

Electronic properties of a one-dimensional two-band model with period randomness

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1993 J. Phys.: Condens. Matter 5 4029

(<http://iopscience.iop.org/0953-8984/5/24/004>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.159

The article was downloaded on 12/05/2010 at 14:09

Please note that [terms and conditions apply](#).

Electronic properties of a one-dimensional two-band model with period randomness

Xiaoshuang Chen[†] and Shijie Xiong^{†‡}

[†] Department of Physics, Nanjing University, Nanjing 210008, People's Republic of China

[‡] China Centre of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

Received 18 November 1992, in final form 20 January 1993

Abstract. In this paper we investigated the electronic properties of a one-dimensional on-site disordered model, which is constructed from a linear composition of two binary compounds with random periods, having two hybridizing bands on every site. Using the improved Dean method and the second-moment formulae, the effects of both disorder and hybridization on the energy spectrum and the property of wavefunctions are studied. The results show that the appearance of some special peaks in the spectrum is due to a particular arrangement of atoms that occurs randomly and the effect of disorder on the energy spectrum decreases in the case of large hybridization. The delocalization of the wavefunctions tends to be enhanced as the hybridization increases. When the hybridization becomes larger than a critical value, some delocalized wavefunctions appear.

Recently, we [1] studied the electronic properties of a one-dimensional (1D) disordered system (a linear composition of two binary compounds with random periods). The results show that some wavefunctions remain delocalized. This is contrary to the general theorem on the absence of such states in a 1D disordered system but is consistent with the conclusion of some recent literature [2–7]. At the same time, in the spectrum some peaks appear which are caused by a particular arrangement of the atoms in the disordered case.

For many realistic systems, several different bands may be important in determining electronic characteristics. Recently, Zhu and Huang [8] have used a multiband model to study the effect of hybridization on the electronic properties in superlattices; they found that hybridization can result in large non-parabolicities in the superlattice subbands. This effect can account for some weak structure in the optical absorption spectrum. Leavitt *et al* [9] have used the two-band model to study the hole properties; the non-parabolic subband structure obtained is capable of accurate predictions of the optical properties of superlattices in an electric field. Leavitt [10] has also used a two-band model to study the electronic states of semiconductor quantum wells and superlattices in an external potential; the conduction subband energies, envelope functions, interband oscillator strength and tunnelling resonance width obtained are highly consistent with the results found elsewhere. At the same time, the electronic, phononic and magnetic properties in 1D disordered or quasiperiodic two-band systems have also been studied by several workers. Dunlap *et al* [11] have constructed a 1D quasiperiodic system with two hybridizing bands. By use of the real-space renormalization group method, Chakrabarti *et al* [12] have studied the electronic properties of a 1D quasiperiodic two-band system; it is found that the hybridization counteracts the effect of disorder in the 1D quasiperiodic two-band system. Buch *et al* [13] have studied the density of states for a spatially disordered two-band system by the use of

the single-chain approximation and the effective-medium approximation and have obtained a qualitative condition for the transition between the extended states and the localized states. It is also useful to extend the work in [1] to a two-band model to study the effect of hybridization on such a disordered system. In the present paper, we propose a model of a 1D disordered system by constructing a linear composition formed from alternating connections of two binary compounds with random periods, having two hybridizing bands on every site. We attempt to investigate the competition between the effects of the disorder and the hybridization on the property of the wavefunctions. The work is also motivated by current studies of a superlattice with artificial random thicknesses which exhibits some unusual properties in experiments [14]. The present 1D model can be used to mimic the structure of these materials in the growth direction and to describe some principal features of electronic states. Despite the complexity of the two-band model, the methods developed for the one-band problems can be extended to this case.

We describe the system by the following tight-binding Hamiltonian:

$$H = \sum_n \epsilon_u(n) |nu\rangle \langle nu| + \sum_n \epsilon_v(n) |nv\rangle \langle nv| + \sum_{n,m} t_1 |nu\rangle \langle mu| + \sum_{n,m} t_2 |nv\rangle \langle mv| + \sum_n \gamma_n (|nu\rangle \langle nv| + |nv\rangle \langle nu|) \quad (1)$$

where $\epsilon_u(n)$ and $\epsilon_v(n)$ are the energy levels of orbital u and orbital v on site n , t_1 and t_2 are the hopping integrals between u and u and between v and v orbitals, respectively, and γ_n is the on-site u - v hybridization term.

