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Reflectionless modes in chains with large-size homogeneous impurities

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Abstract. We study the spectral and localization properties of tight-binding chains with randomly distributed binary blocks of arbitrary size m; one having site energies ϵ_A and the other ϵ_B, respectively. We demonstrate that for block size m greater than one and $\delta = |\epsilon_A - \epsilon_B|$ less than a critical value $\delta_c(m)$ perfect transmission resonance modes exist in the band. Their number is proportional to m and they occur via dominant $1/E^2$ divergencies of the localization length. No transmission is found for $\delta > \delta_c(m)$. Our results are understood by solving exactly the scattering problem from a single homogeneous impurity block of arbitrary size m. In the limit of hard impurities ($m \to \infty$) transmission stops only when $\delta > \delta_c(\infty) = 4V$, V being the intersite matrix element; that is when the pure A and B bands become detached.

1. Introduction

There is intensive current interest for problems concerning electronic transport and wave propagation in disordered lattices [1, 2]. In the theory of Anderson localization for electrons [3–5] the simplest kind of a random potential is usually adopted, that is a random on-site energy value chosen from a set of uncorrelated random numbers. However, the existing disorder in the solid often suggests more complex correlated forms of the random potential, e.g. by permitting large ordered regions to appear. In general, correlations lead to lattice site energies which are no longer independent random variables but relate to the corresponding energies of their neighbours within a potential correlation length. There is not only theoretical interest in correlations; for example, it is known that short-range order due to a spatially correlated potential, when two values of the potential are involved in a single unit cell, is essentially responsible for the presence of gaps in amorphous semiconductors. Another reason for the inevitability of disorder correlations arises from the need to be able to consider wave-like excitations (light, magnons, phonons, etc) propagating in the continuum. It is not usually possible to map these problems to electronic systems with independent site (or bond) disorder but disorder correlations must be included.

Although uncorrelated random models have been extensively studied in the context of Anderson localization [1–5], little attention has been paid to the cases where strong short-range correlations exist. It is expected that they will lead to new interesting phenomena, such as partial delocalization, even in one dimension where all states are expected to be localized [5, 6]. Such a consequence of correlation is familiar from corresponding magnon or phonon studies where delocalization is found at long wavelengths [6].

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In the present paper we focus on the study of random chains with a correlated discrete binary distribution of the random potential. The binary choice made for the potential is also suggested from physical wave-like propagation phenomena in a medium containing homogeneous objects, for example hard spheres, with a density which differs from the rest of the medium. In this case it is implied that m type A and m type B sites are involved in a single unit cell. In order to create the corresponding random chain instead of A and B, large m-site homogeneous blocks, AA...A and BB...B, are randomly distributed with corresponding probabilities p and $q = 1 - p$, respectively. Our simple one-dimensional model of correlation combines short-range order with long-range disorder contrasting with the study of quasi-periodic systems which display long-range order and short-range disorder [7].

In one dimension, within the tight-binding approximation and for independent site-diagonal randomness chosen from a continuous distribution, there is always a positive Lyapunov exponent corresponding to a finite localization length [4, 5]. The situation does not change much for the discrete disorder case of the random A, B binary alloy which corresponds to our model with $m = 1$. Again, all states are localized in accordance with well known theorems but the Lyapunov exponent is no longer a differentiable function of the energy and becomes a weakly singular measure [8].

The results drastically change for the $m = 2$ 'paired' AA, BB random alloy [9–11]. At most two eigenstates can have diverging localization lengths obeying $1/E^2$ singularity laws, where E is the energy measured from the special energies E_0. From another viewpoint the quadratic exponents represent sufficiently strong singularities, being equal to $2/d$ where the dimensionality is $d = 1$. Hence, they satisfy a generalized Harris criterion [12] which inevitably leads to critical behaviour even in one dimension. A corresponding scattering study of the problem [11] revealed that such modes are totally reflectionless and delocalized. Moreover, a previous quantum dynamical study [9] pointed out that these short-range pair correlations may lead to a superfast type of diffusion for the mean squared displacement of a time-evolving wavepacket initially placed at a single site. The superdiffusion is intimately connected with the presence of the reflectionless modes and both only occur for the weakly disordered paired alloys. The conditions for superfast diffusion to exist and reflectionless modes to appear were determined in [9–11]: the difference in the site energies $\delta = |\epsilon_A - \epsilon_B|$, which measures the strength of the disorder, must be less than a critical value $\delta_c(m = 2) = 2V$, where V is the corresponding hopping matrix element. In the strongly disordered case ($\delta > 2V$) the wavepacket localizes at long times. It is interesting to mention that at the intermediate critical disorder $\delta = 2V$ ordinary diffusion is obtained and $1/E$ singularity laws hold instead [9]. Similar results have been shown [6] to hold for magnon or phonon propagation in one-dimensional systems with ordinary uncorrelated continuous disorder in the exchange or force constants, respectively.

