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Delocalization–localization transition in a one-dimensional two-band model with random clusters

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Abstract. We investigate the delocalization–localization transition in a one-dimensional disordered system with two hybridized bands. The effects of both disorder and interband hybridization on the energy spectrum and the properties of wavefunctions are studied by using the improved Dean method and the second-moment formula. The results show that there exist band tails in the gap regions. All subbands are widened by increasing the disorder strength, whereas when the interband hybridization increases, some subbands become narrower and the others are widened. The delocalization of the wavefunctions tends to be enhanced as the hybridization increases. The localization–delocalization transition of the wavefunctions occurs when the interband hybridization becomes larger than a critical value. The competition between disorder and hybridization determines the nature of the electronic states and the energy spectrum.

1. Introduction

Since the pioneering works of Anderson [1] and Mott and Twose [2], electronic and transport properties of randomly disordered systems have been the subject of enduring interest from both fundamental and applied viewpoints. One-dimensional (1D) systems are frequently considered because they turn out to be simpler than those in three dimensions. A great deal of work has shown that for 1D random potentials all electronic states that are solutions of the Schrödinger equation are, in general, localized. From the scaling consideration, one- and two-dimensional systems were expected to become insulators [3]. However, there are some examples of 1D disordered systems where the existence of extended states has been observed. The 1D liquid model shows the existence of nonlocalized states [4]. Azbel [5] and Azbel and Soven [6] have demonstrated that extended states exist in some 1D disordered systems, from which the absence of the localization in experiments can be accounted for [7]. Recently, in a 1D tight-binding random-dimer model, Dunlap *et al* [8, 9] have shown that when one of the site energies is assigned at random to pairs of lattice sites (that is, two sites in succession), $\sqrt{N}$ of the electronic states are delocalized, which is consistent with the theory of Dunlap *et al* [10] and Flores [11]. This is a tight-binding model with site-diagonal disorder and is constructed by randomly inserting a number of identical dimers into

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a purely periodic chain. In our previous paper, the extended states have also been found in other 1D random models, for example, the 1D site-diagonal disordered tight-binding model with random periods [12] and 1D site-diagonal tight-binding random-cluster model [13]. The random-dimer model [8, 9] is also in this class with two atoms in each inserted random cluster. We show numerically and analytically that in the energy spectrum the positions of some extended states depend on the size of the random cluster. In addition, in some particular class of random potentials, the extended states are allowed at selected energies [14]. Very recently, Kozlov *et al* showed that some modes of disorder introducing spatial correlations yielded extended states for particular energies, meaning that the disorder can also provide constructive quantum interference [15]. If the correlated interactions, such as electron–phonon interaction, are introduced in the 1D disordered systems with short-range spatial correlations, the problem will become far more complex [16]; this is beyond the scope of our present work.

For many realistic systems, several different bands may be important in determining electronic characteristics. Leavitt [17] have used the two-band model to study electronic states of semiconductor superlattices, and found that the conduction subband energies, envelope functions and tunnelling resonance width are highly consistent with the results found elsewhere. At the same time, the electronic properties in 1D tight-binding disordered or quasiperiodic two-band systems have also been studied by several workers. By the use of the real-space renormalization group method, Chakrabarti *et al* [18] have studied the electronic properties of a 1D quasiperiodic two-band system; it was found the intra-site interband hybridization counteracts the effect of disorder. Hirose *et al* [19] have found that in GaAs/AlAs quasi-periodic superlattices, the localization character is enhanced due to the interband hybridization. On the other hand, Buch *et al* [20] 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. We have proposed a 1D two-band model with periodic randomness. The results showed that the delocalization of the electronic wavefunction tends to be enhanced as intra-site interband hybridization increases [21]. To our knowledge, so far the effect of inter-site interband hybridization on the electronic properties in 1D disordered two-band systems has remained unexplored. It is thus desirable to study the combined effect of disorder and interband hybridization on the electronic properties in 1D disordered two-band models.