Using the Wannier basis wavefunctions $|i\rangle \equiv \begin{pmatrix} iu \\ iv \end{pmatrix}$, we can write the tight-binding Hamiltonian using 2×2 matrices:

$$H = \sum_{i=-\infty}^{\infty} \tilde{\mathbf{E}}(i) |i\rangle \langle i| + \sum_{i=-\infty}^{\infty} (\tilde{\mathbf{t}}|i\rangle \langle i+1| + \tilde{\mathbf{t}}|i\rangle \langle i-1|) \quad (2)$$

where

$$\tilde{\mathbf{E}}(i) = \begin{bmatrix} \epsilon_u(i) & \gamma(i) \\ \gamma(i) & \epsilon_v(i) \end{bmatrix} \quad \tilde{\mathbf{t}} = \begin{bmatrix} t_1 & 0 \\ 0 & t_2 \end{bmatrix}.$$

The chain is made up of alternating connections of segments of two compounds A and B. A is an atom array of two species a and b : $abab \dots$ B is an array $acac \dots$, where c is another atom species. The $\tilde{\mathbf{E}}(i)$ takes one of $\tilde{\mathbf{E}}_a$, $\tilde{\mathbf{E}}_b$ and $\tilde{\mathbf{E}}_c$, depending on the species of the i th atom.

For a periodic chain, the atom arrangement is

$$\underset{L_A}{abab} \dots \underset{L_B}{acac} \dots \underset{L_A}{abab} \dots \underset{L_B}{acac} \dots$$

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 period randomness, the lengths become random variables and their fluctuations may be expressed by the stochastic functions

$$P(L_A) = \sum_i p_{Ai} \delta(L_A - i) \\ P(L_B) = \sum_i p_{Bi} \delta(L_B - i) \quad (3)$$

where

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

and p_{Ai} and p_{Bi} are the probabilities of finding a segment of compound A and of compound B, respectively, having i atoms. The length of a specific segment is randomly produced from this distribution, and the whole lattice is formed by sequential connections of the segments.

Once the lattice is constructed for given values of the parameters in equation (3), the energy spectrum can be calculated by the Dean method [15]. For a finite chain of N atoms, the number of states with eigenvalues less than ϵ is the number of negative eigenvalues of the $\tilde{U}(i)$ matrices ($i = 1, 2, \dots, N$), and the \tilde{U} matrices are determined from the following relations:

$$\tilde{U}(i) = \tilde{E}(i) - \epsilon \tilde{I} - \tilde{t}^+ \tilde{U}^{-1}(i-1) \tilde{t} \quad i = 2, 3, \dots, N \quad \tilde{U}(1) = \tilde{E}(1) - \epsilon \tilde{I} \quad (4)$$

where $\tilde{U}(i)$, $\tilde{E}(i)$ and \tilde{t} are 2×2 matrices, \tilde{I} is a 2×2 unit matrix, and \tilde{t}^+ is the transpose of \tilde{t} . By the use of this theorem, the density of states is obtained and is shown in figure 1. Figures 1(a) and 1(b) display the results for periodic and random systems, respectively, and figures 1(c) and 1(d) the results for these systems with larger hybridization. It can be seen that, for the random chains, there are some special peaks corresponding to the aa atom clusters, which are absent in the periodic system. The effect of disorder on the spectrum structure decreases at larger hybridization. If the hybridization increases, the separation of the subbands corresponding to two levels on a site becomes larger. In the disordered case, some peaks appear within the gap between these subbands.

In order to study the effect of hybridization on the property of eigenfunctions and to investigate the relation between the second moment of the wavefunctions [17] and the hybridization, we use the improved Dean method [16] to calculate the eigenfunctions. If \tilde{a}_n denotes the amplitude at site n of a wavefunction with eigenvalue E_j , and $\tilde{a}_k \neq 0$, then we choose $|\tilde{a}_k| = 1$ and the other amplitudes can be obtained from the recurrence relations

$$\tilde{a}_{k \pm i} = -\tilde{t} \Delta_{k \pm i}^{\pm} \tilde{a}_{k \pm (i-1)} \quad \text{for } n \geq k \pm i \geq 1 \quad (5)$$

and

$$\Delta_i^{\pm} = 1/[\tilde{E}(i) - E_j \tilde{I} \pm \tilde{t} \Delta_{i \pm 1}^{\pm} \tilde{t}] \quad \text{for } N \geq i + 1 \geq 1$$

$$\Delta_N^+ = 1/[\tilde{E}(N) - E_j \tilde{I}] \quad \Delta_1^- = 1/[\tilde{E}(1) - E_j \tilde{I}]$$

where Δ_i^{\pm} is also a 2×2 matrix, and

$$\tilde{a}_k = \begin{bmatrix} a_u(k) \\ a_v(k) \end{bmatrix}.$$

By adding the subscript j to \tilde{a}_k , the normalized eigenfunction with eigenvalue E_j can be expressed as

