Electron States in a Class of One-Dimensional Random Binary Alloys

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We present a model for alloys of compound semiconductors by introducing a one-dimensional binary random system where impurities are placed in one sublattice while host atoms lie on the other sublattice. The source of disorder is the stochastic fluctuation of the impurity energy from site to site. Although the system is one-dimensional and random, we demonstrate analytically and numerically the existence of a set of extended states in finite systems, whose energy lies close to that of host atoms.

1. Introduction

Electron states in random systems have become an active research topic since the generality of localization phenomena in one dimension (1D) [1]. Although it is well established that almost any nonzero disorder causes exponential localization of all eigenstates in 1D systems, regardless their energy (see, e.g. Ref. [2] and references therein), there exist several exceptions. It is nowadays well known that extended states may arise in random systems where disorder exhibits short-range [3 to 18] or long-range correlations [19, 20]. Spatial correlation means that random variables are not independent within a given correlation length. Suppression of localization by correlations was further put forward for the explanation of high conductivity of doped polyaniline [7] as well as transport properties of random semiconductor superlattices [21].

In this paper, we report further progress along the lines in the preceding paragraph. We turn ourselves to one of the pioneering works in the field, namely the work of Phillips and Wu on polyaniline (see Ref. [7] and references therein). These authors showed that polyaniline can be mapped onto a random dimer model that has a set of extended states, originated by a resonance of a single dimer defect (two neighbor sites with the same energy). Electron states whose energy is close to this resonance turn out to be extended (in the sense that their localization length is larger than the system size) when dimers are placed at random in the 1D system. In this paper, we show that resonances can yield extended states in long-range correlated systems. To this end, we built up a simple model of semiconductor binary alloy, like ternary III–V compounds. In these alloys (say $Al_xGa_{1-x}As$), the cation sublattice is occupied by the same atoms (say As) while anions (say Al and Ga) are randomly distributed over the other sublattice.

We model these alloys by considering a 1D random binary alloy with two species, referred to as A and B atoms hereafter. In order to mimic the disorder present in the anion sublattice, we further assume that the site energy of A atoms is randomly distributed from site to site while that of B atoms is the same over the entire cation sublattice. We demonstrate the occurrence of extended states in the vicinity of the site energy of B atoms *in spite of the fact that the system is purely 1D and random*. From the study of the divergence of the localization length and the density of states (DOS) at the site energy of B atoms we conclude that the number of such extended states scales as the square root of the number of lattice sites.

2. Model

We consider a 1D binary system where A (B) atoms are placed at odd (even) positions of the otherwise regular lattice, whose corresponding site energies are ϵ_{2n-1} (ϵ_{2n}) with $n = 1, 2, \ldots N$, N being the number of unit cells of the alloy. The Schrödinger equation for stationary eigenstates $\psi_n(E)$ is

$$(E - \epsilon_n)\,\psi_n + \psi_{n+1} + \psi_{n-1} = 0\,, \qquad n = 1, 2, \ldots, \mathcal{N}\,, \tag{1}$$

where E is the corresponding eigenenergy, ϵ_n is the site energy and $\mathcal{N} \equiv 2N$ is the number of atoms in the system. According to our model, site energy at even positions is the same and we can set $\epsilon_{2n} = 0$ without loss of generality. The source of disorder in this model arises from the stochastic fluctuations of site energy at odd positions. We assume that $\{\epsilon_{2n-1}\}_{n=1}^N$ is a set of *uncorrelated* random Gaussian variables with mean value v and variance σ^2. Hereafter σ will be referred to as *degree of disorder*. The joint distribution function of a realization of disorder is represented by the direct product of single Gaussians. Thus,

$$\langle \epsilon_{2n-1} \rangle = v\,, \qquad \langle \epsilon_{2n-1}\epsilon_{2n'-1} \rangle = \left(v^2 + \sigma^2\right)\delta_{nn'}\,. \tag{2}$$

The Schrödinger equation (1) can be written via the 2×2 promotion matrix P_n as follows:

$$\begin{pmatrix} \psi_n \\ \psi_{n+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & -E + \epsilon_n \end{pmatrix} \begin{pmatrix} \psi_{n-1} \\ \psi_n \end{pmatrix} \equiv P_n \begin{pmatrix} \psi_{n-1} \\ \psi_n \end{pmatrix}. \tag{3}$$

