL is that σ has an infinite number of centres of local self-similarity [4]. Let σ_{ls} be the set of all such centres. Then, the set, $\Sigma := \{H(E) \mid E \in \sigma_{\mathrm{ls}}\}$, is the second important object to G_σ to characterize σ.

In the trace map formalism, a homomorphism is defined from $\mathcal{F}(A, B)$, the free semi-group generated by the two generators A and B, into $SL(2, \mathbf{R})$ [7, 12, 16]. The image of

$W \in \mathcal{F}$ is called the transfer matrix and is written as $\hat{W}$, which is a product of $\hat{A}$ and $\hat{B}$. The pair of transfer matrices, $\{\hat{A}_n, \hat{B}_n\}$, which are associated with the pair $\{A_n, B_n\} := \sigma^n\{A, B\}$, is an important object in the trace map formalism. A similar pair in the next generation is related to that pair by a recursion relation. If a supplementary transfer matrix is introduced by $\hat{C}_n := \hat{A}_n\hat{B}_n$, the recursion relation yields another one defined for the traces of $\hat{A}_n$, $\hat{B}_n$ and $\hat{C}_n$. The trace map is associated with this recursion relation, and defines a 3D dynamical system over a 3D phase space $\mathbf{R}^3$: $\mathbf{r} \to T\mathbf{r}$ with $\mathbf{r} = (x, y, z)$ [2, 6, 12]. Tx, Ty and Tz are polynomials with integral coefficients. The starting point of an orbit $O(E) := \{\mathbf{r}_n \mid n \in \mathbf{N}\}$ of the TM is given by $\mathbf{r}_1 = (V_A - E, V_B - E, (V_A - E)(V_B - E) - 2)$, which depends on the parameters V_A, V_B and E though the TM itself does not depend on them.

Noncommutativity between $\hat{A}_n$ and $\hat{B}_n$ can be quantified by $I_n := \frac{1}{2}\,\mathrm{Tr}[\hat{A}_n, \hat{B}_n]^2$, which is written as $I_n = I(\mathbf{r}_n)$ with $I(\mathbf{r}) = x^2 + y^2 + z^2 - xyz - 4$ [2]. It follows that $I(\mathbf{r}_1) = (\Delta/2)^2$ with $\Delta := V_B - V_A$. It can be shown generally that there exists a polynomial $P(\mathbf{r})$ such that $[\hat{A}_{n+1}, \hat{B}_{n+1}] = P(\mathbf{r}_n)[\hat{A}_n, \hat{B}_n]$ for a palindromic substitution rule but $[\hat{A}_{n+1}, \hat{B}_{n+1}] = P(\mathbf{r}_n)[\hat{A}_n, \hat{B}_n]\hat{B}_n$ for a quasi-palindromic one [17]. This yields the identity $I(T\mathbf{r}) \equiv [P(\mathbf{r})]^2 I(\mathbf{r})$, where $|P(\mathbf{r})| \equiv 1$ for the conservative case but $\deg(P) \geqslant 1$ otherwise [16]. Hence, $I(\mathbf{r})$ is an invariant of the TM only for the conservative case but $I(\mathbf{r})$ is a semi-invariant for the general case because the TM never changes its sign [6]. Let us assume that $\hat{A}_n$ and $\hat{B}_n$ for $\exists n \in \mathbf{N}$ are not commutative and, besides, that $P(x_n, y_n, z_n) = 0$ for some $E \in \sigma$. Then, $\hat{A}_m$, $\hat{B}_m$ are commutative for $\forall m \geqslant n + 1$, and we can conclude that the relevant eigenstate will be extended as in the case of a periodic system [18]. Different extended states may be obtained from the roots of a similar equation at a different generation. Therefore, an SSL may have an infinite number of extended states unless it is conservative.

The dynamical system defined by the TM, T, is characterized by its limit cycles. If a point in $\mathbf{R}^3$ belongs to a limit cycle with period p, it is a fixed point of T^p and an orbit starting from it is a pure cycle. A necessary and sufficient condition for $E \in \sigma$ to belong to σ_{ls} is that $O(E)$ falls on a limit cycle [5]. If this is satisfied, we can determine the singularity $\alpha = \alpha(E)$ by a linear analysis of T^p around the relevant fixed point [3]. The wavefunction of the corresponding eigenstate is known to be asymptotically self-similar; the spatial ratio of the self-similarity is equal to τ^p [5].