$$|\Psi_j\rangle = \sum_{i=1}^N \tilde{a}_{ij} |i\rangle. \quad (6)$$

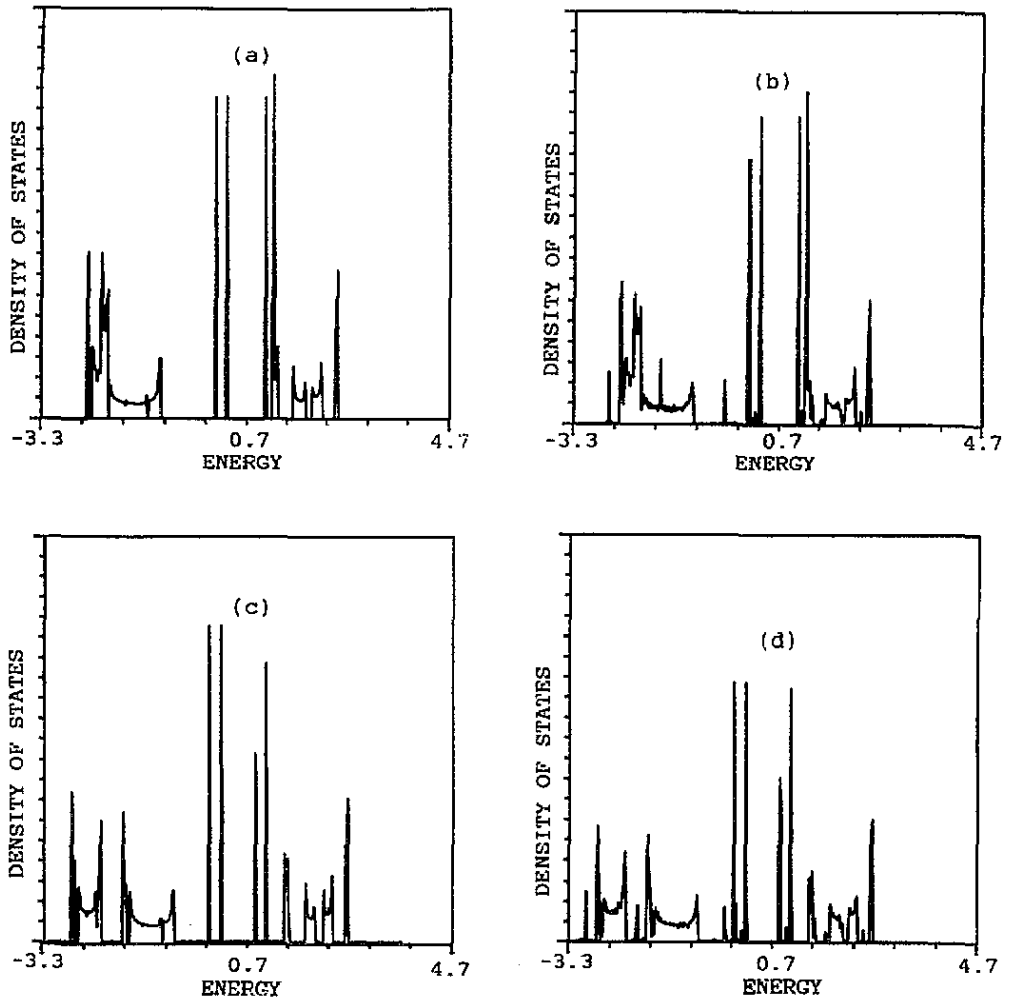


Figure 1. Energy spectrum of the 1D model (5000 atoms). (a) The parameters in equation (3) are

$$p_{Ai} = p_{Bi} = \begin{cases} 1 & \text{for } i = 4 \\ 0 & \text{otherwise} \end{cases}$$

and the parameters in equation (1) are $\epsilon_{au} = -1.0$, $\epsilon_{av} = -2.0$, $\epsilon_{bu} = 1.0$, $\epsilon_{bv} = 0.0$, $\epsilon_{cu} = 2.0$, $\epsilon_{cv} = 1.5$, $t_1 = -1.0$, $t_2 = -0.5$ and $\gamma_1 = \gamma_2 = \gamma_3 = 0.1$. (b) The parameters in equation (3) are

$$p_{Ai} = p_{Bi} = \begin{cases} \frac{9}{10} & \text{for } i = 4 \\ \frac{1}{20} & \text{for } i = 3, 5 \\ 0 & \text{otherwise} \end{cases}$$

and the parameters in equation (1) are the same as those in (a). (c) The parameters in equation (3) are the same as those in (a), and the parameters in equation (1) are the same as those in (a), except for $\gamma_1 = \gamma_2 = \gamma_3 = 0.4$. (d) The parameters in equation (3) are the same as those in (b), and the parameters in equation (1) are the same as those in (c).