We have studied the general AA...A, BB...B random alloy, which consists of homogeneous blocks of arbitrary block size m. Our main result is that for weak disorder ($\delta < \delta_c(m)$) delocalized reflectionless modes occur, exactly as for the $m = 2$ 'paired case'. We similarly demonstrate that partial delocalization occurs via a set of strong $1/E^2$ singularities of the localization length around special energies E_0, whose number is proportional to m. Moreover, we are able to obtain the corresponding phase diagram $\delta_c(m)$, which demonstrates the refectionless transmission region.

Our results are obtained by performing a thorough numerical study of the localization length and the density of states (DOS) of the arbitrary m block size binary sequences for different disorder values as a function of the energy. The numerical method relies on the statistical exploration of the product of the corresponding 2×2 random transfer matrices

whose exponential divergence allows computation of the characteristic Lyapunov exponent. A general mathematical formalism for tackling scattering from a large homogeneous block is also presented and particular cases are exactly solved. These solutions define a simple analytical reasoning which can be used to obtain the critical disorder strength $\delta_c(m)$ for any length m and allow the corresponding phase diagram to be determined. The resonances vanish for $\delta > \delta_c(m)$.

The paper is arranged as follows. In section 2 we introduce the model and results for the DOS and the localization length, specializing for convenience to the $m = 5$ site AAAAA, BBBBB fully random alloy case. In order to interpret these results obtained for a fifty–fifty correlated random alloy we present in section 3 exact general expressions for the reflection coefficient from a single m-site impurity block of B sites embedded in the perfect AAA...AAAA infinite chain. These analytical results are displayed for $m = 5$ and $m = 100$ in section 4. In section 5 the way in which the single large-impurity results can be used to identify the localization length singularities for the fully random AA...A, BB...B alloy sequences is shown. The phase diagram, a brief summary of our results and a related discussion, also by considering possible extensions and applications of the model, can be found in section 6.

2. The Lyapunov exponent for the m-site correlated AA...A, BB...B random alloy

We shall discuss a tight-binding Hamiltonian corresponding to the binary m-site AA...A, BB...B random alloy electronic problem. It is expressed by the following simple difference equation:

$$(E - \epsilon_n)c_n = V(c_{n-1} + c_{n+1}) \tag{1}$$

or, equivalently, via the transfer matrix equation

$$\begin{pmatrix} c_{n+1} \\ c_n \end{pmatrix} = \begin{pmatrix} (E-\epsilon_n)/V & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_n \\ c_{n-1} \end{pmatrix} \qquad n = 0, 1, 2, \ldots, N \tag{2}$$

where E is the energy, V the intersite matrix element c_n the wavefunction amplitude on the nth site and the ϵ_ns take the values ϵ_A or ϵ_B at random subject to the correlation requirement that they are distributed in blocks of m sites each. The object of our study is the asymptotic behaviour of the random matrix product $\prod_{n=1,N} \mathbf{M}_n$, where the $\mathbf{M}_n$ are the independent random 2×2 transfer matrices appearing in equation (2). The real part of the Lyapunov exponent is defined as

$$\gamma = \lim_{N\to\infty} \frac{1}{N} \log \frac{|\prod_{n=1,N}^{N} \mathbf{M}_n z(0)|}{|z(0)|} \tag{3}$$

with a generic starting vector condition $z(0) = \binom{c_1}{c_0}$. The corresponding integrated density of states (IDOS) is computed via the negative eigenvalue theorem [13].

The pure bands due to the A and B sites are centred around $E = \epsilon_A$ and $E = \epsilon_B$ and have corresponding bandwidths $|E - \epsilon_A| \leqslant 2V$ and $|E - \epsilon_B| \leqslant 2V$, respectively. We have chosen to display our results by fixing $\epsilon_A = 0$ and varying $\epsilon_B = \delta \geqslant 0$. In figure 1 we present results for the $m = 5$ site binary alloy, that is for the randomly distributed AAAAA and BBBBB blocks of sites with probabilities $p = q = 0.5$. In the logarithmic y-axis scale

of figure 1 it can be seen seen that the localization length diverges at various E_0 values. We find that it does so following the power law $\xi(E) \sim 1/(E-E_0)^2$. This implies the presence of resonances which occur for $\delta \leqslant \delta_c(m)$ and for $m = 5$ we find that $\delta_c(m=5) = 3.618V$. The corresponding DOS can be extracted from the IDOS which is displayed in the same figure. In the region of critical energies the IDOS is the same as for the pure one-dimensional system implying a DOS which obeys the corresponding pure $E^{-1/2}$ singularity law at the edges. We have verified these mentioned singularities for the localization length and the DOS peaks of our figures by performing numerical multiplications of up to 10^8 transfer matrices.