Though $I(x, y, z)$ is not an invariant of the TM, T, of a limit quasiperiodic lattice, the curved surface defined by the equation $I(x, y, z) = 0$ is an invariant surface [6]. Its restriction, $\mathbf{S}$, into the cube $[-2, 2]^3 \in \mathbf{R}^3$ is a closed surface as shown in figure 2. $\mathbf{S}$ is a ball with tetrahedral point symmetry but has four cusps located at four of the eight corners of the cube [11]. A coordinate system can be introduced into $\mathbf{S}$ by $x = 2\cos(2\pi u)$, $y = 2\cos(2\pi v)$ and $z = 2\cos[2\pi(u + v)]$ with (u, v) being a variable on the 2D torus $\mathbf{T}^2 := \mathbf{R}^2/\mathbf{Z}^2$. Actually, $\mathbf{S}$ is doubly covered by $\mathbf{T}^2$ because $\pm(u, v)$ are mapped onto a single point on $\mathbf{S}$. The origin $(0, 0)$ of $\mathbf{T}^2$ corresponds to $(2, 2, 2)$ in $\mathbf{R}^3$. The TM induces a 2D dynamical system over $\mathbf{T}^2$: $T(u, v) = (u, v)M$ with M being the relevant substitution matrix. With these machineries together with a theory of algebraic number theory, we can determine all the cycles of the dynamical system, which will be presented elsewhere.

We shall consider first a periodic system ($\Delta = 0$). In this case, every 3D orbit of T is confined to $\mathbf{S}$ from the very beginning. The initial state $\mathbf{r}_1$ of the orbit $O(E)$ with $E = -2\cos 2\pi\kappa$ corresponds to $(u_1, v_1) = \pm(\kappa, \kappa)$ on $\mathbf{S}$, where κ is the rationalized wave number of a plane wave state. It follows that $(u_n, v_n) = \pm\big(L_n^{(A)}\kappa, L_n^{(B)}\kappa\big)$ with $L_n^{(A)}$ and $L_n^{(B)}$ being the numbers of the letters in A_n and B_n, respectively. A necessary and sufficient condition for the 2D orbit $\{(u_n, v_n) \mid n \in \mathbf{N}\}$ to converge on $(0, 0) \in \mathbf{S}$ is equivalent to $\kappa \in \mathcal{M}$ [9, 10]. On the other hand, a condition for the 2D orbit to fall on a limit cycle with period p is that $\{(u_{n+p} \mp u_n, v_{n+p} \mp v_n) \mid n \in \mathbf{N}\}$ converges on $(0, 0) \in \mathbf{S}$. Using the fact that the

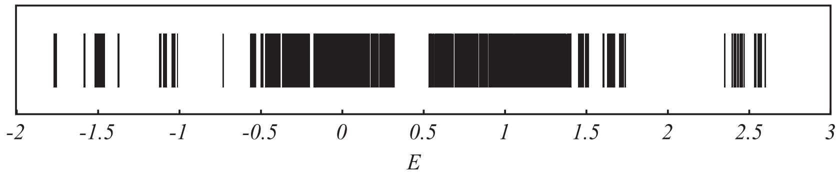

Figure 1. The energy spectrum of the mixed mean lattice with $\Delta := V_B - V_A = 1$.

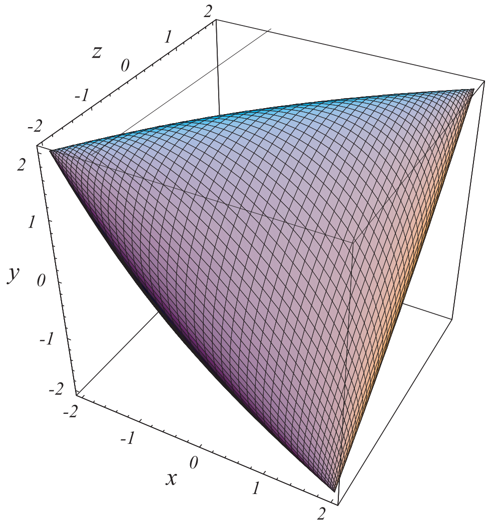

Figure 2. Invariant surface: $I(x, y, z) = 0$.

