Localization in paired correlated random binary alloys

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(Received 14 April 1992; revised manuscript received 20 January 1993)

We study both analytically and numerically the electronic structure and the transport properties of binary chains, when the site energies (ϵ_A or ϵ_B) are random in pairs. We compute the density of states and the localization length versus energy for various strengths of disorder by considering products of 2×2 random matrices in the microcanonical ensemble and also within the usual canonical-ensemble method. The limiting cases of AA,BB correlation, which favor delocalization and AB,BA anticorrelation, which favor localization, as well as intermediate cases involving all pairs AA,AB,BA,BB at random, are distinguished. In the former case, if $\delta=|\epsilon_A-\epsilon_B|$ is less than a critical value $\delta_c=2$, we demonstrate that the density of states has a smooth part and associated dominant $1/E^2$ divergencies of the localization length which for $\delta=\delta_c$ become $1/E$. Our results are explained by considering scattering from single-impurity pairs. The microcanonical-ensemble method is discussed and its limitations are pointed out.

I. INTRODUCTION

There is intensive current interest concerning questions of wave propagation in disordered lattices which is related to the search for optical or acoustic wave localization.[1,2] The well-studied case of electronic systems with independent site (or bond) disorder[3] does not fully cover all cases of such wavelike excitations (light, magnons, phonons, etc.) propagating in the continuum, the new feature being the presence of disorder correlations. As a consequence of correlations for the electronic Anderson model in the tight-binding approximation[3] short-range order is introduced, which implies that the lattice site energies are no longer independent random variables, as usual, but they relate to the corresponding energies of their neighbors within a correlation length. So far, little attention has been paid to disorder correlations where interesting phenomena are expected to appear. For example, although Anderson localization[3-6] is present in one dimension, even for an infinitesimal amount of disorder, in the presence of correlations partial delocalization may arise. This phenomenon is also familiar from corresponding magnon or phonon studies where delocalization is expected at long wavelengths even in one dimension.[7] The present study focuses on random chains with a discrete (binary) correlated distribution of the random potential. A binary potential is suggested from physical wavelike propagation phenomena in a medium containing objects, for example, hard spheres, of different density.

We introduce a "paired" model of correlation which implies that two sites A and B are involved in a single unit cell. Therefore, in order to create the chain instead of A and B, the AA, AB, BA, and BB are distributed at random, with corresponding probabilities P_{AA}, P_{AB}, P_{BA}, and P_{BB}. This simple model of correlation for the case of $P_{AB}=P_{BA}=0$ implies that the corresponding energies ϵ_A and ϵ_B are randomly assigned at every two sites in succession. Such an AA,BB random alloy may be also regarded as a first step for considering propagation in a medium containing impurities of various sizes. In the opposite case, where the AB and BA are distributed at random, the potential is not smooth but two-valued (ϵ_A and ϵ_B) within the unit cell. Our choice of correlation can be contrasted with previous studies[8,9] of first-order Markovian correlated binary one-dimensional systems. In that case, apart from the usual occupation probability P_A ($P_B=1-P_A$), in order to specify correlation an additional parameter had to be defined. The results of Ref. 9 exhibit the role of correlation for weak disorder and are successfully compared to a quasiuniversal theory of localization.

Interesting results for the AA,BB random alloy were recently obtained from the quantum dynamics viewpoint. An initially localized wave packet displays superdiffusion at long times[10] while certain eigenstates have diverging localization lengths. The superfast type of diffusion obeys a $t^{3/2}$ law for the mean-squared displacement of the wave packet and occurs only if the difference in the site energies $\delta=|\epsilon_A-\epsilon_B|$, which measures the strength of the disorder, is less than a critical value $\delta_c=2V$, where $V=1$ is the corresponding hopping matrix element. In the strongly disordered case $\delta>\delta_c$, instead, the wave packet is localized at long times, while for $\delta=\delta_c$ ordinary diffusion is obtained.[10] Similar results have been obtained for magnon propagation in random one-dimensional systems.[7] Superdiffusion with a variable exponent occurs for hierarchical (or more generally power-law) distribution of the hopping probabilities.[11,12] The general characteristic of all these systems is a kind of phase transition from localization to anomalous diffusion with normal diffusion occurring only at the critical point.