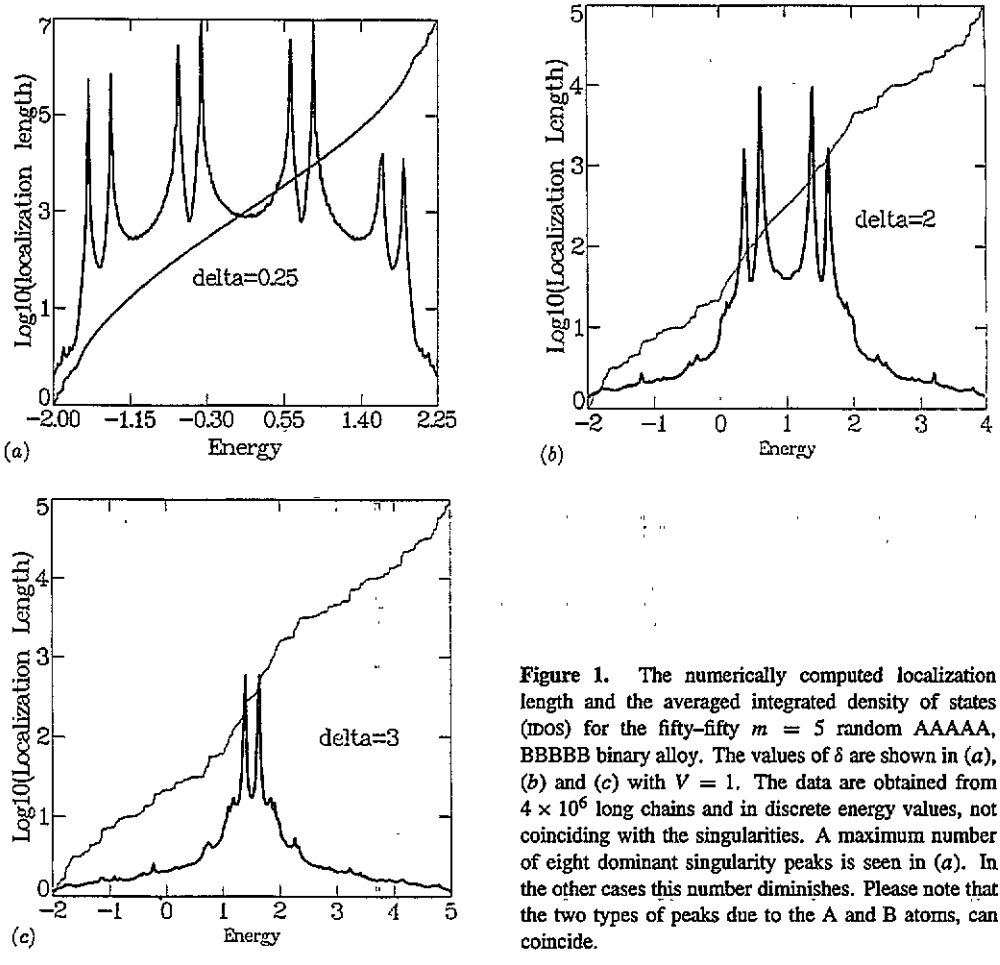


Figure 1. The numerically computed localization length and the averaged integrated density of states (IDOS) for the fifty–fifty $m = 5$ random AAAAA, BBBBB binary alloy. The values of δ are shown in (*a*), (*b*) and (*c*) with $V = 1$. The data are obtained from 4×10^6 long chains and in discrete energy values, not coinciding with the singularities. A maximum number of eight dominant singularity peaks is seen in (*a*). In the other cases this number diminishes. Please note that the two types of peaks due to the A and B atoms, can coincide.

