New Classes of Quasicrystals and Marginal Critical States

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One-dimensional quasilattices, namely, the geometrical objects that represent quasicrystals, are classified into mutual local-derivability (MLD) classes. Besides the familiar class, there exist an infinite number of new MLD classes, and different MLD classes are distinguished by the inflation rules of their representatives. It has been found that electronic properties of a new MLD class are characterized by the presence of marginal critical states, which are considered to be nearly localized states.

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Quasicrystals (QCs) have aperiodic ordered structures, which are different from either crystalline or disordered materials. It has been reported that QCs exhibit quite unique physical properties [1], which should be closely connected with the structure of QCs. A sufficient understanding in this respect is, however, yet to be attained. For instance, in order to understand the transport properties of QCs, further systematic studies on the electronic properties of various types of QCs are necessary.

The atomic positions of an idealized QC form a quasiperiodic object called quasilattice (QL), the classification of which is the principal subject of the crystallography of QCs. One of the important features of QLs is the self-similarity, which is closely connected with the physical properties. Thus, in the first part of this Letter, we shall develop a new classification scheme of QLs based on the self-similarity. One can argue that the different classes of QLs correspond to different universality classes with respect to the electronic properties. We next show that there exists a new class of QLs whose electronic properties are characterized by the presence of *marginal critical states,* which can be thought of as being virtually localized. This feature is essentially different from the case of the standard class of QLs on which most of the previous studies have been done. The transport properties of the new class may be markedly different from the conventional one.

We confine ourselves to one-dimensional (1D) cases. A 1D QL is obtained by projecting a subset of a 2D lattice Λ, the mother lattice, onto a 1D subspace $E_\parallel$ [2,3]. The line $E_\parallel$ is taken to be parallel to $\tau\mathbf{a}_1 + \mathbf{a}_2$ with $\mathbf{a}_1$ and $\mathbf{a}_2$ being the primitive lattice vectors of Λ and τ a quadratic irrational such as $\frac{1}{2}(1 + \sqrt{5})$ (the golden mean), $1 + \sqrt{2}$ (the silver mean), etc. The subset is taken as $\Lambda \cap \Sigma$ with Σ being a parallel strip to $E_\parallel$. If the scales of $E_\parallel$ and $E_\perp$, the physical space and its orthogonal complement, are chosen appropriately, both the projections $\Lambda_\parallel$ and $\Lambda_\perp$ of Λ onto $E_\parallel$ and $E_\perp$, respectively, are given by the dense set $\mathbf{Z}[\tau] \equiv \{p + q\tau \,|\, p, q \in \mathbf{Z}\}$. Thus, a 1D QL is a discrete subset of $\Lambda_\parallel$, where its point density is proportional to the window W, i.e., the width of the strip Σ. According to the relative position of Σ to Λ, an infinite number of QLs are possible with the same W. But they form a single *local-isomorphism class,* and their differences are irrelevant to the physical properties.

For a generic W, one obtains a ternary 1D QL composed of three types of lattice spacings: s, m, and l, referring to short, medium, and long spacings, respectively; they satisfy $|l| = |s| + |m|$. If W is reduced, one obtains another QL as a subset of the original QL. The new spacings, s', m', and l', are composites of the older ones. For an appropriate choice of the reduction of W, the older QL turns out to be a uniform decoration of the newer, i.e., the decoration of l', for example, is common for all l's. The three decorations of the spacings form a substitution rule. The newer QL is then called a *subquasilattice* (SQL) of the older.

If W is reduced by the factor τ^{-n} with n being any positive integer, the resulting QL is locally isomorphic with the scaled version of the original QL with the factor τ^n [4]. The original QL is called self-similar if the new QL is an SQL of the original. Here, the substitution rule, combining the three spacings of the original QL with the newer ones, represents the self-similarity; it is called the *inflation rule*. It can be shown that a QL can be self-similar if and only if its window W belongs to the quadratic field $\mathbf{Q}[\tau] \equiv \{r + s\tau \,|\, r, s \in \mathbf{Q}\}$ [5]; that is, the window must be rational. The inflation rule as well as the minimum power n for the ratio of self-similarity, τ^n, depends on a number theoretical property of W. The following argument will be focused on this rational case.

