Electronic properties of linear compositions of two binary compounds with random layer thicknesses

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The electronic properties of a one-dimensional (1D) disordered system are studied with a model describing the linear composition of two binary compounds with random layer thicknesses; the model is studied with Dean's method, the transfer-matrix method, and Landauer's formula. For certain degrees of randomness, the energy spectrum, some wave functions, and the average resistivity are obtained. The appearance of some special peaks in the spectrum is due to a particular arrangement of atoms that occurs randomly. Some wave functions remain delocalized with disorder, contrary to the general theorem on the absence of such states in 1D disordered systems.

The electronic, phononic, and magnetic properties of one-dimensional (1D) quasiperiodic systems, especially the localization features of the states, have been studied by many authors.[1-7] At the same time, 1D disordered systems have been studied extensively. According to the scaling theory on Anderson localization,[8] the electronic states in 1D disordered models are always localized. Recently, Dunlap, Wu, and Phillips discovered that for a special type of disorder this is not the case, and demonstrated this by showing that there are some delocalized states in a random-dimer model.[9] Dunlap, Kundu, and Phillips[10] and Flores[11] also found delocalization in certain statistically disordered lattices in any spatial dimension. In the present paper we propose another model of a 1D disordered system by constructing a linear composition formed from alternating connections of two binary compounds with random layer thickness. The work is motivated by current studies of GaAs/AlAs superlattices with artificial random thickness which exhibit some unusual properties in experiments.[12] The present 1D model can be used to mimic the structure of these materials in their growth direction and to describe some principal features of electronic states.

We use the tight-binding Hamiltonian

$$H=\sum_{n=-\infty}^{\infty} E(n)|n\rangle\langle n| + \sum_{n=-\infty}^{\infty}(t|n\rangle\langle n+1|+t|n\rangle\langle n-1|) \tag{1}$$

to describe the 1D electronic system, where $|n\rangle$ denotes the Wannier state at the nth site, $E(n)$ is the corresponding energy level, and t is the nearest-neighbor hopping strength. The chain is made of alternating connections of segments of two compounds A and B; A is an atom array consisting of two species a and b: $ababab\cdots$; B is array $acacac\cdots$, with c another atom species. The energy level $E(n)$ takes one of values E_a, E_b, and E_c, respectively for atoms a, b, and c, depending on the species of the nth atom.

For a periodic chain, the atom arrangement is

$$\underbrace{abab\cdots}_{L_A}\underbrace{acac\cdots}_{L_B}\underbrace{abab\cdots}_{L_A}\underbrace{acac\cdots}_{L_B} \tag{2}$$

where L_A and L_B are the lengths of segments A and B, respectively, and the period is L_A+L_B. By introducing random layer thickness, the segment lengths become random variables and their fluctuations may be expressed by the stochastic functions

$$P(L_A)=\sum_i \rho_{Ai}\delta(L_A-i)\,, \qquad P(L_B)=\sum_i \rho_{Bi}\delta(L_B-i)\,, \tag{3}$$

where

$$\delta(l)=\begin{cases}1, & l=0\\ 0, & l\neq 0\end{cases},$$

and $\rho_{A(B)i}$ is the probability of finding a segment of compound $A(B)$ having i atoms. The length of a specific segment is randomly produced from this distribution, and the whole lattice is formed by subsequent connections of the segments.

Once the lattice is constructed for given values of the parameters in Eq. (3), the energy spectrum can be calculated by Dean's method.[13] For a finite chain of N atoms, the number of states with eigenvalues less than ε is the number of negative $U_i (i=1,2,\ldots,N)$, and the U's are determined from following relations:

$$U_i=E(i)-\varepsilon-t^2/U_{i-1}\,, \quad i=2,\ldots,N; \qquad U_1=E(1)-\varepsilon\,. \tag{4}$$