In the present paper, we propose a 1D two-band model with random clusters, having two hybridizing bands at every site. We attempt to investigate the competition between the effects of the disorder and the hybridization on the properties 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 [22]. 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. To our knowledge, there still is no perturbative treatment of the 1D two-band model, even for small enough interband hybridization. A perturbative treatment is also desired for this model. Now, despite the complexity of the two-band model, the numerical methods developed for the one-band problems can be extended to this case.

The paper is organized as follows. In section 2 we describe the 1D on-site disordered model, having two hybridization bands at every site. The density of electronic states is given in section 3. In section 4 we investigate the effects of disorder and interband hybridization on the properties of wavefunctions. The delocalization–localization transition is shown in section 4. The conclusions are given in section 5.

2. Model

We describe the system by the following tight-binding Hamiltonian [19]:

$$H = \sum_n \epsilon_u(n)|nu\rangle\langle nu| + \sum_n \epsilon_v(n)|nv\rangle\langle nv| + \sum_{\langle n,m\rangle} t_{11}|nu\rangle\langle mu| + \sum_{\langle n,m\rangle} t_{12}|nu\rangle\langle mv| + \sum_{\langle n,m\rangle} t_{21}|nv\rangle\langle mu| + \sum_{\langle n,m\rangle} t_{22}|nv\rangle\langle mv| \tag{1}$$

where: $\epsilon_u(n)$ and $\epsilon_v(n)$ are energy levels of orbitals u and v at site n; and t_{11}, t_{22} and t_{12}, t_{21} are the intra-orbital and inter-orbital nearest-neighbour hopping integrals, respectively. We suppose that the hopping integrals are regular but the orbital levels are in a random configuration described below, corresponding to the diagonal disorder. Therefore, this is a two-band version of the tight-binding disordered model.

Using two-component vector basis wavefunctions:

$$|i\rangle \equiv \begin{pmatrix} iu \\ iv \end{pmatrix}$$

we rewrite the tight-binding Hamiltonian in terms of 2×2 matrices:

$$H = \sum_{i=-\infty}^{\infty} \widehat{E}(i)|i\rangle\langle i| + \sum_{i=-\infty}^{\infty} [\hat{t}|i\rangle\langle i+1| + \hat{t}|i\rangle\langle i-1|] \tag{2}$$

where

$$\widehat{E}(i) = \begin{pmatrix} \epsilon_u(i) & 0 \\ 0 & \epsilon_v(i) \end{pmatrix}$$

$$\hat{t} = \begin{pmatrix} t_{11} & t_{21} \\ t_{12} & t_{22} \end{pmatrix}.$$

The lattice is made up of alternating connections of clusters of two species A and B. $\widehat{E}(i)$ takes one of the values $\widehat{E}_A$ and $\widehat{E}_B$, depending on the species which is present at the ith site. We consider a particular random distribution in which the lengths of A segments are fixed and the lengths of B segments are random. This means that the length of a particular B segment is a random variable. So the 1D chain arrangement is

$$\begin{array}{ccccccccc} \ldots\mathrm{AAA}\ldots\mathrm{BBB}\ldots\mathrm{AAA}\ldots\mathrm{BBB}\ldots\mathrm{AAA}\ldots\mathrm{BBB}\ldots \\ m \qquad L_i \qquad m \qquad L_{i+1} \qquad m \qquad L_{i+2} \end{array}$$

where m is the length of segment A and L_i is the length of the ith B segment. We denote as $P_B(L_i)$ the distribution function of the lengths of B segments. The form and the extent of disorder are controlled by this function. Here, we consider a distribution as follows:

$$P_B(L_i) = \sum_j p_{Bj}\delta(L_i - j) \tag{3}$$

where

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

and p_{Bj} is the probability of finding a segment of B having j sites. The whole lattice is formed by sequential connections of A and B segments.