Several QLs associated with the silver mean are presented in Table I. The first two are binary but others ternary. The QLs except for C and E have self-similarities whose ratios are presented in the sixth column. The QL C is not self-similar but is changed to the once-inflated version of A by the substitution rule in the seventh column. A similar relation holds between the pair $\{D, E\}$. The QL A is an SQL of B with the substitution rule, $s' = s$, $l' = sm$, and the QL F is an SQL of G with $s' = m$, $m' = l$, $l' = msm$. Though the two QLs G and H are similar, there exists no inflation rule which combine them.

We introduce an important relationship between QLs: two QLs are *mutually locally derivable* if all the sites of

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TABLE I. Several 1D QLs associated with the silver mean, $\tau = 1 + \sqrt{2}$. The first three belong to the type I MLD class, while others belong to type II MLD classes.

	W	$\lvert s\rvert$	$\lvert m\rvert$	$\lvert l\rvert$	Ratio	Inflation rule (or substitution rule)
A	$\sqrt{2}$	1	$\cdots$	τ	τ	$s' = l,\ l' = sll$
B	$1 + \sqrt{2}$	1	$\sqrt{2}$	$\cdots$	τ	$s' = sm,\ m' = sms$
C	$3 - \sqrt{2}$	1	$\sqrt{2}$	τ	$\cdots$	$(s' = sm,\ m' = sll)$
D	$1 + \frac{1}{2}\sqrt{2}$	1	$\sqrt{2}$	τ	τ	$s' = sm,\ m' = sl,\ l' = sll$
E	$\sqrt{2} + \frac{1}{2}\sqrt{2}$	1	$\sqrt{2}$	τ	$\cdots$	$(s' = sm,\ m' = ssm,\ l' = slsm)$
F	$\frac{1}{2} + \sqrt{2}$	1	$\sqrt{2}$	τ	τ^2	$s' = smsl,\ m' = smsmsl,\ l' = smsllsmsl$
G	$\frac{3}{2} + \sqrt{2}$	τ^{-1}	1	$\sqrt{2}$	τ^2	$s' = msm,\ m' = mlmmsm,\ l' = mlmlmmsm$
H	$\frac{1}{2} + \frac{1}{2}\sqrt{2}$	1	τ	$\sqrt{2}\,\tau$	τ^2	$s' = msm,\ m' = mlmmsm,\ l' = mlmlmmsm$

one of them are determined *locally* from the structure of the other and vice versa [6]. All the QLs derived from a single mother lattice are classified into an infinite number of *mutual local-derivability* (MLD) classes. The MLD class to which a given QL belongs is determined by a number theoretical property of $W \in \mathbf{Q}[\tau]$. We only present a necessary condition: *if two QLs belong to a single MLD class, the relevant two windows have a common denominator when they are represented as simple fractions in the quadratic field*. A QL and its any SQL belong to the same MLD class. The eight QLs in Table I are divided into three MLD classes: $\{A, B, C\}$, $\{D, E\}$, and $\{F, G, H\}$. It can be shown that (i) every MLD class includes at least one self-similar member, which can be taken as a representative of the class, and (ii) every QL in the MLD class has an SQL which is similar to the representative; that is, any non-self-similar QL is a uniform decoration of a self-similar QL.

The structure factor of a QL is composed of Bragg peaks, whose intensities are determined by the size of the window. For example, the three QLs, C, D, and F in Table I, have windows of similar sizes, and their structure factors are not so much different. They nevertheless belong to different MLD classes.

We shall call a QL to be type I or II according to whether its window belongs to $\mathbf{Z}[\tau]$ or not, respectively. All the type I QLs for a given τ form a single MLD class, as seen in Table I. Previous investigations on the electronic properties of 1D QLs have been almost exclusively done on the basis of models on type I QLs [7–9]. It has been proved that a type I QL and its any decoration belong to a common universality class of electronic properties [10], which are dominated by the structures of the inflation rule. On the other hand, we may expect that type II QLs belong to different universality classes, because their inflation rules are different from that of the type I class.

