Electronic states in one-dimensional self-similar alloy with $(3^1, 3^2, \dots, 3^N)$ periods

Takashi Nagatani

College of Engineering, Shizuoka University, Hamamatsu 432, Japan

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The one-dimensional $A_{1-x}B_x$ alloy is presented to study electron properties of binary alloys intermediate between periodicity and randomness. The system studied is represented by a tight-binding Hamiltonian with diagonal elements given by $\sum_{n=1}^N \epsilon_B f(\cos(2\pi i/3^n + 2\pi/3))$, where if $x=1$ then $f(x)=1$, otherwise $f(x)=0$, and ϵ_B indicates the site energy of the B atom. The Hamiltonian is exactly renormalized with the use of a decimation technique. Densities of states and band structures are calculated by the recursion relations. It is shown that the bands break up into narrower subbands with increasing N . It appears that when N becomes $N+1$ each band breaks up into triplet subbands, and as $N \rightarrow \infty$ the density of states approaches a limit with an infinite number of band gaps.

In recent years, there has been much interest in crystalline solids with incommensurate lattice potentials.¹⁻⁵ The solids form a class of solids intermediate between crystalline and disordered. Fractals also provide useful models for physical systems intermediate between periodicity and randomness.⁶⁻⁹

In this Rapid Communication, we present the one-dimensional (1D) model of the self-similar alloy which is composed of two kinds of constituent atoms with self-similar configurations. The densities of states per site and band structures of an electron are studied by the tight-binding Hamiltonian with diagonal elements given by

$$\sum_{n=1}^N \epsilon_B f(\cos(2\pi i/3^n + 2\pi/3))$$

where, if $x=1$ then $f(x)=1$, otherwise $f(x)=0$, and ϵ_B indicates the site energy of a B atom. The self-similar model is interesting from several viewpoints. (a) It is a natural intermediate case between periodicity and randomness. It may be expected that the electronic states of the self-similar alloy with the number N of iterations alter from crystalline to disordered accordingly as N increases. (b) The Hamiltonian can be exactly renormalized by a decimation technique and reduced to the recursion relations for the diagonal and off-diagonal parts. (c) It may be related to electron properties of solids intermediate between crystalline and disordered. The 1D binary alloy is constructed by making use of the Koch curve. The first two construction stages of the Koch curve are shown by Fig. 1(a). The apexes of the Koch curve are replaced by the B atoms and other sites by the A atoms. In this way, we can construct the 1D binary alloy with the self-similar configurations, which is displayed by Fig. 1(b). An electron in the 1D binary alloy is scattered self-similarly from B atoms which take the form of $\sum_{n=1}^N 3^n$ periods in the chain.

We consider here a tight-binding Hamiltonian with nearest-neighbor interaction only. Shifting the origin of energy to the site energy of A atom and choosing the off-diagonal elements to be equal to unity, we have that the Schrödinger equation in the site representation is

$$E \cdot a_i = \epsilon_i a_i + a_{i+1} + a_{i-1}, \quad (1)$$

where a_i and ϵ_i are, respectively, the amplitude of the state and the site energy of an electron at the i th site. The site

energy ϵ_i takes one of the two possible values $\epsilon_A (=0)$ and ϵ_B . In the configuration shown by Fig. 1, the self-similar modulation potential is given by

$$\epsilon_i = \sum_{n=1}^N \epsilon_B f(\cos(2\pi i/3^n + 2\pi/3)), \quad (2)$$

where if $x=1$ then $f(x)=1$ or else $f(x)=0$ and $i=0, 1, 2, \dots$. We apply the standard decimation procedure^{10,11} to the tight-binding Hamiltonian where the decimation technique is schematically indicated in Fig. 2. The crossed sites in the upper chain are eliminated, producing the renormalized lower chain. The renormalization procedure, as described above, yields a new Hamiltonian with renormalized diagonal and off-diagonal matrix elements. This procedure can be automatically repeated to the N th time. We obtain, after the n th renormalization, the following recursion relations for the renormalized site and transfer

(a)

(b)

FIG. 1. Construction stages of the 1D self-similar alloy $A_{1-x}B_x$. (a) The first two construction stages of the Koch curves with $D=\ln 3/\ln 2$. The apexes (2nd, 5th, 6th, and 8th points) of the Koch curve are replaced by the B atoms and other sites by the A atoms. (b) The linear chain with the self-similar configurations constructed by the above method.

