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LETTER TO THE EDITOR

An exact systematized renormalization-group approach for periodic and aperiodic systems

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Abstract. A systematized renormalization-group approach is present to study systematically the physical properties of the one-dimensional systems arranged in the 1D sequence which are constructed by the inflation rule $\{A, B\} \rightarrow \{A^{m_{11}}B^{m_{12}}, B^{m_{21}}A^{m_{22}}\}$. A basic decimation rule is introduced, which is intuitive, simplified and exact, to investigate the electronic properties of the systems which contain crystals and quasicrystals. As typical examples, the spectra of global electronic bands of the 1D systems with $(m_{11}, m_{12}, m_{21}, m_{22}) = (1, 1, 0, 1)$, $(1, 1, 1, 1)$, and $(1, 1, 2, 1)$ are numerically calculated

Lattices containing a periodic and quasiperiodic (aperiodic) modulating potential, which are called the crystals and the quasicrystals respectively, have received considerable attention [1–7]. A most effective theory is the renormalization-group (RG) theory which was developed to study the physical properties in periodic and aperiodic lattices by Wiecko *et al* [2] Kohmoto *et al* [3] and Nori *et al* [4]. In recent years, due to the aperiodic but regular structure and rich physical properties of aperiodic lattices, it has become more important to extend the RG theory to study the physical properties in aperiodic lattices. Some typical one-dimensional (1D) aperiodic lattices such as the Fibonacci [3, 5] and generalized Fibonacci [6] quasicrystals, and the Thue-Morse [7] and generalized Thue-Morse [8] aperiodic lattices were extensively studied and several separated real-space RG methods have been developed to investigate individually the global energy spectra [3, 5–8] and the local electronic properties [9]. Lately, a notion of approximant crystals has been introduced [10] which can be considered as approximate systems successively approaching quasicrystals. Because of their very interesting physical properties and easy fabrication by the molecular beam epitaxy in these systems, the apparent systems have attracted wide attention. Odagaki *et al* [11] developed a hyperinflation technique to determine systematically the constructions of the 1D quasiperiodic systems, and used the hyperinflation rule to calculate successfully the spectrum of energy bands of the Fibonacci lattice [12]. Based on the hyperinflation rule, we present here a new systematized RG approach to study the physical properties, for example the global energy spectrum, of the 1D systems which contain the crystals, the quasicrystals and other aperiodic lattices.

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In general, we focus here on the 1D systems which are arranged in the sequences constructed by the inflation rule

$$A \to A^{m_{11}}B^{m_{12}} \qquad B \to B^{m_{21}}A^{m_{22}} \tag{1}$$

or by the recursion relation

$$\begin{pmatrix}\Omega_{l+1}^{A}\\ \Omega_{l+1}^{B}\end{pmatrix}=\begin{pmatrix}m_{11} & m_{12}\\ -m_{22} & -m_{21}\end{pmatrix}\begin{pmatrix}\Omega_{l}^{A}\\ \Omega_{l}^{B}\end{pmatrix} \qquad l\geqslant 0 \tag{2}$$

with the initial conditions $\Omega_0^A=\{A\}$ and $\Omega_0^B=\{B\}$, where m_{11}, m_{12}, m_{21} and m_{22} are non-negative integers, and the symbol '$-$' denotes shifting of Ω_l^A and Ω_l^B to one another, for instance, $(\Omega_l^A)^{-1}$ can be written as Ω_l^B. Denoting by F_l^A and F_l^B the numbers of tiles A and B in the lth generation Ω_l^A and Ω_l^B, respectively, we obtain from (1) the following recursion relations:

$$F_{l+1}^{A}=(m_{11}+m_{21})F_l^{a}+(m_{12}m_{22}-m_{11}m_{21})F_{l-1}^{A} \tag{3a}$$

$$F_{l+1}^{B}=(m_{11}+m_{21})F_l^{B}+(m_{12}m_{22}-m_{11}m_{21})F_{l-1}^{B} \tag{3b}$$

with initial conditions $F_0^A=1$ and $F_1^A=m_{11}+m_{12}$ for (3a) and $F_0^B=1$ and $F_1^B=m_{21}+m_{22}$ for (3b). Let τ be the value to which the ratio F_{l+1}^A/F_l^A tends as $l\to\infty$. From relation (3a), τ can be given as