If we take the atom spacing as the unit of length, the second moment of the wavefunctions [17] is defined as

$$S_j = \frac{1}{N} \left[\sum_{i=1}^N i^2 |\tilde{\mathbf{a}}_{ij}|^2 - \left(\sum_{i=1}^N i |\tilde{\mathbf{a}}_{ij}|^2 \right)^2 \right]^{1/2}. \quad (7)$$

It is a measure of the extension of the wavefunction.

For a given E_j , the second moment is numerically calculated for different hybridizations and is shown in figure 2. The result shows that the second moment increases when the hybridization increases. When the hybridization becomes larger than a critical value, the second moment is invariable and almost becomes a constant, which is just that for the extended states [18]. We also calculate the second moment for other energy locations and find that the same behaviour appears if the energy is located in the smooth part of the energy spectrum. This means that some wavefunctions become delocalized, which is consistent with the result of [13]. Since the hybridization enhances the tendency towards delocalization, whereas the disorder tends to produce the opposite effect, the competition between them determines the nature of the electronic eigenfunctions and the energy spectrum. We also found that some wavefunctions remain localized when the hybridization increases.

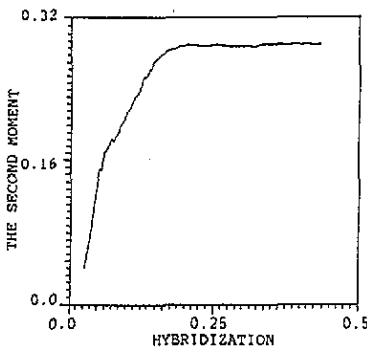


Figure 2. The second moment of wavefunctions for different hybridizations. The parameters except for γ are the same as those in figures 1(b) and 1(d) and $E_j = -1.499$.

In summary, we have studied an on-site model of a special random chain with two hybridizing bands. The energy spectrum, the wavefunctions and their second moment are numerically calculated. The results show that some special peaks appear in the spectrum because of a particular arrangement of atoms in such a random chain, and the effect of disorder on the electronic structure is counteracted by the effect of hybridization. When the hybridization reaches a critical value, some wavefunctions become delocalized. This is consistent with the conclusion of some recent literature on one-band models [1-7] as well as on a two-band model [13].

Acknowledgments

This work was supported by the National Fund of Natural Sciences of China.

References

- [1] Chen Xiaoshuang and Xiong Shijie 1992 *Phys. Rev. B* **46** 12004
- [2] Lavarda F C, Galvao D S and Laks B 1992 *Phys. Rev. B* **45** 3107
- [3] Dunlap D H, Wu H-L and Phillips P W 1990 *Phys. Rev. Lett.* **65** 88
- [4] Dunlap D H, Kundu K and Phillips P W 1989 *Phys. Rev. B* **40** 10999
- [5] Flores J C 1989 *J. Phys.: Condens. Matter* **1** 8471
- [6] Dunlap D H and Phillips P W 1990 *J. Chem. Phys.* **92** 6093
- [7] Wu H-L and Phillips P 1991 *Phys. Rev. Lett.* **66** 1366
- [8] Zhu B and Huang K 1987 *Phys. Rev. B* **36** 8102
- [9] Leavitt R P, Bradshaw J L and Towner F J 1991 *Phys. Rev. B* **44** 11266
- [10] Leavitt R P 1991 *Phys. Rev. B* **44** 11270
- [11] Dunlap R A, McHenry M E, O'Handley R C, Srinivas V and Bahadur D 1989 *Phys. Rev. B* **89** 1942
- [12] Chakrabarti A, Karmakar S N and Moitra R K 1990 *Mod. Phys. Lett. B* **4** 797
- [13] Buch I J, Logan D E, Madden P A and Winn M D 1989 *J. Phys.: Condens. Matter* **1** L8735
- [14] Yamamoto T, Kasu M, Noda S and Safari A 1990 *J. Appl. Phys.* **68** 5318
Kasu M, Yamamoto T, Noda S and Safari A 1990 *Japan. J. Appl. Phys.* **29** 828
- [15] Dean P 1972 *Rev. Mod. Phys.* **44** 127
- [16] Zhang Z-B 1986 *J. Phys. C: Solid State Phys.* **19** L689
- [17] Chao K A 1982 *J. Phys. C: Solid State Phys.* **14** L385
- [18] Severin M and Riklund R 1989 *Phys. Rev. B* **39** 10362