We now present a brief review on the electronic properties of type I QLs. The main observations, obtained from the case of the Fibonacci lattice as well as some of its associates, are [7] (i) *the energy spectrum is purely singular continuous or, equivalently, fractal-like,* and (ii) *all the eigenfunctions are critical, i.e., neither extended nor localized in the usual meaning.* The energy spectrum and the eigenfunctions have also been found to exhibit self-similar structures, which can be directly related to the inflation rule of the underlying QL by a real-space renormalization-group approach [8].

The energy spectrum of any homogeneous 1D system obeys locally a scaling law. The local scaling at the reference energy E_r is represented by the scaling exponent $\alpha = \alpha(E_r)$ satisfying $0 \leq \alpha \leq 1$ [7]. While α represents the local dimension of the energy spectrum, it also characterizes the localization character of the eigenfunction of the energy level E_r. In particular, an isolated energy level of a localized state has a vanishing exponent, $\alpha = 0$, while inside an absolutely continuous spectrum, which confirms extended states, $\alpha = 1$. A purely singular-continuous spectrum being characterized by fractional exponents confirms critical eigenfunctions. The energy spectrum of a type I QL is, in general, a multifractal [11], and is characterized by the $f(\alpha)$ spectrum. The support of the $f(\alpha)$ is an interval $[\alpha_{\min}, \alpha_{\max}]$ with $0 < \alpha_{\min} < \alpha_{\max} < 1$; α ranges from $\alpha_{\min}$ to $\alpha_{\max}$, so that every energy level is characterized by fractional power-law scaling [7].

Although the above observations are common in the case of type I QLs, electronic properties of type II QLs have been scarcely investigated. In the following, we show some numerical as well as analytical evidence that the type II QL listed as D in Table I and shown in Fig. 1 indeed exhibits a new scaling property. Let us take a *binary* atomic chain, which is obtained by decorating this QL as follows: (i) atoms of type X are located on all the lattice points, (ii) one atom of type Y is located on each spacing of type m, and (iii) a pair of type Y atoms is located on each spacing of type l. The densities of the two types of atoms in the chain are equal. More remarkably, the chain is invariant against the exchange of two types of atoms, X and Y. We employ the tight-binding model on this atomic chain, $t\Psi_{j-1} + V_j\Psi_j + t\Psi_{j+1} = E\Psi_j$, where we assume that $t = -1$ for the transfer integrals and $V_X = 0$ and $V_Y = V$ for the relevant site energies.

Because of the aforementioned symmetry of the atomic chain, the energy spectrum becomes symmetrical which is confirmed by the numerical result as shown in Fig. 2.

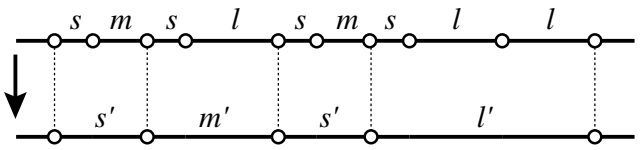

FIG. 1. A ternary 1D QL given as D in Table I. It is self-similar with the inflation rule in the table. The ratio of the self-similarity is the silver mean, $\tau = 1 + \sqrt{2}$. The frequencies of the three spacings s, m, and l are shown to be proportional to $\tau^{-1}:\tau^{-2}:\tau^{-1}$ $(2\tau^{-1} + \tau^{-2} = 1)$.

The energy spectrum is divided into two equivalent clusters, and the left cluster exhibits a hierarchical trifurcation, which will reflect the nature of the leftmost level, i.e., the ground state. The trifurcation can be understood in terms of a perturbational real-space renormalization-group approach similar to that introduced by Niu and Nori for the case of the Fibonacci lattice [8]. The approach is based on the recursive structure of the QL and assumes $V \gg 1$. In the zeroth approximation, the spectrum consists of two equally degenerate energy levels at $E = 0$ and V, while the eigenstates are the Wannier states themselves. To see the splitting of the level originating from the X atoms, all the Y atoms are decimated as shown in Fig. 3. This yields three types of effective transfer integrals between X atoms, $t_s = -1$, $t_m \approx -1/V$, and $t_l \approx -1/V^2$, which are all negative and satisfy the inequalities:

$$|t_s| \gg |t_m| \gg |t_l| . \tag{1}$$

In the first approximation, we take only the leading effective transfer integral t_s into account. Since the type s spacings are isolated, the energy spectrum consists of three sublevels at $E = 0$ and $E = \pm t_s (= \mp 1)$; the central level is derived from isolated atoms, while the two satellites are derived from isolated diatomic "molecules." The weights of the three sublevels have the ratios $\tau^{-1}:\tau^{-2}:\tau^{-1}$, which agree with the numerical results. To see the trifurcation of the level derived from the molecular bonding states, we shall consider the molecules to be the "atoms" of the second generation. Because of the self-similarity of the QL, there appear three types of effective transfer integrals between the new atoms as shown in Fig. 3:

$$t_s' \approx \frac{1}{2} t_m, \qquad t_m' \approx \frac{1}{2} t_l, \quad \text{and} \quad t_l' \approx \frac{1}{2} \frac{t_l^2}{t_s}, \tag{2}$$

where the numerical factor $1/2$ appears as the square of the bonding amplitude $1/\sqrt{2}$. Since the new parameters satisfy the same inequalities as Eq. (1), we can return now to the point after Eq. (1) and continue the discussion *recursively*. Thus, we obtain a hierarchical trifurcation spectrum. The ground state is understood to be a hierarchical composite of molecular bonding states, as shown in Fig. 4.

To make a quantitative argument, we introduce two positive parameters as the ratios between the effective transfer integrals of the nth generation:

$$f_n = \frac{t_m^{(n)}}{t_s^{(n)}}, \qquad g_n = \frac{t_l^{(n)}}{t_m^{(n)}} . \tag{3}$$

Equation (2) yields the two-dimensional map, $f_{n+1} \approx g_n, g_{n+1} \approx f_n g_n$, which converges to the origin of the fg plane. This means that the atoms are increasingly isolated as n is increased. We can linearize this 2D map with new variables, $\ln f_n$ and $\ln g_n$, and obtain the asymptotic expression

$$f_n \approx g_{n-1} \sim \exp[-c\tau_{\mathrm{G}}^n] = \exp[-c\tau^{n\nu}], \tag{4}$$

with $\tau_{\mathrm{G}} = (1 + \sqrt{5})/2$, i.e., the golden mean, and $\nu = \ln\tau_{\mathrm{G}}/\ln\tau \approx 0.546$. Note that τ_{G} is the leading eigenvalue of the 2×2 matrix associated with the linearized map and c a positive constant depending on V.

The bandwidth w_n of the subcluster of the nth generation is estimated to be $w_n \approx 2|t_s^{(n)}|$. The relation $t_s^{(n+1)} \approx \frac{1}{2} t_m^{(n)}$ as in Eq. (2) can be used to prove $w_{n+1}/w_n \approx t_s^{(n+1)}/t_s^{(n)} \approx \frac{1}{2} f_n \sim \exp[-c\tau^{n\nu}]$, which tends to zero as $n \to \infty$. This is observed in Fig. 2. Then, it can be proved that $w_n \sim \exp[-c'\tau^{n\nu}]$ with c' being another positive constant. Since size L of the atom of the nth generation is proportional to τ^n, we find $w_n \sim \exp[-(L/\xi)^\nu]$, i.e., a stretched exponential, with ξ

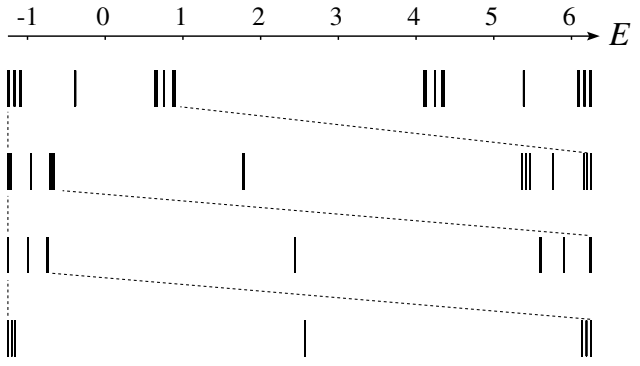

FIG. 2. A singular-continuous energy spectrum of the type II QL given in Fig. 1. It was obtained numerically from a finite approximant composed of 1970 atoms with $V = 5.0$. The left cluster of energy levels exhibits trifurcating behavior when it is expanded successively.