$$\tau=\tfrac{1}{2}\{(m_{11}+m_{21})+[(m_{11}-m_{21})^2+4m_{12}m_{22}]^{1/2}\} \tag{4}$$

for the sequence Ω_∞^A. For the generalized Fibonacci sequences [6], $(m_{11}, m_{12}, m_{21}, m_{22})=(m, n, 0, 1)$. From (4) we have $\tau=[m+(m^2+4n)^{1/2}]/2$, and particularly $\tau=(1+\sqrt{5})/2$ for the Fibonacci sequence ($m=n=1$). As to the generalized Thue–Morse sequences [8], $(m_{11}, m_{12}, m_{21}, m_{22})=(m, n, n, m)$ and it follows from (4) that $\tau=m+n$. In particular, $\tau=2$ for the Thue–Morse sequence ($m=n=1$) [7].

To deal with the electronic properties of 1D lattices, the Hamiltonian studied is often written as the tight-binding model [1]

$$H=\sum_i[|i\rangle\varepsilon_i\langle i|+|i\rangle t_{i-1,i}\langle i-1|+|i\rangle t_{i,i+1}\langle i+1|] \tag{5}$$

where $|i\rangle$ is the Wannier state centred at site i, the nearest-neighbour coupling parameter $t_{i,j}$ takes t_A and t_B arranged in Ω_l^A which is arranged by the periodic lattice, and the site energy ε_i generally takes one of the following five values:

$$\varepsilon_i=\begin{cases}\varepsilon_\alpha & \text{if } t_{i-1,i}=t_{i,i+1}=t_A\\ \varepsilon_\beta & \text{if } t_{i-1,i}=t_A,\ t_{i,i+1}=t_B\\ \varepsilon_\gamma & \text{if } t_{i-1,i}=t_B,\ t_{i,i+1}=t_A\\ \varepsilon_\delta & \text{if } t_{i-1,i}=t_{i,i+1}=t_B\\ \varepsilon_\sigma & \text{if site } i \text{ is the boundary site of the unit cell}\end{cases} \tag{6}$$

corresponding to its surrounding environment. The sites possessing the site energies ε_α, ε_β, ε_γ, ε_δ and ε_σ are called the sites of types α, β, γ, δ and σ, respectively. When $m_{12}=1$ and $m_{21}=0$ in particular, the site energies often assume ε_α, ε_β, ε_γ and ε_σ while there is no site of type δ in the 1D lattice with $m_{12}=1$ and $m_{21}=0$.

For a 1D lattice of which the unit cell Ω_l^A is constructed by the recursion relation (2), following calculations can be obtained. Transferring the 1D lattice with the unit cell Ω_l^A by the decimation rule which is contrary to the inflation rule (1) (see also

figure 1), the renormalized 1D sublattice is created, in which the site parameters are renormalized as ε_i' ($i=\alpha, \beta, \gamma, \delta$ and σ), t_A' and t_B'. The unit cell of the renormalized sublattice is Ω_{l-1}^{A} which is also constructed by the recursion relation (2). According to the geometric properties of the decimation rule (see figure 2) which is contrary to the inflation rule (1), a set of RG equations of above transformation is generally given from equation (5) as follows

$$\varepsilon_\alpha' = \varepsilon_\gamma + \frac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \frac{t_B R_{m_{11}-1,m_{12}-2}}{R_{m_{11}-1,m_{12}-1}} \tag{7a}$$

$$\varepsilon_\beta' = \varepsilon_\delta + \frac{t_B R_{m_{11}-1,m_{12}-2}}{R_{m_{11}-1,m_{12}-1}} + \frac{t_B W_{m_{22}-2,m_{21}-1}}{W_{m_{22}-1,m_{21}-1}} \tag{7b}$$

$$\varepsilon_\gamma' = \varepsilon_\alpha + \frac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \frac{t_A W_{m_{22}-1,m_{21}-2}}{W_{m_{22}-1,m_{21}-1}} \tag{7c}$$

$$\varepsilon_\delta' = \varepsilon_\beta + \frac{t_A W_{m_{22}-1,m_{21}-2}}{W_{m_{22}-1,m_{21}-1}} + \frac{t_B W_{m_{22}-2,m_{21}-1}}{W_{m_{22}-1,m_{21}-1}} \tag{7d}$$