3. Density of states

Once the lattice is constructed for given values of the parameters in equation (3), the energy spectrum can be calculated by the Dean method [23]. For a finite lattice of N sites, the number of states with eigenvalues less than ϵ is the number of negative eigenvalues of the matrices $\widehat{U}(i)$ $(i = 1, 2, \ldots, N)$, and the $\widehat{U}$-matrices are determined by the following relations:

$$\begin{aligned} &\widehat{U}(i) = \widehat{E}(i) - \epsilon\widehat{I} - \hat{t}^{\mathrm{t}}\widehat{U}^{-1}(i-1)\hat{t} \qquad i = 2, 3, \ldots, N \\ &\widehat{U}(1) = \widehat{E}(1) - \epsilon\widehat{I} \end{aligned} \tag{4}$$

where $\widehat{U}(i)$, $\widehat{E}(i)$ and $\hat{t}$ are 2×2 matrices, $\widehat{I}$ is a 2×2 unit matrix and $\hat{t}^{\mathrm{t}}$ is the transpose of $\hat{t}$. By the use of this theorem, the density of states is obtained and it is shown in figure 1. Generally, the parameters used are $\epsilon_{Au} = -\epsilon_{Bu} = 2.0$, $\epsilon_{Av} = -\epsilon_{Bv} = 1.0$, $t_{11} = t_{22} = 1.0$ and $t_{12} = t_{21} = 1.0$, which are similar to those of reference [18]. One can see that the density of states is symmetrically distributed on the two sides of the spectrum. Figure 1(a) and figure 1(b) display the results for the periodic and random systems, respectively. The density of states for the periodic system shows the existence of the gap caused by the interband hybridization. We can see that the Van Hove singularities, characterized as $D(E) \sim 1/\sqrt{E}$, appear on both sides of the gaps. For the random system, besides the two subbands appearing near the centre of the spectrum, other subbands are widened by disorder and there exist band tails in the gap regions, as expected for amorphous materials. In the density of states, subbands B_1 and B_2 merge with C_1 and C_2 (marked with arrows in figure 1(b)), respectively, and all of the gaps become narrower or disappear due to the introduced disorder. In figure 1(c) and figure 1(d), the parameters are the same as those in figure 1(b), except that the inter-orbital hoppings $t_{12(21)}$ are changed to 0.7 and 1.2, respectively. By comparison of figure 1(b) and figure 1(c), we find that the two central subbands develop into one band in a symmetric way as the inter-orbital hybridization decreases. The widening of the A_1- and B_1-subbands of figure 1(c) is larger than that in figure 1(b). These results imply that the A_1- and B_1-subbands become narrower, the central band is divided into two subbands and the central band gap appears on increasing the hybridization, whereas the other subbands become wider. The same trend can also be seen in figure 1(d).

4. Delocalization–localization transition

In the work on the 1D disordered systems, the wavefunction behaviour is considered as the most solid evidence of localization. To study the localization of 1D disordered systems, some criteria, such as the first moment, the inverse participation ratio, the structural entropy, the Thouless number and the second moment, have been introduced and used [25–27]. The numerical results have indicated that the second moment is successfully used as a single localization criterion for 1D aperiodic systems [25, 26]. In order to study the effect of interband hybridization on the properties of eigenfunctions, we will mainly discuss the dependence of the second moment of the wavefunctions on the interband hybridization. The eigenfunctions are obtained by the improved Dean method [24]. If $\hat{a}_n$ denotes the amplitude at site n of a wavefunction with eigenvalue E_j, and $\hat{a}_k \neq 0$, we can choose $|\hat{a}_k| = 1$ and the other amplitudes can be obtained from the recurrence relations

$$\hat{a}_{k\pm i} = -\Delta^{\pm}_{k\pm i}\hat{t}\hat{a}_{k\pm(i-1)} \qquad \text{for } N \geqslant k \pm i \geqslant 1 \tag{5a}$$