ratios $L^{(A)}_{n+p}/L^{(A)}_n$ and $L^{(B)}_{n+p}/L^{(B)}_n$ tend to τ^p as n goes to infinity, we can show that a necessary and sufficient condition for that condition to be satisfied is given by $(\tau^p - 1)\kappa \in \mathcal{M}$ or $(\tau^p + 1)\kappa \in \mathcal{M}$, which is equivalent to the condition $\kappa \in \mathbf{Q}[\omega] - \mathcal{M}$ with $\mathbf{Q}[\omega] := \{s + t\omega \mid s, t \in \mathbf{Q}\}$. Thus, the behaviour of the TM of a periodic system has been completely revealed. Since the energy spectrum of the periodic system is absolutely continuous, $\alpha(E)$ takes 1.[3] Two states with wave numbers $\pm\kappa$ degenerate in energy and the corresponding two orbits of the TM are identical, so that we can assume $0 \leqslant \kappa \leqslant 1/2$. The number κ is nothing but the normalized value per one site of the number of nodes in the relevant sinusoidal wave. Since $H(E)$ is related to $\kappa = \kappa(E)$ by the equation $H = 2\kappa(E)$, the asymptotic behaviour of the TM at the energy E is determined by the value of $H(E) \in [0, 1]$.

We will proceed to the case of a non-periodic system ($\Delta \neq 0$). Since an LQL (limit quasiperiodic lattice) has reflection symmetry, every energy level has its own parity with respect to the centre of symmetry. If Δ is changed adiabatically from zero to the present value, every energy level will change continuously because double degeneracies present at $\Delta = 0$ do not matter if the parity is specified. It follows that κ remains the normalized number of nodes. Then, the asymptotic behaviour of the TM will be determined by the value $H = H(E)$, and the rule is the same as described above for the periodic system. Thus, we can conclude that $\Sigma = \mathbf{Q}[\omega] \cap [0, 1]$, which is a similar result to the one obtained in [4] for the case of the Fibonacci lattice. A remarkable property of the TM of an LQL is its *universality*. It is based on the two points: (1) the TM does not explicitly depend on the parameters Δ and E. (2) It

[3] However, $\alpha = 1/2$ for the case where E is located at a band edge.

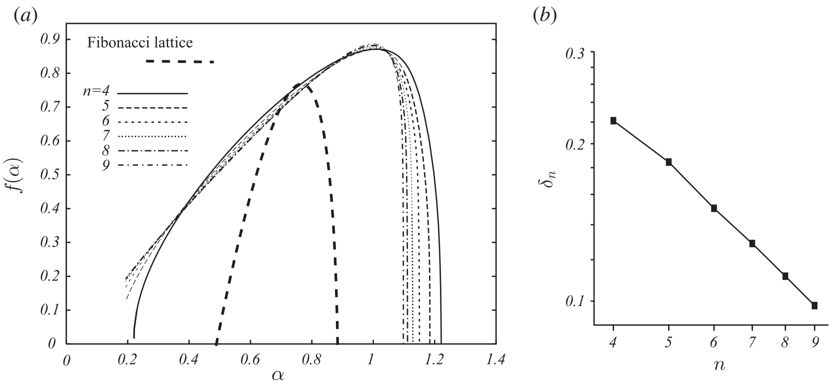

Figure 3. The $f(\alpha)$-spectra of the energy spectra of periodic approximants for the mixed mean lattice (*a*) and a log–log plot of $\delta_n := \alpha_{\max}^{(n)} - 1$ versus the generation number n (*b*). The data from the fourth to the ninth generations are used. The data in the region $\alpha < 0.2$ are cut because their accuracies are insufficient on account of the presence of marginal critical states. The $f(\alpha)$-spectra of the Fibonacci lattice are superposed for comparison. The asymptotic linearity of the plot in (*b*) concludes that δ_n tends to zero in an inverse power law for n as n goes to infinity.