In the general case of arbitrary size m homogeneous impurities we have observed similar singular behaviour which ceases at the critical value $\delta_c(m)$. We have obtained estimates for the ratio $\delta_c(m)/V$, which is zero for $m = 1$ and varies from 2 for $m = 2$ to 4 for $m = \infty$. Moreover, the maximum number of singularities is proportional to $2(m-1)$ for the very small δ values, it decreases for larger $\delta \leqslant \delta_c(m)$ and vanishes for $\delta > \delta_c(m)$. Following the same reasoning as in [6, 9–11] the divergence of $\xi(E)$ for a finite chain of length N implies $\sqrt{N}$ propagating states around $|E| = E_0$ having ξs equal or longer than the system size [9]. It must be pointed out that the results of figure 1 principally concern the disordered ($p = q = 0.5$) binary AAAAA, BBBBB alloy. The position and form of the dominant

singular behaviour is not affected by varying the concentration—only the corresponding intensities change [11].

3. Scattering from a single m-site homogeneous impurity block

In order to understand the results obtained in the previous section for the AA...A, BB...B random alloy we have solved exactly the problem of a single BB...B impurity of size m embedded in an infinite pure A chain. For this purpose the large BB...B homogeneous impurity is placed on the m consecutive sites contained in $n = 0$ to $m - 1$; the rest of the sites being only of the kind A. The corresponding initial conditions in terms of the reflection and transmission coefficients R, T are:

$$c_n = \begin{cases} e^{ikn} + Re^{-ikn} & \text{for } n \leqslant -1 \\ Te^{ikn} & \text{for } n \geqslant m \end{cases} \tag{4}$$

while the amplitudes $c_0, c_1, \ldots, c_{m-1}$ are the solutions of the following equations:

$$(E - \epsilon_B)c_n = V(c_{n-1} + c_{n+1}) \qquad n = 0, 1, 2, \ldots, m-1. \tag{5}$$

The equation for the pure A chain is

$$(E - \epsilon_A)c_n = V(c_{n-1} + c_{n+1}) \qquad n \leqslant -1, n \geqslant m \tag{6}$$

and the energy dispersion without the impurity BB...B is simply $E = \epsilon_A + 2V\cos k$.

From equations (4)–(6) we easily obtain c_0 and c_{m-1}, i.e. the amplitudes on the first and last sites inside the impurity, which are given by

$$c_0 = 1 + R \tag{7}$$

and

$$c_{m-1} = Te^{ik(m-1)} \tag{8}$$

respectively. On the other hand, if equation (5) is written in a transfer matrix form we obtain, for the amplitudes on the last site inside the impurity and the immediate site outside,

$$\begin{pmatrix} c_m \\ c_{m-1} \end{pmatrix} = \begin{pmatrix} (E - \epsilon_B)/V & -1 \\ 1 & 0 \end{pmatrix}^m \begin{pmatrix} c_0 \\ c_{-1} \end{pmatrix} \tag{9}$$

with

$$c_{-1} = e^{-ik} + Re^{ik} \qquad c_m = Te^{ikm} \tag{10}$$

from equation (4). Equation (9) defines the matrix $\mathbf{Q}$

$$\mathbf{Q} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \equiv \begin{pmatrix} (E - \epsilon_B)/V & -1 \\ 1 & 0 \end{pmatrix}^m \tag{11}$$

which has the following symmetry properties:

$$Q_{12} = -Q_{21} \tag{12a}$$

$$\det(\mathbf{Q}) = -1. \tag{12b}$$

Combining equations (7)–(12) we finally obtain a general expression for the reflection probability amplitude:

$$|R|^2 = \frac{(Q_{11} - Q_{22} + 2Q_{12}\cos k)^2}{(Q_{11} - Q_{22} + 2Q_{12}\cos k)^2 + 4\sin^2 k}. \tag{13}$$

We may now apply this formula to obtain results valid for any m.

4. Results for a single 5-site homogeneous impurity

We have obtained complete analytical expressions for scattering from impurities of various sizes m. As an example we choose, again, the case of $m = 5$ to display our results. The calculation is lengthy but the result for the reflection coefficient is simply given by

$$|R|^2 = |A|^2/|B|^2 \tag{14}$$

where

$$A = \delta_-((E(E-2\epsilon_B) - \tfrac{3}{2}V^2 + \epsilon_B^2)^2 - \tfrac{5}{4}V^4) \tag{15}$$

and

$$|B|^2 = A^2 + 4V^{10}\sin^2 k. \tag{16}$$

It can be shown that $|R|^2$ vanishes at the following points:

$$\delta_- = \epsilon_A - \epsilon_B = 0 \tag{17a}$$

$$E_0 = E_{\pm\pm} \equiv \epsilon_B \pm V\sqrt{\tfrac{1}{2}(3 \pm \sqrt{5})}. \tag{17b}$$