$$\varepsilon_\sigma' = \begin{cases} \varepsilon_\sigma + \dfrac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \dfrac{t_B R_{m_{11}-1,m_{12}-2}}{R_{m_{11}-1,m_{12}-1}} & \text{if } l \text{ is an odd integer} \\ \varepsilon_\sigma + \dfrac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \dfrac{t_A W_{m_{22}-1,m_{21}-2}}{W_{m_{22}-1,m_{21}-1}} & \text{if } l \text{ is an even integer} \end{cases} \tag{7e}$$

$$t_A' = t_A t_B / R_{m_{11}-1,m_{12}-1} \qquad t_B' = t_A t_B / W_{m_{22}-1,m_{21}-1} \tag{7f}$$

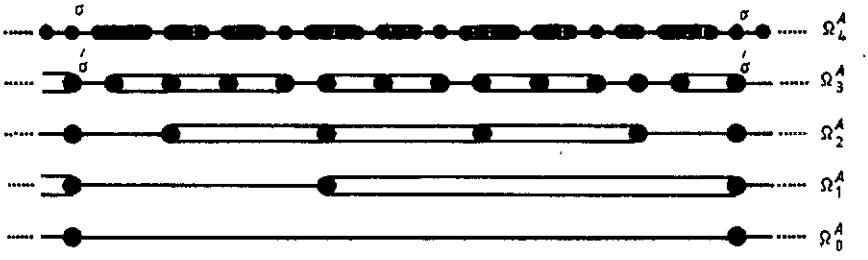

Figure 1. The decimation for the unit cell Ω_4^A in which $(m_{11}, m_{12}, m_{21}, m_{22})=(1, 1, 2, 1)$.

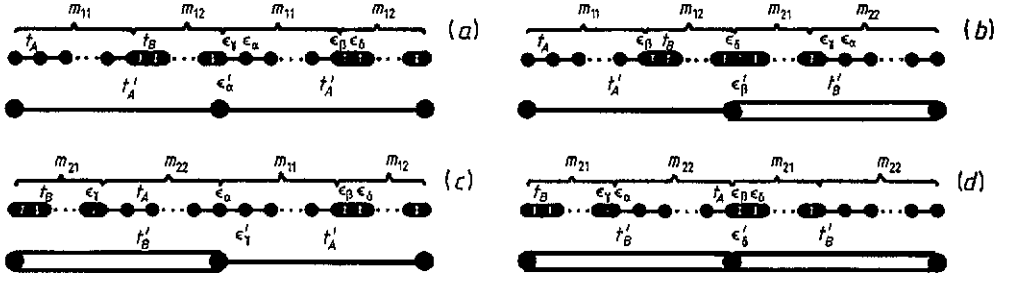

Figure 2. Four types of renormalized sites α, β, γ and δ, which are obtained by the application of the decimation rule. (*a*) α-type renormalized site; (*b*) β-type renormalized site; (*c*) γ-type renormalized site; (*d*) δ-type renormalized site.

where $m_{21} \neq 0$, l is the number of Ω_l^A's generation and

$$g = (E - \varepsilon_\alpha)/2t_A \qquad h = (E - \varepsilon_\delta)/2t_B \tag{8a}$$

$$P_i = (E - \varepsilon_\beta)\mathcal{U}_i(g) - t_A\mathcal{U}_{i-1}(g) \tag{8b}$$

$$Q_i = (E - \varepsilon_\gamma)\mathcal{U}_i(g) - t_B\mathcal{U}_{i-1}(g) \tag{8c}$$

$$R_{i,j} = P_i\mathcal{U}_j(h) - t_B\mathcal{U}_i(g)\mathcal{U}_{j-1}(h) \tag{8d}$$

$$W_{i,j} = Q_i\mathcal{U}_j(h) - t_A\mathcal{U}_i(g)\mathcal{U}_{j-1}(h) \tag{8e}$$

where $\mathcal{U}_N(X) = \sin[(N+1)\cos^{-1}(X)]/\sin[\cos^{-1}(X)]$ is the Nth Chebyshev Polynomial of the second kind which satisfies the recursion relation

$$\mathcal{U}_N(X) = 2X\mathcal{U}_{N-1}(X) - \mathcal{U}_{N-2}(X) \qquad N \geqslant 1 \tag{9}$$