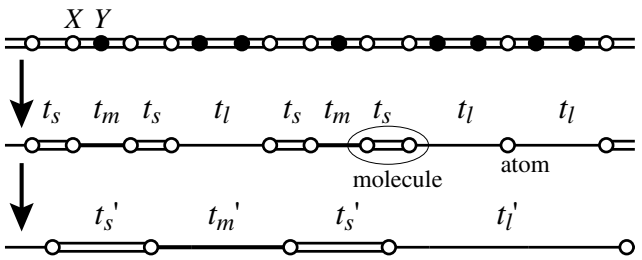

FIG. 3. A perturbational real-space renormalization-group treatment of the ground state. "Molecules" are separated by three types of spacings, which are arranged similarly to the underlying QL.

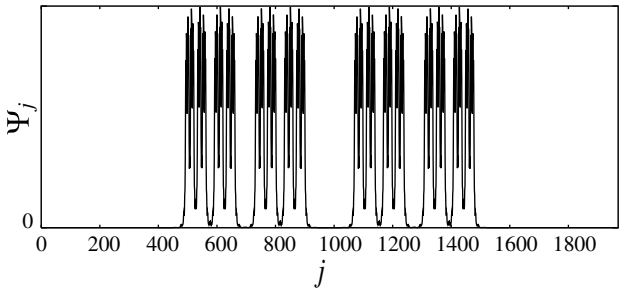

FIG. 4. The ground state wave function of the approximant composed of 1970 atoms with $V = 1.0$. Ψ_j is the probability amplitude on the jth site. This figure exhibits the molecular bonding state of the eighth generation, where hierarchical internal structure is observed.

being a characteristic length. This is manifestly different from the case of usual critical states exhibiting a power law, $w_n \sim L^{-1/\alpha}$, and has never been observed in energy spectra of type I QLs. Note that a power-law scaling could be observed if the ratio w_{n+1}/w_n had tended to a finite value.

The above argument proves that the exponent α of the ground state vanishes. This does not mean, however, that the ground state is localized, because the ground state level is not isolated from other levels. The length ξ, which decreases as V is increased and diverges as $V \to 0$, represents the size of almost isolated atoms. The presence of a characteristic length implies that the ground state wave function, shown in Fig. 4, is not self-similar, although it still remains critical. We may call the ground state a *marginal critical state*, whose presence is closely connected with the self-similarity of the present QL.

The exact real-space renormalization-group formalism proposed by Ashraff and Stinchcombe [9] can also be adapted to study the ground state properties. There appears a 7D map but its asymptotic behavior is dominated by its behavior in a 2D subspace corresponding to the fg plane. The map being reduced to the subspace is essentially the same as above. It has also been numerically confirmed that each energy level at a band edge, where energy levels accumulate only from one side, gives the equivalent fixed point of the 7D map to that of the ground state level.

The presence of marginal critical states causes vanishing of the left end $\alpha_{\min}$ of the support $[\alpha_{\min}, \alpha_{\max}]$ of the relevant $f(\alpha)$ spectrum. This is an important feature of electronic properties of type II QLs, and has also been confirmed for several other type II QLs including the one whose ratio of self-similarity is τ_G^3. The exponent ν introduced above is a proper number to the relevant MLD class but satisfies $0 < \nu < 1$. It is surprising that QLs derived from a single mother lattice can belong to different universality classes of electronic properties.

The binary sequence of atoms in the atomic chain used above to investigate electronic properties of type II QLs is found to be one of the circle sequences investigated in detail by Aubry *et al.* [12]. Some other type II QLs can also be transformed to circle sequences if they are decorated appropriately, but a general relationship between the type II QLs and the circle sequences awaits further investigation. We should remark, however, that an indication of an unusual electronic property of a circle sequence was first reported by Luck [13].

The present report is summarized as follows: (i) 1D QLs can be classified into an infinite number of MLD classes, which are distinguished from each other by the inflation rules of their representatives, and (ii) there exists a "type II" MLD class whose electronic properties are characterized by the presence of marginal critical states.

A full account of the exact real-space renormalization-group treatment of marginal critical states will be presented elsewhere. The present results can also be extended to 2D and 3D QLs because these QLs are related to 1D QLs through the Ammann bars or planes [3], and the results will be reported elsewhere.

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