We consider the localization properties of the model by determining the corresponding electronic structure and the quantum transport quantities. They are derived by exploring the statistics of the product of the corresponding 2×2 random transfer matrices. The exponential divergence of this product allows the estimation of the

characteristic Lyapunov exponent and its real and imaginary parts give the inverse localization length and the density of states (DOS), respectively. The analytical determination of the Lyapunov exponent remains a very difficult task, although perturbational results[5,6,13] and for special cases[14] analytical expressions are possible. In one dimension for independent site-diagonal randomness, chosen from a continuous distribution, there is always a positive Lyapunov exponent corresponding to a finite localization length.[5,6] For the binary-alloy site-diagonal randomness considered here the Lyapunov exponent can go to zero and due to the discrete potential is, in general, a nondifferentiable function of the energy.[15,16] We do not expect any singular behavior in models with a smooth distribution of the site energies.[6]

We also employ an analytical formula for the evaluation of the Lyapunov exponent recently derived.[14] It exploits the fact that the corresponding transfer matrices are of two types, A and B, and appear in the product with probability p and $q=1-p$, respectively. Therefore a microcanonical-ensemble average can be defined, where the number of type-A and type-B matrices is not allowed to vary from sample to sample.[14] This implies that in the different realization of the product of N matrices are involved exactly pN matrices of type A and qN matrices of type B. The microcanonical-ensemble average includes, of course, the fluctuations due to the random positions of the A and B types of matrices in the product. In this paper we examine the usefulness of this appealing Deutsch and Paladin[14] method, when applied to the correlated case.

Using both the above methods we have carried out a thorough study of the DOS and the localization length as a function of energy for different disorder values. In the case of the AA,BB random sequence our main result is that the DOS has a smooth part corresponding to delocalized states. In this case, although the majority of states are localized, transport is expected at special energies. On the contrary, for the case of anticorrelation, that is, when AB,BA are randomly distributed ($P_{AA}=P_{BB}=0$) or for the more complicated case involving all four pairs AA, AB, BA, and BB at random, our results are consistent with localization for every energy and degree of disorder.

The paper is arranged as follows. In Sec. II we present the model and the formalism of the two methods we used. In Sec. III we present results of the DOS and the localization length for the AA,BB random-alloy case. For weak disorder ($\delta<\delta_c$) we demonstrate partial delocalization via the presence of $1/E^2$ singularities of the localization length and a corresponding partially pure DOS. We also present results within the microcanonical-ensemble method and some limitations of the method are pointed out. In Sec. IV we consider the general AA, AB, BA, and BB alloy cases. In Sec. V expressions for the reflection coefficient from single-impurity pairs are presented which are used to identify the localization-length singularities for the paired-alloy model. A brief summary of our results and a related discussion considering possible extensions of the correlated model can be found in Sec. VI.

II. RANDOM MATRIX PRODUCT AND THE LYAPUNOV EXPONENT

We shall discuss a tight-binding Hamiltonian corresponding to the binary-alloy electronic problem which is expressed by the simple difference transfer matrix equation

$$\begin{bmatrix} c_{n+1} \\ c_n \end{bmatrix} = \begin{bmatrix} \frac{E-\epsilon_n}{V} & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} c_n \\ c_{n-1} \end{bmatrix}, \quad n=0,1,2,\ldots,N , \tag{1}$$

where E is the energy and c_n the wave-function amplitude on the nth site. The ϵ_n's take the value ϵ_A or ϵ_B at random, subject to the correlation requirement that they are distributed in pairs. The four pairs AA, AB, BA, and BB have corresponding probabilities P_{AA}, P_{AB}, P_{BA}, and P_{BB} of occurring in the chain. The object of our study is the asymptotic behavior of the random matrix product $\prod_{n=1,N}^{N}\mathbf{M}_n$, where the $\mathbf{M}_n$ are independent random 2×2 matrices. The corresponding real part of the Lyapunov exponent is defined as

$$\gamma=\lim_{N\to\infty}\frac{1}{N}\ln\frac{\left|\prod_{n=1}^{N}\mathbf{M}_n z(0)\right|}{|z(0)|} , \tag{2}$$

with a generic starting vector condition

$$z(0)=\begin{bmatrix} c_1 \\ c_0 \end{bmatrix} .$$

The Lyapunov exponent γ is a random quantity and apart from the usual numerical calculation its mean value can also be computed by taking averages on the microcanonical ensemble, as suggested in Ref. 14. In this case only the position of the A's and B's is allowed to fluctuate. For the uncorrelated alloy model with A and B drawn from a Bernoullian distribution with probabilities $p=P_A$ and $q=1-p=P_B$ the corresponding transfer matrices are

$$\mathbf{M}_n=\begin{bmatrix} \frac{E-\epsilon_n}{V} & -1 \\ 1 & 0 \end{bmatrix} , \tag{3}$$

where $n=A$ or B, that is, $\epsilon_n=\epsilon_A$ or ϵ_B, respectively. The Lyapunov exponent is subsequently given by the formula

$$\bar{\gamma}(p)=q\ln(q)+p\ln(p)+\ln\lambda_1(\bar{x})-q\ln(\bar{x}) , \tag{4}$$

where the saddle point $\bar{x}$ is derived from the equation

$$\bar{x}\frac{\partial\lambda_1(\bar{x})}{\partial\bar{x}}=q\lambda_1(\bar{x}) \tag{5}$$

and the function $\lambda_1(\bar{x})$ is determined from the largest eigenvalue of the matrix $\mathbf{M}_A+\mathbf{M}_B x$.