By iterating this equation we can relate (ψ_n, ψ_{n+1}) and (ψ_0, ψ_1) with $\psi_0 \equiv 0$,

$$\begin{pmatrix} \psi_n \\ \psi_{n+1} \end{pmatrix} = \prod_{k=n}^{1} P_k \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} \equiv M_n \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}, \tag{4}$$

where M_n is referred to as the transfer matrix. We find most convenient to deal with the promotion matrix of the (diatomic) unit cell instead of that corresponding to a single atom (3), namely $T_n \equiv P_{2n}P_{2n-1}$. For real E and ϵ_n, the promotion matrix T_n can be regarded as an element of the SO(1,2) group, isomorphic to SL(2,R). It can be cast in the following form via the Pauli matrices σ_μ:

$$T_n = \left[\frac{E}{2}\left(E - \epsilon_{2n-1}\right) - 1\right]\mathcal{I}_2 - \frac{E}{2}\left(E - \epsilon_{2n-1}\right)\sigma_3$$

$$+ \frac{\epsilon_{2n-1}}{2}\sigma_1 + i\left(E - \frac{\epsilon_{2n-1}}{2}\right)\sigma_2\,, \tag{5}$$

where $\mathcal{I}_m$ denotes the $m \times m$ unit matrix. It is easy to demonstrate the following useful property $T_n^{-1} = \sigma_2 T_n^{\dagger} \sigma_2$. The transfer matrix of the entire system (N unit cells) is obtained as $M_N = \prod\limits_{n=N}^{1} T_n$. Oseledec's theorem [22] states that the following limiting matrix Γ exists:

$$\Gamma = \lim_{N \to \infty} \left(M_N^{\dagger} M_N \right)^{1/2N}, \tag{6}$$

with eigenvalues e^{γ}.

3. Existence of Extended States

In order to find the localization length one should calculate the matrix $M_N^{\dagger} M_N$ for large N. We will perform this task following the technique developed in Ref. [23]. By using the formula for the decomposition of the product of two spin-1/2 states into the direct sum of scalar and spin-1 states, we have

$$(T_j)_{\alpha'}^{\alpha} (T_j^{-1})_{\beta}^{\beta'} = \frac{1}{2} (\delta)_{\beta}^{\alpha} (\delta)_{\alpha'}^{\beta'} + \frac{1}{2} (\sigma^{\mu})_{\alpha'}^{\beta'} \Lambda_j^{\mu\nu} (\sigma^{\nu})_{\beta}^{\alpha}, \tag{7}$$

where

$$\Lambda_j^{\mu\nu} = \frac{1}{2} \mathrm{Tr} \left(T_j \sigma^{\mu} T_j^{-1} \sigma^{\nu} \right) \tag{8}$$

is the spin-1 part. Multiplying the expression (7) by the left and right by σ_2 we have

$$(T_j)_{\alpha'}^{\alpha} (T_j^{\dagger})_{\beta}^{\beta'} = \frac{1}{2} (\sigma_2)_{\beta}^{\alpha} (\sigma_2)_{\alpha'}^{\beta'} + \frac{1}{2} (\sigma^{\mu}\sigma_2)_{\alpha'}^{\beta'} \Lambda_j^{\mu\nu} (\sigma^{\nu}\sigma_2)_{\beta}^{\alpha}. \tag{9}$$

Now we should take into account the disorder and calculate the average of Γ by random distribution of ϵ_{2n-1} at odd sites

$$\langle \Gamma \rangle = \frac{1}{2} \sigma_2 \otimes \sigma_2 + \frac{1}{2} (\sigma^{\mu}\sigma_2) \otimes (\sigma^{\nu}\sigma_2) \left(\prod_{j=1}^{N} \langle \Lambda_j \rangle \right)^{\mu\nu}, \tag{10}$$

where Λ_j is defined by (8). According to Oseledec's theorem [22], the Lyapunov exponent of the ensemble for an energy value E, which is nothing but the inverse of the localization length λ^{-1}, where λ is given in units of the length of the unit cell, will be given by

$$\lambda^{-1} = \log \left[\xi(E) \right], \tag{11}$$

where $\xi(E)$ is the closest to unity eigenvalue of $\langle \Lambda_j \rangle$, whose elements are