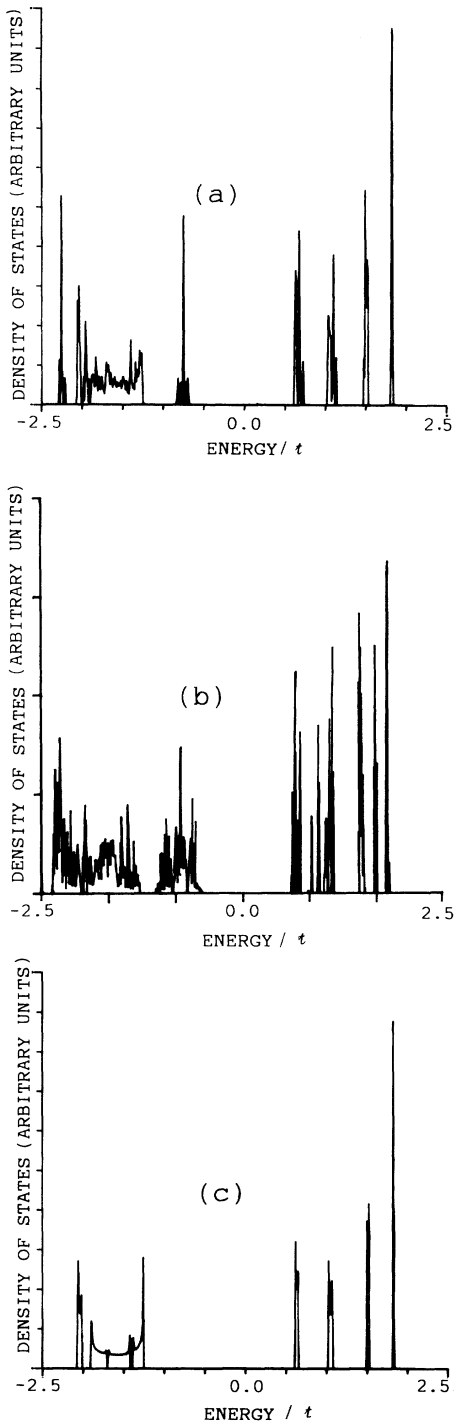

FIG. 1. Energy spectrum of 1D model in text with 5000 atoms. The parameters in Eq. (3) are

$$\text{(a)}\ \rho_{Ai}=\rho_{Bi}=\begin{cases}0.75 & \text{for } i=4\ ,\\ 0.25, & \text{for } i=3\ ,\\ 0\ , & \text{otherwise}\ .\end{cases}$$

$$\text{(b)}\ \rho_{Ai}=\rho_{Bi}=\begin{cases}1/3\ , & \text{for } 5\geq i\geq 3\\ 0\ , & \text{otherise}\ .\end{cases}$$

$$\text{(c)}\ \rho_{Ai}=\rho_{Bi}=\begin{cases}1\ , & \text{for } i=4\\ 0\ , & \text{otherwise}\ .\end{cases}$$

By use of this theorem, the density of states is obtained and shown in Fig. 1. By comparing the results for random chains and a periodic one, it can be seen that for random chains, there are two peaks at $E=-0.75$ and $E=-2.25$, that are produced by *aa* atom clusters, which are absent in the periodic system. It can also be seen that more structures appear as the randomness is increased.

To calculate the wave functions, we use the improved Dean's method.[14,15] If a_n denotes the amplitude at site n of a wave function with eigenvalue E_j, and $a_k\neq 0$, then we choose $a_k=1$ and the other amplitudes can be obtained from the recurrence relations:

$$a_{k\pm i}=-t\Delta^{\pm}_{k\pm i}a_{k\pm(i-1)}\ ,\quad \text{for } N\geq k\pm i\geq 1\ , \tag{5}$$

and

$$\Delta^{\pm}_i=1/[E(i)-E_j+t^2\Delta^{\pm}_{i\pm 1}]\ ,\quad \text{for } N\geq i\pm 1\geq 1\ ,$$

$$\Delta^{+}_N=1/[E(N)-E_j]\ ,$$

$$\Delta^{-}_1=1/[E(1)-E_j]\ .$$

For a random chain two calculated wave functions are shown in Fig. 2. The state shown in Fig. 2(a) is obviously localized, while the state in Fig. 2 (b) seems to be delocal-