and

$$\Delta^{\pm}_{i} = 1/[\widehat{E}(i) - E_j\widehat{I} - \hat{t}\Delta^{\pm}_{i\pm1}\hat{t}\,] \qquad \text{for } N \geqslant i + 1 \geqslant 1 \tag{5b}$$

where

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

(where $\Delta_i^{\pm}$ is a 2×2 matrix) and

$$\hat{a}_k = \begin{pmatrix} a_u(k) \\ a_v(k) \end{pmatrix}.$$

By adding the state index j to the subscript of $\hat{a}_k$, the normalized eigenfunction with eigenvalue E_j can be expressed as

$$|\psi_j\rangle = \sum_{i=1}^{N} \hat{a}_{ij}|i\rangle. \tag{6}$$

If we take the site spacing as the unit of length, the second moment of the wavefunctions [25] is defined as

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

In order to demonstrate the extended characteristics of the states, we calculated the wavefunctions of a sample model with $m = 3$. The length of lattice considered is 3000. For a given energy $E_j = -2.40$, the wavefunction of an unscattered state is shown in figure 2. From figure 2, it is obvious that the wavefunction is delocalized in this disordered system, in agreement with the situation in [20, 21] and in the single-band case of [13]. This is due to the specific short-range spatial correlation in the disorder for the system. On the other hand, for the localization of the electronic states in 1D disordered systems, people usually study the dependence of the localization on the energy and size. For example, if one wants to calculate the transmission property of the electronic states as a function of energy in the above-mentioned system, one can find that the transmission coefficient is almost unity at the energy $E_j = -2.40$. However, here our focus is on how the competition between disorder and hybridization determines the properties of the electronic states in the 1D two-band disordered system. So, we mainly discuss the effect of the interband hybridization on the behaviour of the wavefunction for the fixed system and some definite energies. In addition, if the interband hybridization (t_{12} and t_{21}) is equal to zero, the 1D two-band model is reduced to two independent 1D single-band models, some particular delocalized wavefunctions still exist at some fixed energies, similar to that in figure 2, which has been very thoroughly treated [13]. As mentioned above, the second moment can be readily used to measure the localization of the wavefunction [25, 26]. Next, the second moments as a function of interband hybridization are numerically calculated for different energies. The result is shown in figure 3. For $E_j = -2.50$, figure 3(a) shows that the second moment increases when the hybridization increases. The delocalization of the electronic wavefunction is enhanced as the interband hybridization increases. It is also found that the second moment increases more steeply as the interband hybridization increases up to the value 0.7, and then when the interband hybridization becomes larger than a value 1.0, the second moment reaches a maximum and almost becomes a constant, $1/\sqrt{12}$, which is just the critical value for the extended states in a 1D aperiodic system [26]. It has been pointed out that $S_j = 1/\sqrt{12}$ in the case of delocalized wavefunctions and decreases to a small value in the case of localized states [26]. Therefore, we find that at the energy $E_j = -2.50$, the delocalization–localization transition of the electronic states appears at the hybridization value 1.0. For another energy $E_j = -3.00$, we show in figure 3(b) that when the interband hybridization increases the second moment also increases at first, then increases more steeply as the hybridization exceeds the value 0.9 and finally reaches the critical value $1/\sqrt{12}$ at the