$$\langle \Lambda_j^{11} \rangle = \frac{1}{2} \left(2 + E^4 + 4Ev - 2E^3v - \sigma^2 - v^2 + (\sigma^2 + v^2 - 4) E^2 \right),$$

$$\langle \Lambda_j^{12} \rangle = -\frac{i}{2} \left(E^4 - 2E^3v + \sigma^2 + v^2 + (\sigma^2 + v^2 - 2) E^2 \right),$$

$$\langle \Lambda_j^{13} \rangle = -E^3 - v + 2E^2v - (\sigma^2 + v^2 - 2) E$$

$$\langle \Lambda_j^{21} \rangle = \frac{i}{2} \left(E^4 + 4Ev - 2E^3v - \sigma^2 - v^2 + (\sigma^2 + v^2 - 2) E^2 \right),$$

$$\langle \Lambda_j^{22} \rangle = \frac{1}{2} \left(2 + E^4 - 2E^3 v + \sigma^2 + v^2 + (\sigma^2 + v^2)\, E^2 \right),$$

$$\langle \Lambda_j^{23} \rangle = -i \left(E^3 + v - 2E^2 v + (\sigma^2 + v^2)\, E \right),$$

$$\langle \Lambda_j^{31} \rangle = -2E + E^3 + v - E^2 v,$$

$$\langle \Lambda_j^{32} \rangle = -i \left(E^3 - v - E^2 v \right),$$

$$\langle \Lambda_j^{33} \rangle = 1 - 2E^2 + 2Ev. \tag{12}$$

Delocalized states have an infinite localization length and, therefore, at some particular energy E, the matrix $\langle \Lambda_j \rangle$ should have an eigenvalue equal to unity. Hence we get the following condition for obtaining delocalized states:

$$\det \left[\mathcal{I}_3 - \langle \Lambda_j \rangle \right] = -2\sigma^2 E^2 = 0. \tag{13}$$

As we see, there is a delocalized state at $E = 0$. This result is also supported by the fact that the state with $E = 0$ is the solution of the Schrödinger equation (1) for an infinite system, for which $\psi_{2n+1} + \psi_{2n-1} = 0$. Thus, the state with $E = 0$ spreads uniformly over the entire lattice since the probability amplitude $|\psi_{2n+1}|^2$ at odd sites is constant. Futhermore, the main point of the present method relies in the fact that one can calculate the localization length for any arbitrary state with $E \neq 0$. To get some insight into this result, let us expand (11) around $E = 0$ to get

$$\lambda^{-1} = \begin{cases} -\dfrac{\sigma^2}{4v} E + \mathcal{O}(E^2); & E < 0, \\[2mm] 2v^{1/2} E^{1/2} + \mathcal{O}(E^{3/2}); & E > 0, \end{cases} \tag{14}$$

for $v > 0$. Notice that the localization length is asymmetric around the energy of the extended state since it scales as $\sim E$ at the left and $\sim E^{1/2}$ at the right. The situation is just the opposite for $v < 0$. Remarkably, the prefactor at the left depends on the degree of disorder of the alloy but becomes independent of disorder at the right.
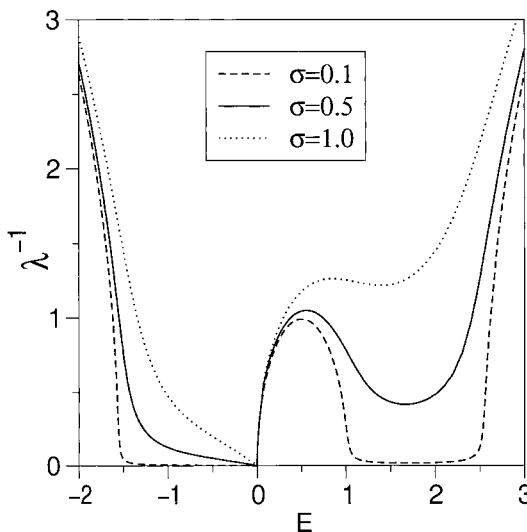
When the degree of disorder vanishes ($\sigma = 0$), the alloy is simply a diatomic periodic chain with site energies 0 and v in each unit cell and, consequently, there are two allowed bands. The lower band ranges from $v/2 - (v^2/4 + 4)^{1/2}$ up to 0 while the upper band ranges from v up to