with $\mathcal{U}_{-1}(X) = 0$ and $\mathcal{U}_0(X) = 1$. When $m_{21} = 0$ in particular, corresponding to the decimation rule which is contrary to the inflation rule (1), we obtain from equation (5) the following set of RG equations:

$$\varepsilon'_\alpha = \varepsilon_\gamma + \frac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \frac{t_B R_{m_{11}-1,m_{12}-2}}{R_{m_{11}-1,m_{12}-1}} \tag{10a}$$

$$\varepsilon'_\beta = \varepsilon_\gamma + \frac{t_B R_{m_{11}-1,m_{12}-2}}{R_{m_{11}-1,m_{12}-1}} + \frac{t_A\mathcal{U}_{m_{22}-2}(g)}{\mathcal{U}_{m_{22}-1}(g)} \tag{10b}$$

$$\varepsilon'_\gamma = \varepsilon_\alpha + \frac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \frac{t_A\mathcal{U}_{m_{22}-2}(g)}{\mathcal{U}_{m_{22}-1}(g)} \tag{10c}$$

$$\varepsilon'_\delta = \varepsilon_\alpha + \frac{2t_A\mathcal{U}_{m_{22}-2}(g)}{\mathcal{U}_{m_{22}-1}(g)} \tag{10d}$$

$$\varepsilon'_\sigma = \begin{cases} \varepsilon_\sigma + \dfrac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \dfrac{t_B R_{m_{11}-1,m_{12}-2}}{R_{m_{11}-1,m_{12}-1}} & \text{if } l \text{ is an odd integer} \\ \varepsilon_\sigma + \dfrac{t_A R_{m_{11}-2,m_{12}-1}}{R_{m_{11}-1,m_{12}-1}} + \dfrac{t_A\mathcal{U}_{m-2}(g)}{\mathcal{U}_{m-1}(g)} & \text{if } l \text{ is an even integer} \end{cases} \tag{10e}$$

$$t'_A = t_A t_B / R_{m_{11}-1,m_{12}-1} \qquad t'_B = t_A/\mathcal{U}_{m_{22}-1}(g) \tag{10f}$$

in which g, h, P_i, Q_i and $R_{i,j}$ are given as equations (8a)-(8d), respectively.

According to the self-similar properties of the decimation rule which is contrary to the inflation rule of the sequence Ω_l^A, the 1D lattice with the unit cell Ω_l^A can be reduced to the simple periodic lattice with the renormalized site energy ε'_σ and the renormalized coupling parameter t'_A because all the types of sites α, β, γ and δ have been removed after l transformations. This shows that for an aperiodic system Ω_∞^A, many physical properties can be reduced to those of the periodic system (i.e. the 1D simple crystal), which is easy to study. For instance, the energy spectrum of bands in a lattice with unit cell Ω_l^A is identical to those in the final renormalized lattice which is the simple periodic lattice. According to the Bloch-like formula, the energy spectrum of a lattice with the final renormalized parameters ε'_σ and t'_A is determined by the solution to the implicit equation

$$E = \varepsilon'_\sigma + 2t'_A\cos(kL) \tag{11}$$

where $L = F_l^A d$ (d is the distance between two sites).

As typical examples, the spectra of energy bands in the Ω_3^As in which $(m_{11}, m_{12}, m_{21}, m_{22}) = (1, 1, 0, 1)$, $(1, 1, 1, 1)$, and $(1, 1, 2, 1)$ are calculated numerically in figures 3 and 4, respectively. For the well known Fibonacci lattice with $(1, 1, 0, 1)$, figure 3(a) and 3(b) are the spectra of energy bands of Ω_3^A and Ω_4^A, respectively, in which $\varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma = \varepsilon_\sigma = 0$, and $t_A/t_B = 1.5$. One can see that the numbers F_3^A and F_4^A of tiles A and B in Ω_3^A and Ω_4^A are, respectively, equal to 5 and 8 which are identical to the numbers of the energy bands in the spectrum shown in figures 3(a) and 3(b). For the other lattices with $(m_{11}, m_{12}, m_{21}, m_{22}) = (1, 1, 1, 1)$ and $(1, 1, 2, 1)$, their energy spectra of bands are shown in figures 4(a) and 4(b), respectively, in which $\varepsilon_i = 0$ ($i = \alpha, \beta, \gamma, \delta$ and σ) and $t_A/t_B = 1.5$. The numbers of the energy bands in the spectrum given in figures 4(a) and 4(b) are equal to the numbers F_3^A of 8 and 13 of tiles A and B in Ω_3^A, respectively. In figure 4(a), it is also shown that the spectrum of energy bands in the Thue–Morse system for the off-diagonal tight-binding model are symmetrical at the energy $E = 0$. Comparing figures 3(a) with figure 3(b), it is found that the number of the bands increases by the recursion relation (3a) and the gaps between two nearest-neighbour bands become dense as l increases. These results obtained here are similar to those obtained by other RG schemes [3, 6].