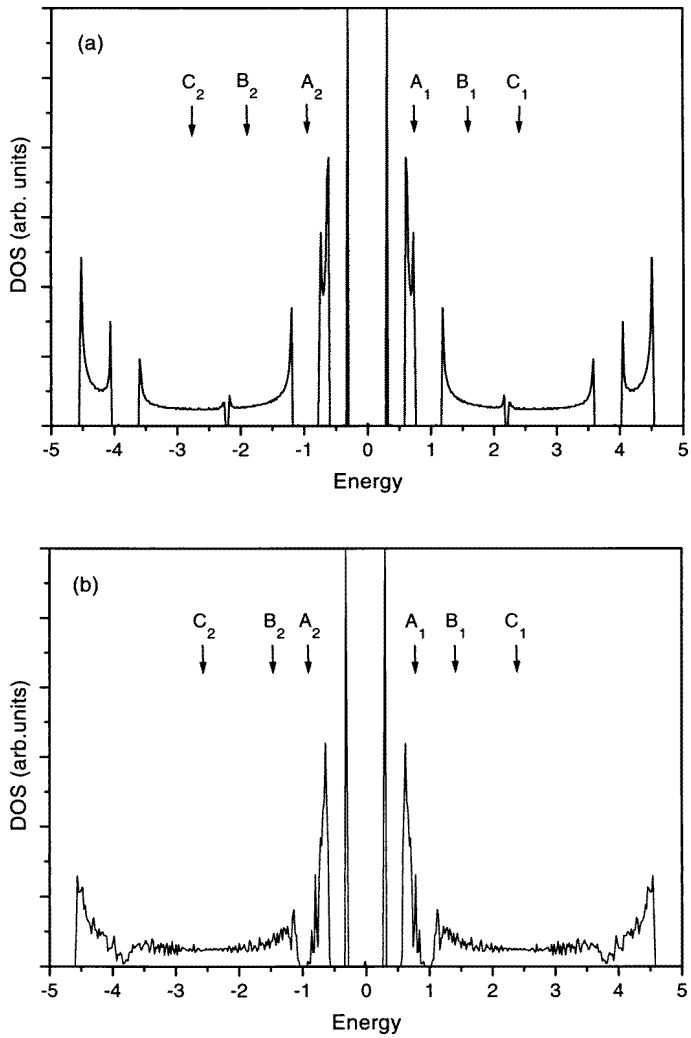

Figure 1. The density of states for the 1D model with 3000 sites. (a) The periodic system and the parameters in equation (1) are $\epsilon_{Au} = -\epsilon_{Bu} = 2.0$, $\epsilon_{Av} = -\epsilon_{Bv} = 1.0$, $t_{11} = t_{22} = 1.0$ and $t_{12} = t_{21} = 1.0$. A_1, B_1, C_1, A_2, B_2 and C_2 indicate different subbands. (b) The parameters in equation (3) are $p_{Bi} = 1/3$ for $1 \leqslant i \leqslant 3$, $p_{Bi} = 0$ otherwise and the parameters in equation (1) are the same as those in (a). A_1, B_1, C_1, A_2, B_2 and C_2 are in agreement with those in (a). (c) The parameters in equation (3) are the same as those in (b) and the parameters in equation (1) are the same as those in (a) except that $t_{12} = t_{21} = 0.8$. (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 (a) except that $t_{12} = t_{21} = 1.2$.

hybridization value 1.2, which is similar to the behaviour in figure 3(a). This indicates that for this energy state, the transition appears at the hybridization value 1.2. We also calculate the second moment for other energies and find that the same behaviour appears if the energy is located in the smooth part of the spectrum. This means that some wavefunctions become delocalized, which is consistent with the conclusion of references [20, 21]. In addition, in the energy located near the edge of subband, e.g., the energy of the state in figure 3(b), for small