The form of the expected singular behaviour is obtained if we expand the corresponding inverse reflection probability near each of the four resonance points E_0. We find

$$\frac{1}{|R|^2} = \frac{|B|^2}{\delta_-^2(E-E_{++})^2(E-E_{+-})^2(E-E_{-+})^2(E-E_{--})^2} \tag{18}$$

where

$$|B|^2 = \sum_{n=0}^{8} \frac{b_n}{n!}(E-E_0)^n. \tag{19}$$

The corresponding coefficients near the point $E_0 = E_{++}$ are: $b_0 = -V^8(\delta_-^2 - 3.2360\delta_- V - 1.3819V^2)$, $b_1 = V^7(2\delta_- V - 3.2360V^2)$, $b_2 = V^6(104.721\delta_-^2 - 2V^2)$, $b_3 = 1103.49\delta_-^2 V^5$, $b_4 = 6123.94\delta_-^2 V^4$, $b_5 = 21476.5\delta_-^2 V^3$, $b_6 = 48459.6\delta_-^2 V^2$, $b_7 = 65239.1\delta_-^2 V$, $b_8 = 40320\delta_-^2$, and if we replace V by $-V$ we obtain the coefficients of the expansion near $E_0 = E_{-+}$. Near the point $E_0 = E_{+-}$ we obtain: $b_0 = -V^8(\delta_-^2 - 1.2360\delta_- V - 3.6180V^2)$, $b_1 = V^8(2\delta_- - 1.2360V)$, $b_2 = V^6(15.2786\delta_-^2 - 2V^2)$, $b_3 = 23.4891\delta_-^2 V^5$, $b_4 = -315.938\delta_-^2 V^4$, $b_5 = -1083.53\delta_-^2 V^3$, $b_6 = 3380.43\delta_-^2 V^2$, $b_7 = 24919.1\delta_-^2 V$, $b_8 = 40320\delta_-^2$, and by replacing V by $-V$ we obtain the coefficients near $E_0 = E_{--}$.

The behaviour of the reflection probability $|R|^2$ for $m = 5$ with $\epsilon_A = 0$, $\epsilon_B = \delta \geqslant 0$ for various choices of δ/V: (a), 0.25; (b), 2; and (c) 3 is shown in figure 2. In figure 3 similar results are shown but for $m = 100$. If m increases further a band of resonances can be seen.

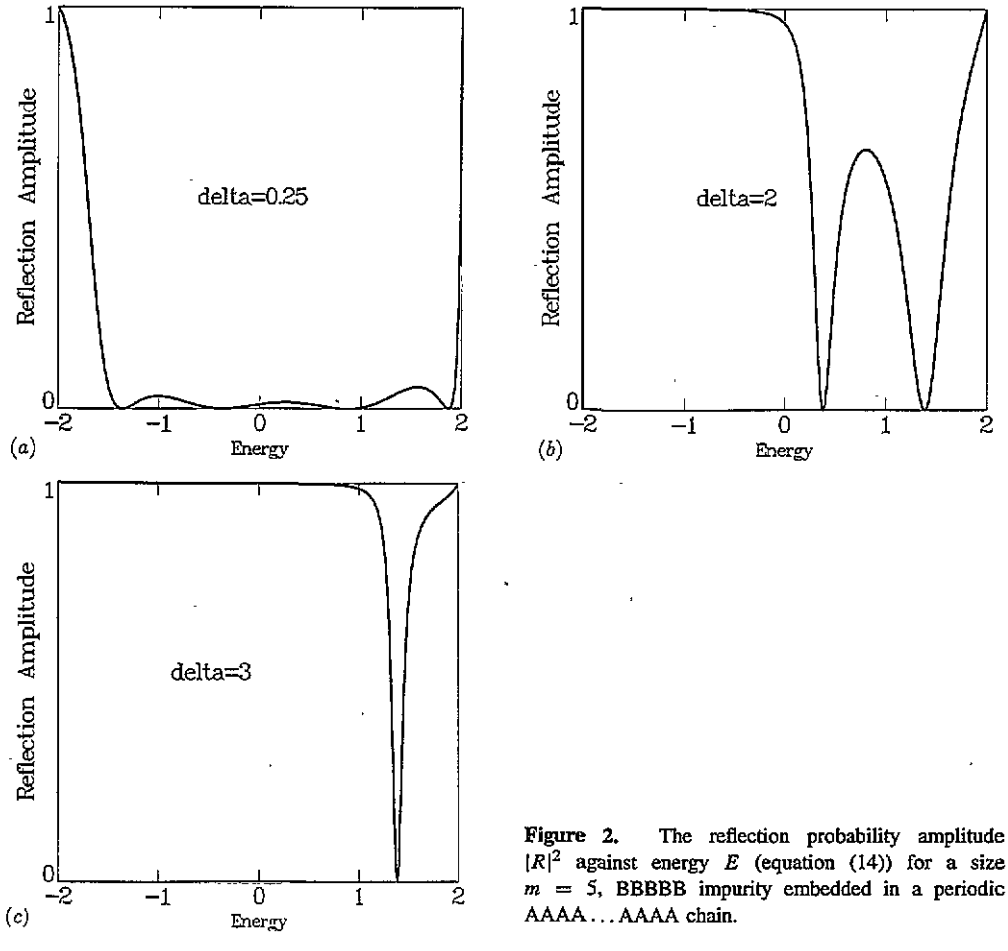
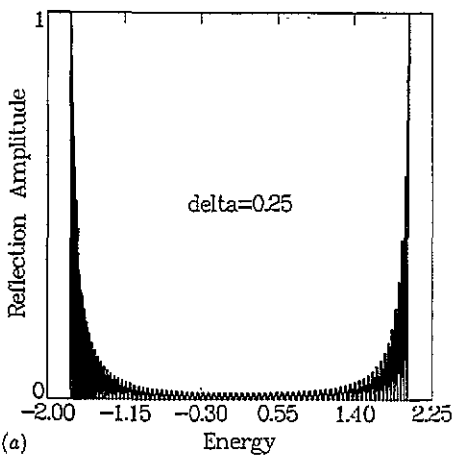