Fig. 1. Inverse of the localization length as a function of energy when $v = 1$ and $\sigma = 0.1$, 0.5 and 1.0. Notice that $\lambda \to \infty$ at $E = 0$

$v/2 + (v^2/4 + 4)^{1/2}$ for $v > 0$. In this case all eigenstates are Bloch functions and spread over the entire chain. Localization occurs as soon as a small degree of disorder is introduced in the system. But, according to our previous result, the eigenstate with $E = 0$ remains extended. This is clearly seen in Fig. 1, where the inverse of the localization length obtained from (11) is plotted against E for $v = 1$ and different degrees of disorder σ. In all cases the inverse of the localization length is nonzero except at $E = 0$, where $\lambda^{-1} = 0$. This suggests the occurrence of a delocalized state at $E = 0$. We leave the discussion on finite systems for the next section.

4. Numerical Results

To confirm the above analytical results we have also numerically diagonalized the Schrödinger equation (1). We will mainly focus our attention on the normalized DOS (DOS per unit length) $\rho(E)$, and on the degree of localization (inverse participation ratio, IPR) for the states at energy E. They are defined, respectively, as follows [24]:

$$\rho(E) = \frac{1}{\mathcal{N}} \left\langle \sum_k \left(\frac{1}{R}\right) \theta \left[\frac{R}{2} - |E - E_k|\right] \right\rangle, \tag{15}$$

$$L(E) = \frac{1}{\mathcal{N}\rho(E)} \left\langle \sum_k \left(\frac{1}{R}\right) \theta \left[\frac{R}{2} - |E - E_k|\right] \left(\sum_{n=1}^{\mathcal{N}} a_{kn}^4\right) \right\rangle, \tag{16}$$

where the angular brackets indicate an average over an ensemble of disordered linear chains and a_{kn} is the eigenvector of (1) corresponding to the eigenvalue E_k with $k = 1, 2, \ldots, \mathcal{N}$. Here R is the spectral resolution and θ is the Heaviside step function. The IPR behaves like $1/\mathcal{N}$ for delocalized states spreading uniformly over the entire system on increasing $\mathcal{N}$. In particular, the IPR can be exactly computed for the eigenstates of the periodic lattice. In doing so we obtain the expected behavior for $\mathcal{N} \to \infty$. On the contrary, localized states exhibit much higher values. In the extreme case, when the eigenstate is localized at a single site, the IPR becomes unity.

We have fixed $v = 1$ and studied several values of the degree of disorder σ, ranging from 0.1 up to 1.0. The highest value of the degree of disorder considered in the present work means that the typical fluctuations of the site energy are of the order of the nearest neighbor coupling. The maximum number of atoms in the chain was $\mathcal{N} = 1000$ (500 unit cells) although larger systems were also studied to check that our main results are independent of the size. The results comprise the average over 100 realizations of the disorder for each given pair of parameters v and σ. The spectral resolution was $R = 4 \times 10^{-3}$.

Let us comment the results we have obtained numerically. Figure 2 shows the DOS for two different values of the degree of disorder ($\sigma = 0.1$ and 1.0) when the system size is $\mathcal{N} = 1000$ and $v = 1$. The DOS presents the usual U-shape within the bands when the degree of disorder is small. The singularities at the edge of the allowed bands are smeared out on increasing the degree of disorder except at $E = 0$, where the divergence remains even for the largest degree of disorder ($\sigma = 1.0$). This result suggests the state at $E = 0$ is delocalized.

The degree of localization (IPR) presents an overall increase when the degree of disorder increases, meaning that the larger the degree of disorder, the smaller is the localization length. This is clearly observed in Fig. 3, where we show the IPR as a func-
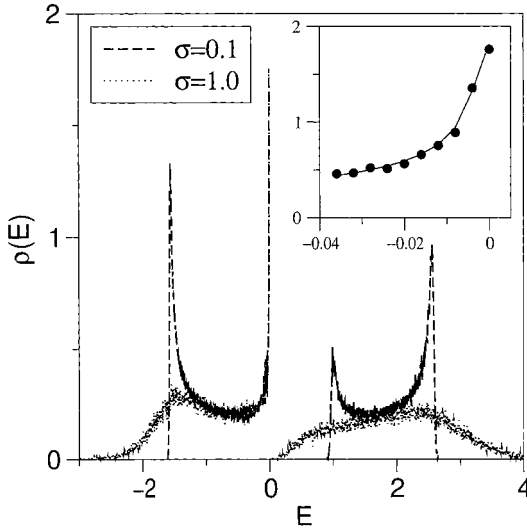
Fig. 2. Density of states as a function of energy when the lattice size is $\mathcal{N} = 1000$, $v = 1$ and the degree of disorder is $\sigma = 0.1$ and 1.0. The inset shows an enlarged view close to the top of the lower band for $\sigma = 1.0$ and the solid line is the $\sqrt{-E}$ fit