In summary, we have presented a systematized RG approach to study the electronic properties of 1D systems constructed by the inflation rule $\{A, B\} \to \{A^{m_{11}}B^{m_{12}}, B^{m_{21}}A^{m_{22}}\}$, where m_{11}, m_{12}, m_{21} and m_{22} are non-negative integers. By applying the decimation rule which is contrary to the above inflation rule, the RG equations corresponding to the decimation are obtained and the final renormalized site parameters ε_i' and t_{ij}' are exactly calculated. This is a much more intuitive, straightforward and exact approach to investigate systematically the electronic properties, for instance the spectra of energy

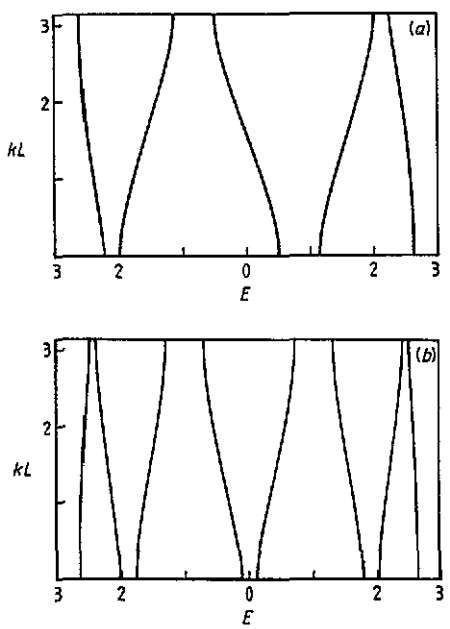

Figure 3. The energy bands for the lattice with $(1, 1, 0, 1)$, where $\varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma = \varepsilon_\sigma = 0$ and $t_A/t_B = 1.5$. (a) Five-bands structure in Ω_3^A; (b) eight-bands structure in Ω_4^A.

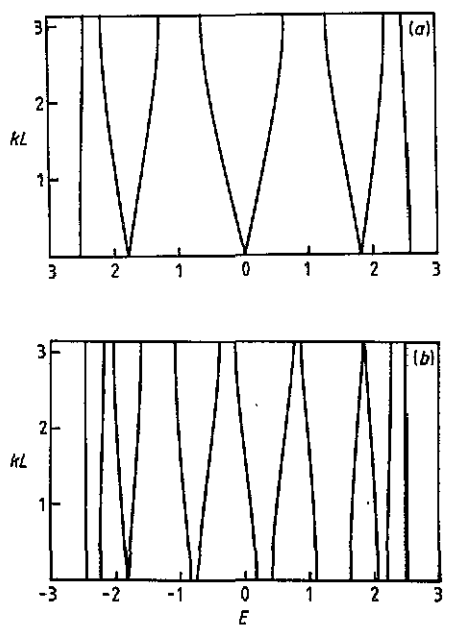

Figure 4. The energy bands for the lattice with the unit cell Ω_3^A, where $\varepsilon_i = 0$ ($i = \alpha, \beta, \gamma, \delta$ and σ), $t_A/t_B = 1.5$ and $(m_{11}, m_{12}, m_{21}, m_{22}) = (a)$ $(1, 1, 1, 1)$; (b) $(1, 1, 2, 1)$.

bands, in 1D systems containing crystals and quasicrystals. As typical examples, the spectra of energy bands in the 1D lattices with $(1, 1, 0, 1)$, $(1, 1, 1, 1)$, and $(1, 1, 2, 1)$ are numerically calculated. Some results which are similar to those of other physicists are obtained.

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