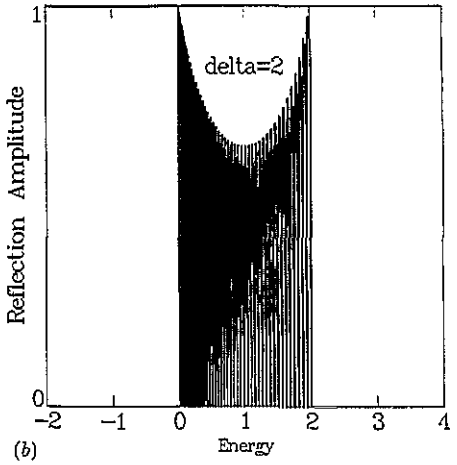
Figure 2. The reflection probability amplitude $|R|^2$ against energy E (equation (14)) for a size $m = 5$, BBBBB impurity embedded in a periodic AAAA...AAAA chain.

5. Comparison between the random AA...A, BB...B alloy and the single BB...B impurity results

The first important result of this paper was the exact solution for scattering from a single large homogeneous impurity block, as presented in the previous sections. The second is recognition of the validity of our single impurity block interpretation for the complete problem of the random m-site AA...A, BB...B alloy. In this section we compare the fully random AA...A, BB...B alloy with the results obtained for a single BB...B homogeneous impurity. We show that the introduction of a percentage of homogeneous BB...B scatterers does not change the perfect transmission abilities of the special modes already present for a single block. This extrapolation is shown to work perfectly well near the energies where the reflectionless modes are found. Therefore, we can conclude the validity of the single large homogeneous scatterer results at any concentration.

In order to demonstrate how the single BB...B block results embedded in the infinite A chain enable us to recover the observed singular behaviour we adopt the expansion of $|R|^{-2}$ from equation (18) in the vicinity of the special zero reflection energies E_0 (equation (17*b*)). The localization length ξ for the fully random block binary alloy is proportional to $[\frac{1}{2}\log(1-|R|^2)]^{-1}$, which for small $|R|^2$ near the special modes becomes $\xi \propto 2/|R|^2$. The effect of the many-impurity blocks on the localization length decreases





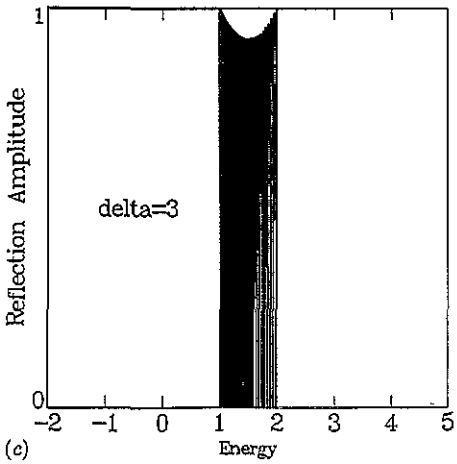


Figure 3. The same as in figure 2 but for $m = 100$. Now, a denser set of singularities can be clearly seen.

the corresponding intensity but not the position and form of the singular laws.