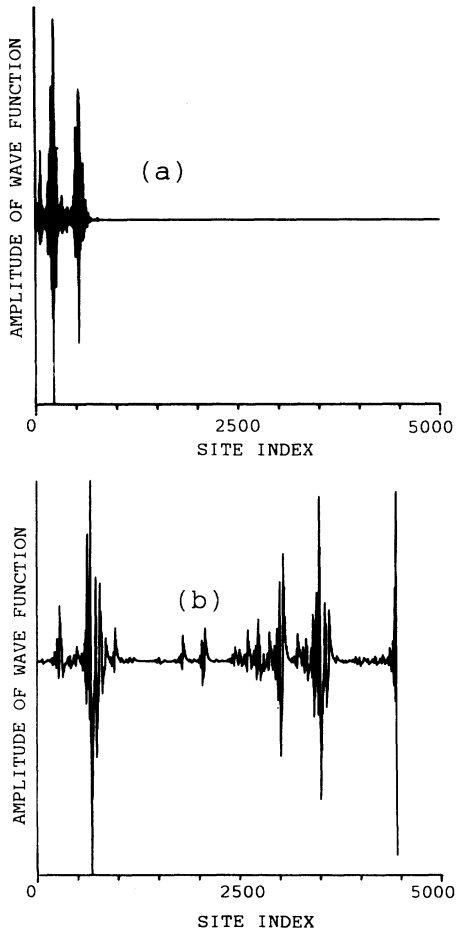

FIG. 2. Two wave functions of a random chain. The parameters of randomness are the same as those of Fig. 1(a). The corresponding eigenvalue is (a) $E=-1.9820t$. (b) $E=-1.9851t$.

ized. Thus, we have also been led to the unusual conclusion previously obtained in Refs. 9–11.

To further confirm this conclusion, we use Landauer's formula, together with the transfer-matrix method, to calculate the resistivity, which is a plausible quantity for estimating the localization and can be examined, in principle, by experiment. This method has been used by several authors to investigate the localization in disordered and incommensurate models.[5,16,17] As a first step implementing the method, we embed a segment of the present random chain containing $N+1$ atoms in an infinite and perfectly conducting chain. By setting $t=1$, the equation for amplitudes in the segment of a wave function with eigenvalue ε becomes

$$[\varepsilon - E(n)]a_n - a_{n+1} - a_{n-1} = 0 \ , \quad \text{for } N+1 \geq n \geq 1 \ . \tag{6}$$

The relation connecting both ends of the segment can be expressed by the transfer matrix

$$\begin{bmatrix} a_{N+2} \\ a_{N+1} \end{bmatrix} = \left[\prod_{i=1}^{N+1} \begin{bmatrix} \varepsilon - E(i) & -1 \\ 1 & 0 \end{bmatrix} \right] \begin{bmatrix} a_1 \\ a_0 \end{bmatrix} \equiv V_N \begin{bmatrix} a_1 \\ a_0 \end{bmatrix} \ . \tag{7}$$

The wave function in rest of the system, which is a perfect conductor separated into two parts by the random segment, can be expressed as plane waves. We then consider a particle being injected into the segment from left of the perfect parts with unit incident amplitude. If the amplitudes of the reflection and transmission waves are r_N and t_N, respectively, then we have

$$a_n = \begin{cases} \exp(ikn) + r_N \exp(-ikn) \ , & n \leq 0 \ , \\ t_N \exp(ikn) \ , & n \geq N+1 \ . \end{cases} \tag{8}$$

We define another transfer matrix T_N as

$$T_N \begin{bmatrix} r_N \\ 1 \end{bmatrix} \equiv \begin{bmatrix} T_{N11} T_{N12} \\ T_{N21} T_{N22} \end{bmatrix} \begin{bmatrix} r_N \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ t_N \end{bmatrix} \ , \tag{9}$$

so

$$|r_N|^2 = |T_{N12}|^2 / |T_{N11}|^2 \ , \tag{10}$$

$$|t_N|^2 = 1 / |T_{N11}|^2 \ . \tag{11}$$

From Eqs. (7)–(9), T_N can be calculated as

$$T_N = \theta S^{-1} V_N S \ , \tag{12}$$

where

$$\theta = \begin{bmatrix} \exp[ik(N+1)] & 0 \\ 0 & \exp[-ik(N+1)] \end{bmatrix} \ , \tag{13}$$

$$S = \begin{bmatrix} \exp(-ik) & \exp(ik) \\ 1 & 1 \end{bmatrix} \ .$$

The energy-dependent and dimensionless resistance $R(\varepsilon, N)$ of the segment is defined by Landauer's formula:

$$R(\varepsilon, N) = |r_N|^2 / |t_N|^2 = |T_{N12}|^2 \ . \tag{14}$$

To find an effective criterion for localization of a wave function, we use an average resistivity defined as

$$\bar{\rho}(\varepsilon, N) = \frac{1}{N} \sum_{i=1}^{N} R(\varepsilon, i)/i \ . \tag{15}$$