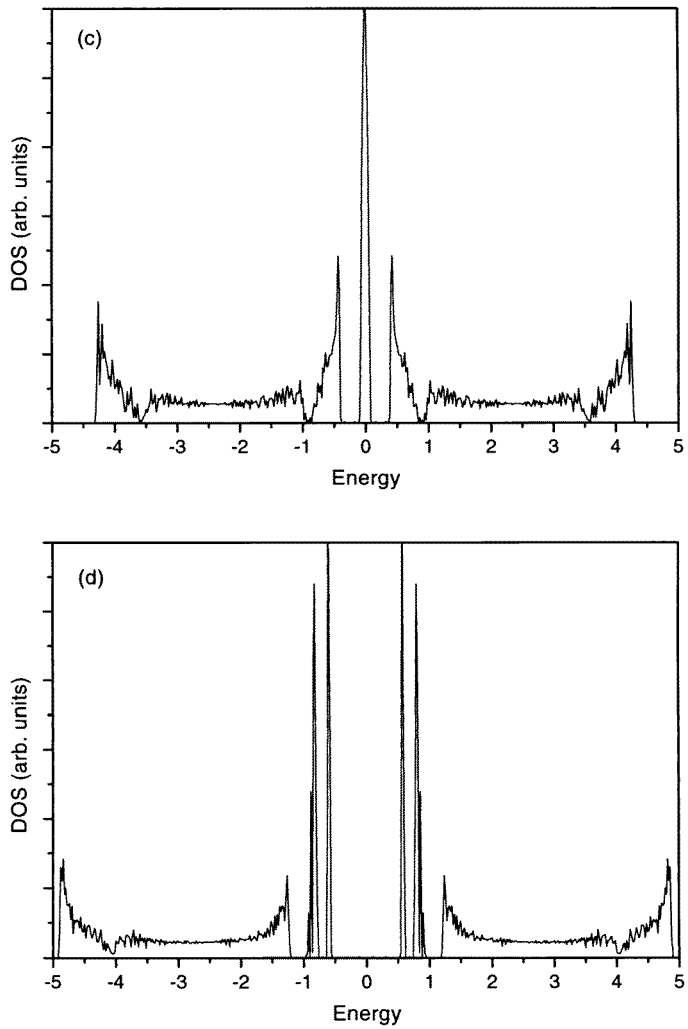

Figure 1. (Continued)

hybridization the state is completely localized and the second moments are almost zero, whereas for the energy located near the band centre like that in figure 3(a), the second moments are finite for small hybridization. These results indicate that the delocalization of wavefunctions near the band centre is more enhanced than that of edge states under the same degree of disorder. If the energy is located in the other part of the energy spectrum, we find that the second moment also increases but cannot reach the critical value as the interband hybridization increases. This implies that some wavefunctions remain localized but the localization is weakened with increasing hybridization. Since the interband 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 wavefunctions and the energy spectrum. In addition, the fluctuations in the curves of the second moments in figure 3 can be attributed to the finite size of the system. At different interband hybridization but with the same energy

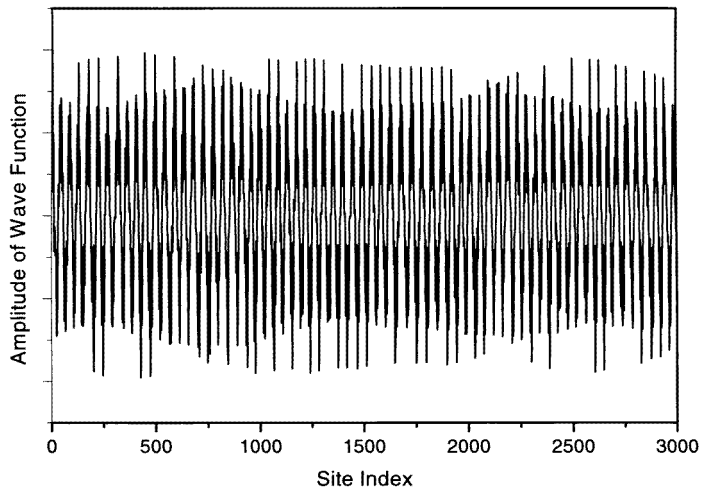

Figure 2. The wavefunction of the 1D model with 3000 sites with energy $E_j = -2.4$. The parameters are the same as those of figure 1(b).

E_j, the wavefunctions have different repeated periods. When the length of the system is not equal to an integer times the period of the wavefunctions, different amplitudes of envelope wavefunctions appear at the end of the system which lead to the fluctuations of the second moment. On the other hand, if the wavefunctions are completely localized in the finite sample, the amplitudes of the wavefunctions at the end are almost zero; the fluctuations are very small as can be seen from the second moment at small hybridization in figure 3(b). Furthermore, in our calculations, we find that the behaviour of the second moment is different for different choices of disorder. If the degree of disorder is increased, the second moment approaches the critical value $1/\sqrt{12}$ at larger hybridization strength. This again confirms that the competition between the disorder and the interband hybridization determines the nature of the electronic wavefunctions and the energy spectrum.