FIG. 2. Schematic representation of the decimation technique. The crossed sites in the upper chain are eliminated, producing the renormalized lower chain.

FIG. 3. Allowed energies for $\epsilon_B = 0.5$. The band structures are shown for $N = 1, 2, \dots, 10$. Band edges are indicated by the bars.

FIG. 4. Graphs of the band structures with the interval $\Delta E = 0.01$ are plotted against the site energy ϵ_B . (a) $N = 2$. (b) $N = 3$. (c) $N = 4$.

energies:

$$\epsilon_{n+1} = \epsilon_n + \frac{V_n^2(2E - 2\epsilon_n - \epsilon_B)}{[(E - \epsilon_n)(E - \epsilon_n - \epsilon_B) - V_n^2]}, \quad (3)$$

$$V_{n+1} = \frac{V_n^3}{[(E - \epsilon_n)(E - \epsilon_n - \epsilon_B) - V_n^2]}, \quad (4)$$

where $\epsilon_0 = 0$ and $V_0 = 1$.

The renormalized chain obtained after the N th iterations

appears to be the ordered single-atomic chain with the site energy ϵ_N and the transfer energy V_N . An allowed region of the spectrum is given by

$$|E - \epsilon_N| \leq 2|V_N|. \quad (5)$$

The density of states per site is also given by

$$D(E) = \theta(2|V_N| - |E - \epsilon_N|) / \pi [4V_N^2 - (E - \epsilon_N)^2]^{1/2}. \quad (6)$$

Figure 3 shows forbidden and allowed energies as a function

FIG. 5. Densities of states per site are shown for $\epsilon_B = 0.5$. (a) $N=2$. (b) $N=3$. (c) $N=4$.

of N for $\epsilon_B = 0.5$. Notice that the allowed regions break up into narrower subbands with larger N . The band gaps and allowed regions less than the interval $\Delta E = 0.01$ are not shown in Fig. 3. Band edges are indicated by the bars. In Fig. 4 the graphs of the band structures with the interval $\Delta E = 0.01$ are plotted against the site energy ϵ_B , obtained after two, three, and four iterations. For large ϵ_B , the bands get narrower. The densities of states obtained after two, three, and four iterations are shown in Fig. 5 for

$\epsilon_B = 0.5$. We can now identify that when $N = 1$ becomes $N = 2$ three bands break up into nine bands. Gaps and bands with the interval $\Delta E = 0.01$ are not shown in Fig. 4 but it appears that when N becomes $N + 1$ 3^N bands break up into 3^{N+1} bands. Density of states become more peaked structures with increasing N , which is characteristic of the disordered chain. It appears that as $N \rightarrow \infty$ the density of states approaches a limit with an infinite number of band gaps and all states are localized.

¹S. Aubry, in *Solid State Sciences: Solitons and Condensed Matter Physics*, edited by A. P. Bishop and T. Schneider (Springer-Verlag, Berlin, 1978), Vol. 8, p. 264.

²M. Ya. Azbel, Phys. Rev. Lett. **43**, 1954 (1979).

³J. B. Sokoloff, Phys. Rev. B **23**, 6422 (1981).

⁴K. S. Dy and T. C. Ma, J. Phys. C **15**, 6971 (1982).

⁵M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).

⁶B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, San

Francisco, 1982).

⁷Y. Gefen, A. Aharony, and B. B. Mandelbrot, J. Phys. A **16**, 1267 (1983); **17**, 435 (1984).

⁸D. Ben-Avraham and S. Havlin, J. Phys. A **16**, L559 (1983).

⁹E. Domany, S. Alexander, D. Bensimon, and L. P. Kadanoff, Phys. Rev. B **28**, 3110 (1983).

¹⁰L. P. Kadanoff and A. Houghton, Phys. Rev. B **11**, 377 (1975).

¹¹C. E. T. Goncalves da Silva and B. Koiller, Solid State Commun. **40**, 215 (1981).