tion of the energy for the same parameters as in Fig. 1. However, the increase of the IPR strongly depends on energy, being more pronounced close to the center of both allowed bands. Interestingly, the IPR at $E = 0$ becomes independent of the degree of disorder although depends on the system size, as expected. This peculiarity manifests the delocalized character of the state at $E = 0$. Finally, notice the good correspondence between Fig. 1 (analytical result) and Fig. 3 (numerical result).

Some words concerning the relevance of this extended state in transport properties are now in order. From a rigorous mathematical point of view, Eq. (14) demonstrates the existence of a single extended state in *infinite* systems. However, the divergence of the localization length λ at the resonant energy points out that several states present localization length larger than the system size in *finite* systems. We can roughly calculate the number of such states from some basic considerations: It is apparent from the divergence of the normalized DOS at the resonant energy (see Fig. 2) that there exists a number of states close to the top of the lower band even in the presence of disorder.

We can safely admit that the DOS diverges as $\rho(E) \sim 1/\sqrt{-E}$, like periodic systems, close to the top of the lower band *even* in disordered systems (see inset of Fig. 2 for the higher value of the degree of disorder considered in this work, namely $\sigma = 1.0$). From (14) it is clear that the localization length is larger than the system
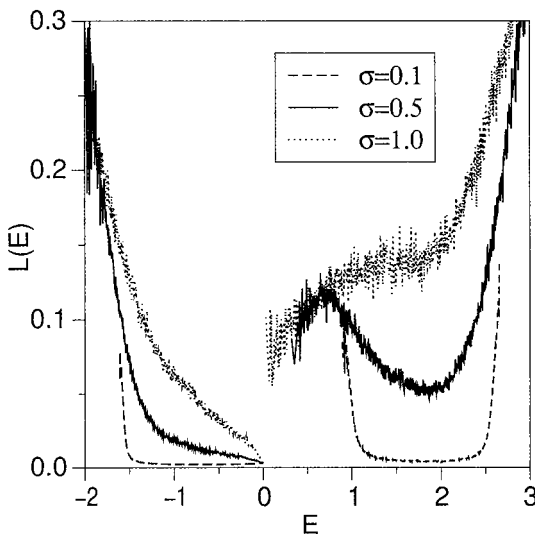
Fig. 3. Inverse participation ratio for the same cases as shown in Fig. 1. Notice the overall increase on increasing the degree of disorder except at $E = 0$

size for those states whose energy lies within the range $E = E_c \equiv -4v/N\sigma^2$ up to $E = 0$. The number of such states is then

$$\int\limits_{E_c}^{0} \mathcal{N}\rho(E)\,\mathrm{d}E \sim \sqrt{\mathcal{N}}\,.$$

Therefore, we are led to the conclusion that the localization length of $\sim \sqrt{\mathcal{N}}$ states is larger than the system size. Remarkably, a similar scaling was found in the random dimer model [4].

5. Conclusions

In this paper, we have considered electron dynamics in a one-dimensional model of binary alloy where disorder lies in one of the two sublattices. Although the system is one-dimensional and random, we have demonstrated analytically the existence of a de-localized state in infinite systems at an energy matching that of atoms of the other sublattice. The relevance of such a state on the transport properties is still an open question since the advent of the random dimer model [4]. Most important from a practical point of view, we have obtained a closed expression for the divergence of the localization length around this particular energy. Numerical results from the evaluation of the DOS and IPR (degree of localization) strongly suggest that there exist *many* ($\sim \sqrt{\mathcal{N}}$) states close to the resonant energy that remain extended in finite systems, in the sense that their localization length is larger than the system size.

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