For the paired correlated problem the corresponding matrix expressions are obtained by multiplying the two

consecutive type-A or type-B matrices together. Four different matrices should be involved, which reduce to two in the limiting cases of the AA,BB ($P_{AB}=0$, $P_{BA}=0$) or the AB,BA ($P_{AA}=0$, $P_{BB}=0$) random alloys, respectively. For the AA,BB random alloy with $p=P_{AA}$ and $q=1-p=P_{BB}$, respectively, the matrices are

$$\mathbf{M}_{AA}=\begin{bmatrix} \left[\frac{E-\epsilon_A}{V}\right]^2-1 & -\left[\frac{E-\epsilon_A}{V}\right] \\ \frac{E-\epsilon_A}{V} & -1 \end{bmatrix}, \tag{6}$$

$$\mathbf{M}_{BB}=\begin{bmatrix} \left[\frac{E-\epsilon_B}{V}\right]^2-1 & -\left[\frac{E-\epsilon_B}{V}\right] \\ \frac{E-\epsilon_B}{V} & -1 \end{bmatrix}. \tag{7}$$

The real part of the Lyapunov exponent via Eq. (2) gives directly the inverse localization length following a well-established approach (see, e.g., Ref. 5). It relies on the application of Furstenberg's theorem,[6] which guarantees self-averageability, so that for very long chains γ converges to its mean value. The DOS was subsequently more conveniently computed using an eigenvalue counting theorem,[17] which gives directly the integrated density of states (IDOS). The DOS can be obtained in a histogram form by differentiating the corresponding IDOS, using a finite-energy step.

III. CORRELATED AA,BB ALLOY: THE DOS AND THE LOCALIZATION LENGTH

A. Usual canonical-ensemble method

The bands due to the pure A and B sites are centered around $E=\epsilon_A$ and $E=\epsilon_B$, and the corresponding band-