In order to demonstrate our previous conclusion we show in figure 4 the localization length for a random 5-site block alloy, with $p = 0.9$, $q = 0.1$, and various δ/V values. In comparison with figure 1 we observe that the number of singularities remains unaffected except for the fact that some peaks now have a reduced intensity. The dominant intensity modes are due to the minority BB...B blocks embedded in the sea of the A chain. The rest of the peaks belong to the reverse situation, that is of the AA...A blocks embedded in the B chain. From figure 4 we visualize how the results for one BB...B block can expain the localization length for the fully random case by plotting $2/|R|^2$, where $|R|^2$ is obtained in equation (14). The position for the rest of the smaller peaks which appear in figure 4 can also be easily deduced via equation (17*b*) by interchanging the parameters ϵ_A and ϵ_B in the single impurity calculation. We should mention that for some values of δ/V some of the peaks, from the two types of scatterers A and B, can coincide (figure 4). Finally, in the mostly disordered case of $p = 0.5$ and $q = 0.5$ the two types of peaks acquire equal contibutions in intensity.

6. Discussion

We have studied a one-dimensional tight-binding model with binary-alloy-type site

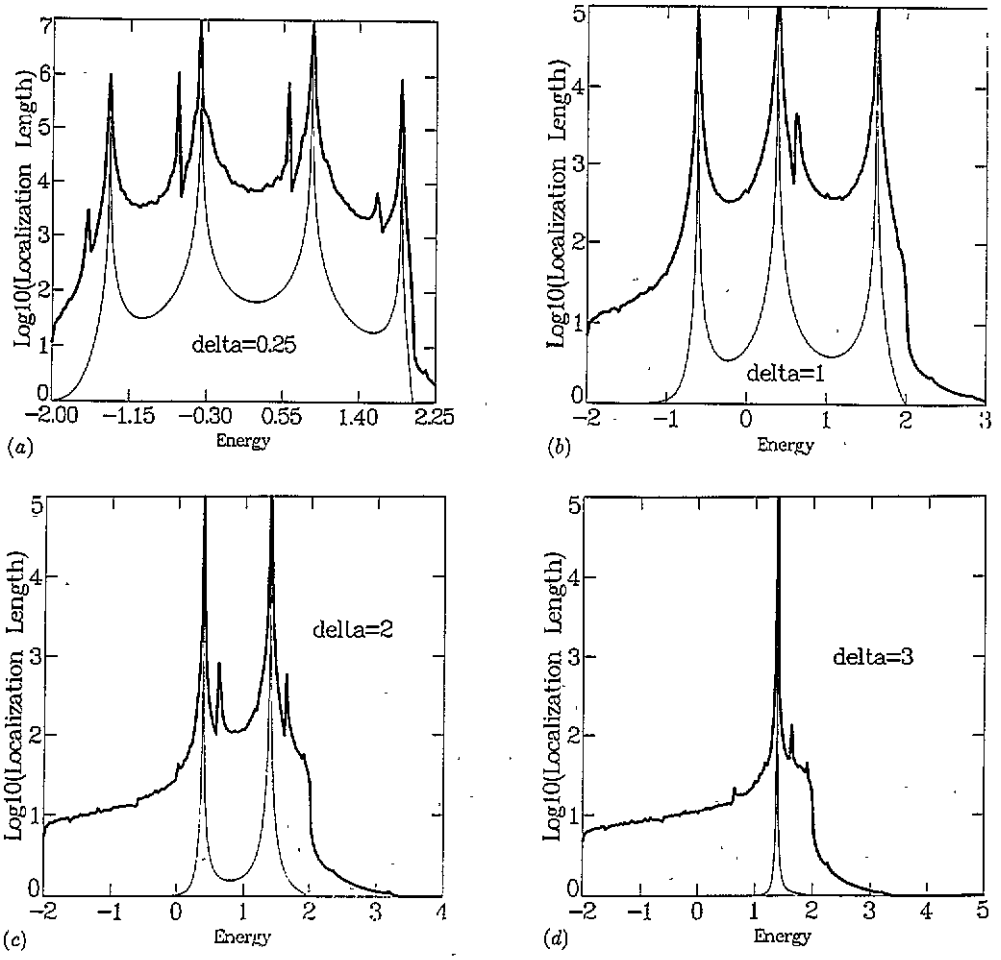


Figure 4. The computed localization length for $m = 5$ but at unequal concentrations of the two species. The AAAAA block occurs with probability $p = 0.9$ and the BBBBB block with $q = 0.1$. The localization length estimated from the single 5-site BBBBB single homogeneous impurity results is also shown by thin lines. A similar type of calculation but for an AAAAA impurity embedded in the BBBB...BBBB chain would reproduce the rest of the weaker peaks in the figure (replacing ϵ_A with ϵ_B in equation (17*b*)).