For delocalized states, the reflection coefficient is smaller than unity, so

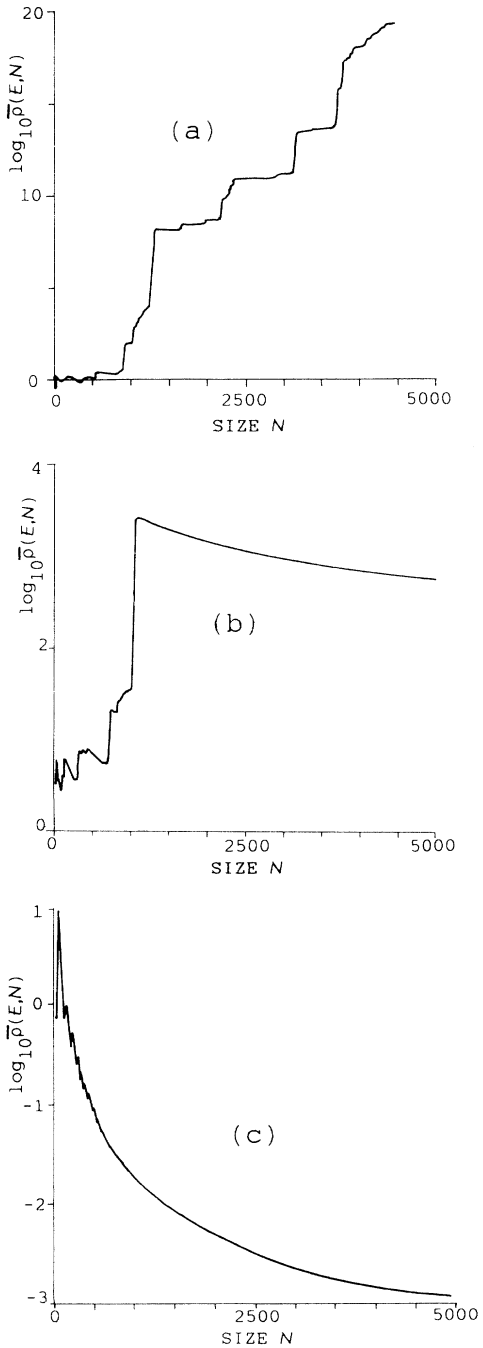

FIG. 3. Logarithm of average dimensionless resistivity as a function of the size of the system. The parameters of randomness are the same as those of Fig. 1(a). The corresponding wave function is (a) The wave function shown in Fig. 2(a). (b) The wave function with energy level $E=-1.9845t$. (c) The wave function shown in Fig. 2(b).

$$R(\varepsilon,i)/i=|r_i|^2/i(1-|r_i|^2)\to 0 \quad \text{when } i\to\infty \ ,$$

and

$$\bar{\rho}(\varepsilon,N)\to 0 \quad \text{when } N\to\infty \ . \tag{16}$$

Thus, after reaching some value of N, the average resistivity monotonically decreases with increasing N for extended state, and increases with N for localized state.

The logarithm of average resistiviity as a function of the size of the random segment is plotted in Fig. 3. The localized behavior of the corresponding wave function can be seen in Fig. 3(a), while the wave functions used for calculation of Fig. 3(b) and Fig. 3(c) are delocalized.

In summary, we have studied an on-site model of a special random chain. The energy spectrum, wave functions and the specially defined resistivity are numerically calculated. It is found that randomness causes some specific structure in the energy spectrum to appear. By increasing the randomness the band width is enlarged. From studying the results of the calculations of the wave functions and resistivity, it is shown that the delocalized states still exist when the system is disordered. This differs from Anderson's localization theorem, but is consistent with the conclusion of some recent literature.[9-11,18]

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