is essentially of 3D character, and not confined to a 2D manifold as in the conservative case. Thus, the attractor is independent of the value of Δ, and identical to that of the periodic system. It follows that the $f(\alpha)$-spectrum of σ is universal. Moreover, we can conclude that $\alpha = 1$ for every centre of local self-similarity of σ (see footnote 3), and, consequently, $\alpha_{\max} = 1$. We will show it explicitly here for the case of the mixed mean lattice, for which $\tau = 1 + \sqrt{3}$ and $\omega = \tau/2$. The condition $(\tau^p - 1)\kappa \in \mathcal{M}$ is satisfied for this case by $p = 1$ and $\kappa = 1/3$, and the relevant 3D orbit of T converges to a 1-cycle. The scaling parameter determined by a linear analysis of T around the relevant fixed point, $(-1, -1, -1)$, is shown as exactly equal to τ^p with $p = 1$, so that $\alpha = 1$.

The gap-labelling theorem concludes that $G_\sigma = \mathcal{M} \cap [0, 1]$ [15], which is expected, also, from a perturbative consideration. The gap labelled by $H \in G_\sigma$ is bounded by two energy levels located at band edges. However, the corresponding fixed point $(2, 2, 2)$ of the TM is a singularity of $\mathbf{S}$, and we cannot conclude that $\alpha = 1/2$ for these two energy levels. Surprisingly, it turns out that $\alpha_{\min} = 0$, so that the relevant states are *marginal critical states*, which we can prove by a similar technique to the one used in [19][4]. This and the result $\alpha_{\max} = 1$ are consistent with the $f(\alpha)$-spectrum being universal because there is no reason why the value of $\alpha_{\min}$ or $\alpha_{\max}$ must take an odd value. We show in figure 3 the $f(\alpha)$-spectrum of the energy spectrum in figure 1. The broadness of the $f(\alpha)$-spectrum means that the energy spectrum of an LQL is more inhomogeneous than that of a conservative SSL. Since both Σ and G_σ are determined solely by the substitution matrix, we expect that, if there are several symmetrical isomers, their $f(\alpha)$-spectra belong to a common universality class although their TMs are different.

The TM derived from a conservative SSL is a 2D map on the curved surface $I(x, y, z) = (\Delta/2)^2$. Since this surface depends on the value of Δ, the $f(\alpha)$-spectrum as well as $\alpha_{\min}$ and $\alpha_{\max}$ are not universal. This is consistent with the known fact that $\alpha_{\min} > 0$ and $\alpha_{\max} < 1$ for every conservative SSL (see figure 2) [2, 5]. The conservative SSLs are actually minorities in $\Pi_{\mathrm{I}}^{\mathrm{s}}$, and one-electron properties of nonconservative SSLs in $\Pi_{\mathrm{I}}^{\mathrm{s}}$ have not been investigated

[4] A marginal critical state is a peculiar critical state discovered for the case of a *ternary* SSL in [19]. It exhibits a non-power-law scaling.

yet. The present theory is basically applicable to this case; the only modification needed is to replace the Fourier module by $\mathcal{M} = (1+\omega)^{-1}\mathbf{Z}[\omega]$. Thus, among isomers belonging to $\Pi_{\mathrm{I}}^{\mathrm{s}}$, only the conservative member is nonuniversal. Note, for example, that the substitution rule, $(ABA, ABABA)$, produces a conservative SSL but its isomer, $(ABA, BAAAB)$, does not.

Although no substance which takes a structure represented by an LQL as its thermodynamically stable phase is known, such a structure is realizable as an artificial superlattice. Since a transfer matrix formalism can be applied for more general 1D Schrödinger equations, the results of this letter apply to the electronic state in such an artificial superlattice as well [20]. Furthermore, it is basically applicable to a propagation in a stratified substance of an ultrasonic wave, an electromagnetic wave (light) and a spin wave as well. If, for example, a lower marginal critical state is used as a channel of light, the speed of light will fall dramatically.

In conclusion, one-electron properties of limit quasiperiodic lattices exhibit a universality in contrast to the case of quasiperiodic ones, and a universality class is specified solely by the substitution matrix.

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