(diagonal) disorder assigned randomly to every m sites in succession. The need for considering the random distribution of whole words of sites instead of just letters also has a profound significance from a statistical information theory viewpoint, as a means of storing information [14]. We have discussed here the quantum transport properties in these correlated disorder models following recent findings that for words of length $m = 2$ the exhibited behaviour is markedly different from the usual localization picture obtained for $m = 1$.

We have studied the localization length and the DOS for the general large m-long words extending the usual transfer matrix techniques. Our numerical results are displayed both as a function of the energy and the degree of disorder expressed by the difference $\delta = |\epsilon_A - \epsilon_B|$ and show that the localization length displays many $1/E^2$ singularity peaks. The larger the blocks the richer the set of energies where the singularities exist. This singular behaviour corresponds to delocalized states in the band while the rest of the states are localized. The

reason for the partial delocalization is due to the local order introduced via correlation. We obtain a partial explanation of our results by studying scattering from a single impurity block. Although the single large-impurity results should only be valid in the limit where the impurity concentration is close to zero, it turns out that they remain essentially valid at any concentration. The corresponding phase diagram in figure 5 demonstrates the region of the resonance states for an arbitrary length of the blocks.

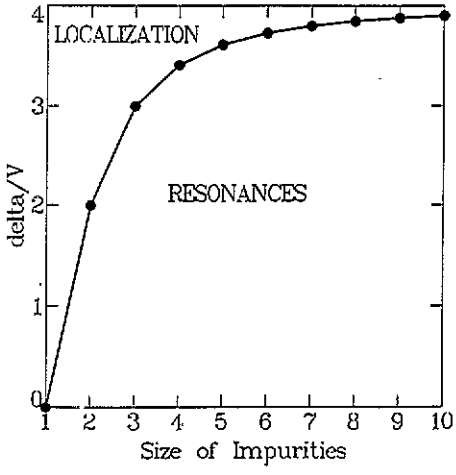


Figure 5. The phase diagram showing the critical $\delta_c(m)/V$ values against the block size m evaluated from the exact results of sections 3 and 4. This diagram holds accurately for arbitrary concentration of the BB...B impurity blocks but is essentailly valid for the random AA...A, BB...B block alloy for any p and q.

It must be mentioned that the strong singular behaviour found in this paper is unrelated to the familiar A, B alloy behaviour at energies where the DOS vanishes and the localization length is weakly singular. It must also be stressed that, although the present study has been limited to the binary distribution, we expect similar results for any arbitrary discrete distribution. Our results can easily be extended to account for a generalized model where the two species have different arbitrary sizes m_A and m_B, respectively. It is obvious that if one of the species has a length equal to one there will be no peaks due to the corresponding atoms. For instance if $m_A = 1$ and $m_B \geqslant 2$ the peaks will only be due to the B blocks. If $m_A \geqslant 2$ and $m_B \geqslant 2$ peaks due to both types will appear in numbers according to their m values. In models with a smooth distribution of the site energies, another type of singular behaviour in the band is expected as shown in [15]. In fact, the complicated invariant measure and the perturbation theory techniques derived for continuous models enabled the localization length and the DOS near the special energies for the 'paired' $m = 2$ random alloy to be calculated [15]. However, our straightforward approach is much simpler and, as shown in this paper, extendable to any length m of the impurities.

In summary, we focused on the conditions under which partial delocalization occurs for weakly disordered 'block correlated' random binary alloys via dominant $1/E^2$ singularities of the localization length. In the present study accurate numerical results demonstrate that if $\delta < \delta_c(m)$ partial delocalization exists, a critical situation is expected for $\delta = \delta_c(m)$ and ordinary localization is obtained if $\delta > \delta_c(m)$. We have further estimated $\delta_c(m)$ for large homogeneous impurities at any concentration. Preliminary studies have also shown that the reflectionless modes are responsible for a superdiffusive quantum wavepacket transport at long times, as was found for $m = 2$ in [9]. In the range of possible applications for our results the properties of one-dimensional conductors, such as polyaniline, as well as molecular beam epitaxy grown structures consisting of random and quasi-periodic mixtures could be included. We can also consider propagation in a medium containing large-size

impurities where the novel effects discussed above should appear as a result of the introduced short-range spatial correlations. Many other interesting questions still remain in this area with the most obvious being the extension of our study of a binary alloy in the presence of short-range order to higher dimensions.

Acknowledgments

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