5. Conclusions

We investigate the delocalization–localization transition in a particular 1D diagonal disordered model which has two hybridized bands. By using the improved Dean method and second-moment formula, the effects of both disorder and interband hybridization on the energy spectrum and the properties of wavefunctions are studied. The results show that for the random system, there exist band tails in the gap region, as expected for amorphous materials. In the spectrum of the density of states, two pairs of subbands with a smaller gap merge into continuous bands, and all subband gaps become narrower on introducing the disorder. All subbands are widened with increasing degree of disorder. On the other hand, the symmetrical A_1- and A_2-subbands become narrower, and other subbands become wider when interband hybridization increases. We also show that the delocalization of wavefunctions tends to be enhanced as the hybridization increases. The localization–delocalization transition of wavefunctions appears when the interband hybridization becomes larger than a critical value. Since the interband 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 wavefunctions and the energy spectrum.

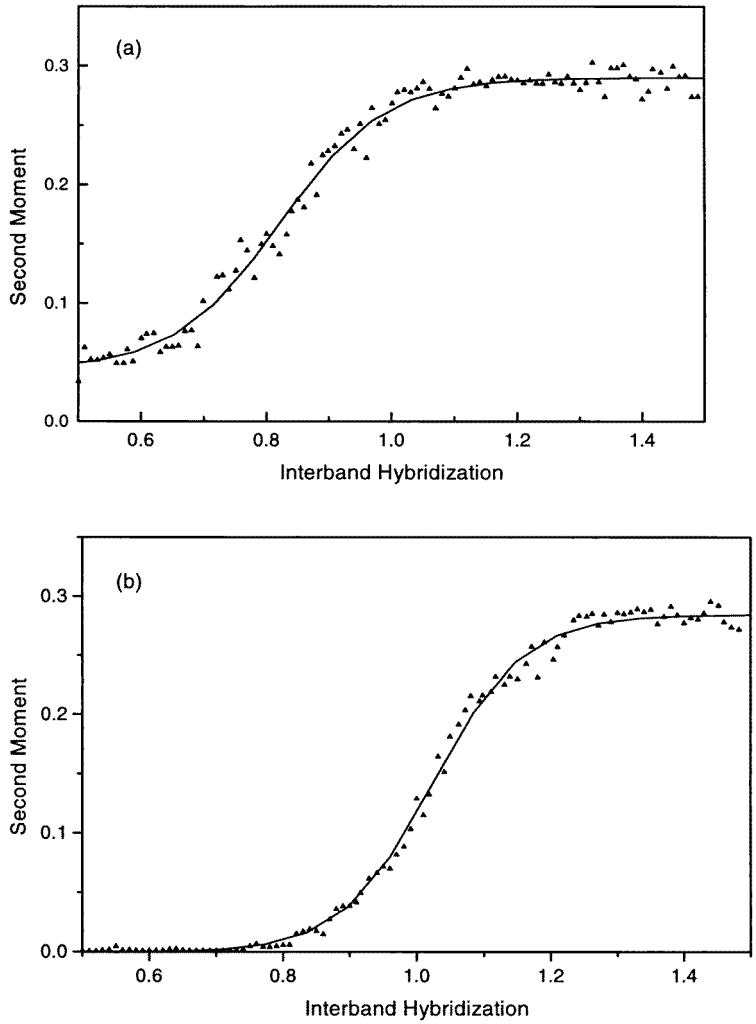

Figure 3. The second moment of the wavefunctions as a function of the interband hybridization. The black triangles represent the numerical results, which are fitted by the solid curves. The parameters except for t_{12} and t_{21} are the same as those in figure 1(b). (a) $E_j = -2.5$ and (b) $E_j = -3.0$.

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