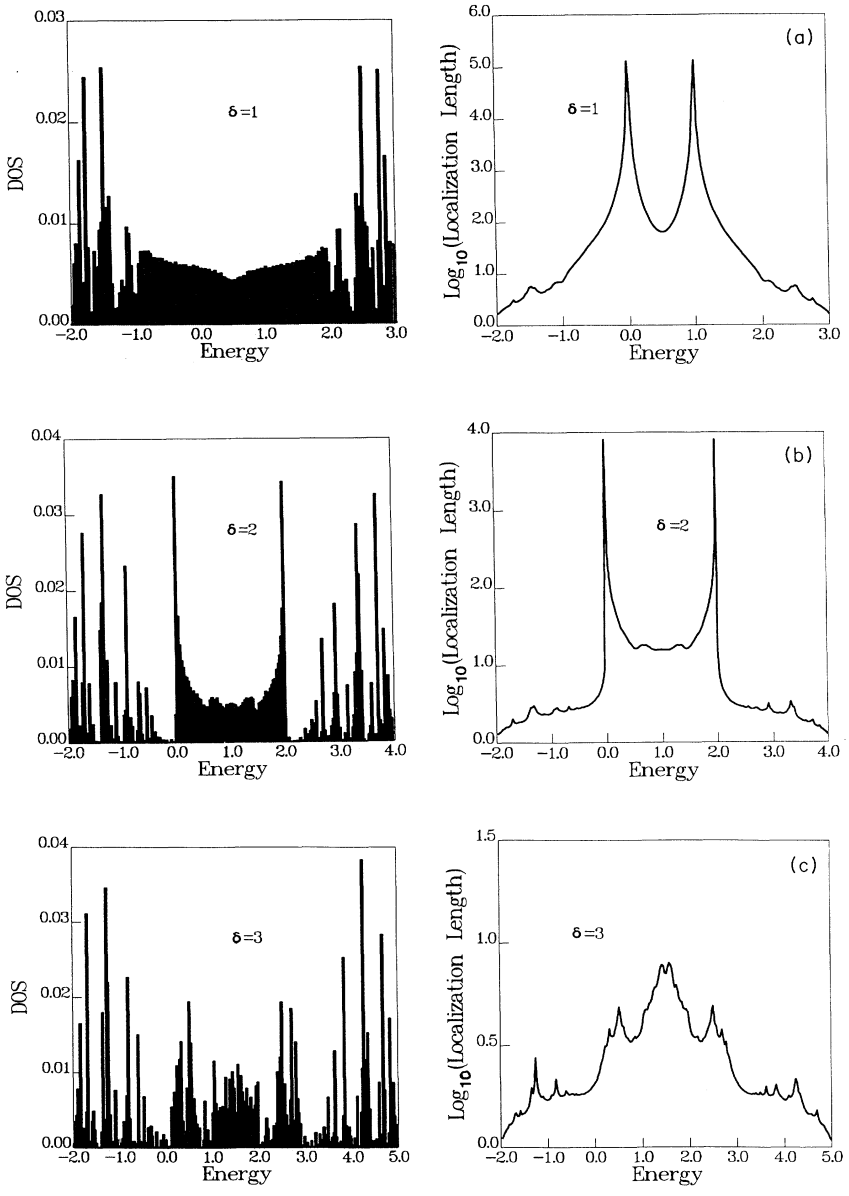

FIG. 1. The numerically computed averaged density of states (DOS) and the localization length for a random AA,BB correlated binary alloy with $P_{AA}=P_{BB}=0.5$ for the three δ values shown in (a), (b), and (c). The data are obtained from 4×10^6 long chains and in discrete energy values, not coinciding with the singularities. It should be stressed that the two dominant singularity peaks occur at the pure A and B band centers $\epsilon_A=0$ and $\epsilon_B=\delta$, respectively.

widths are $|E-\epsilon_A| \leq 2V$ and $|E-\epsilon_B| \leq 2V$, respectively. If we consider the AA,BB-ordered alloy with various $\delta=|\epsilon_A-\epsilon_B|$ values a four-band spectrum is obtained by

$$E=\tfrac{1}{2}(\delta_+ \pm \{\delta_-^2+8V^2 \pm 4V[\delta_-^2+4(1+\sin^2 2k)V^2]^{1/2}\}^{1/2}) , \quad (8)$$

with $\delta_\pm=\epsilon_A \pm \epsilon_B$. The two middle bands contain ϵ_A and ϵ_B only if $\delta \leq 2V$. For $\delta=2V$ the outerband edges of these bands coincide with ϵ_A and ϵ_B, while for $\delta>2V$ they move inside the energy range defined by ϵ_A and ϵ_B. The first and the fourth bands are always outside these special energies.

The random AA,BB binary alloy has a drastically different band structure (see Fig. 1). We display our results making the choice of a constant $\epsilon_A=0, V=1$ and a varying $\epsilon_B=\delta \geq 0$. We observe that the two outside bands of the periodic AA,BB alloy split into localized states while the two middle bands join together into one band, which splits only if $\delta>2$. We find that the localization length diverges at $E=\epsilon_A$ or ϵ_B as $\xi(E) \sim 1/E^2$ for $\delta<2$ [Fig. 1(a)]. The DOS at these energies is smooth, the same as for the pure system. Exactly at $\delta=2$ [Fig. 1(b)] the localization length is still singular but we encounter a $\xi(E) \sim 1/E$ singularity instead while the DOS in this case obeys the corresponding pure band edge $E^{-1/2}$-singularity law. The localization-length singularity becomes weaker than $1/E$ and the DOS is also highly divergent for $\delta>2$, implying localized states [Fig. 1(c)]. It must also be pointed out that the values of the localization length seen in the logarithmic scale of Fig. 1(a) are much higher than the values of Fig. 1(c).

We have verified the above-mentioned singularities at the localization length and the DOS peaks of our figures by performing additional numerical multiplications of up to 10^8 transfer matrices. For $\delta<2$, due to the divergence of $\xi(E)$, for a finite chain of length N the states around $|E|=0$ have ξ's equal to or longer than the system size. These propagating states lie in a window $\Delta E \sim 1/\sqrt{N}$ around the special energies and their number is proportional to $\sqrt{N}$.[10]

The results of Fig. 1 concern the mostly disordered $p=q=0.5$ binary AA,BB alloy. In order to see what is the effect of varying the concentration on this behavior we show more results in Fig. 2 for $\delta=2$ and $p=0.9$, $q=0.1$. We observe that the variation of the concentration does not affect the position and the form of the dominant singular behavior, only its intensity. The peaks at ϵ_A and ϵ_B occur now according to the occupation probability of AA and BB.

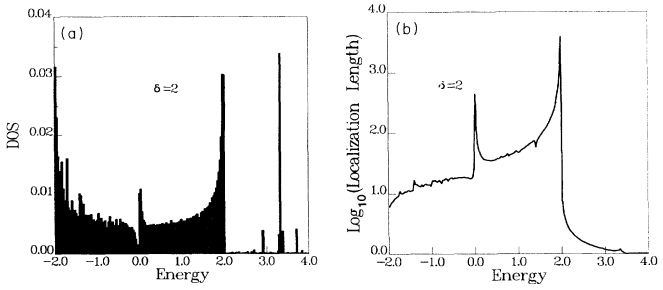

FIG. 2. The numerically computed (a) averaged DOS and (b) the localization length for $\delta=2$ with $P_{AA}=0.9$ and $P_{BB}=0.1$

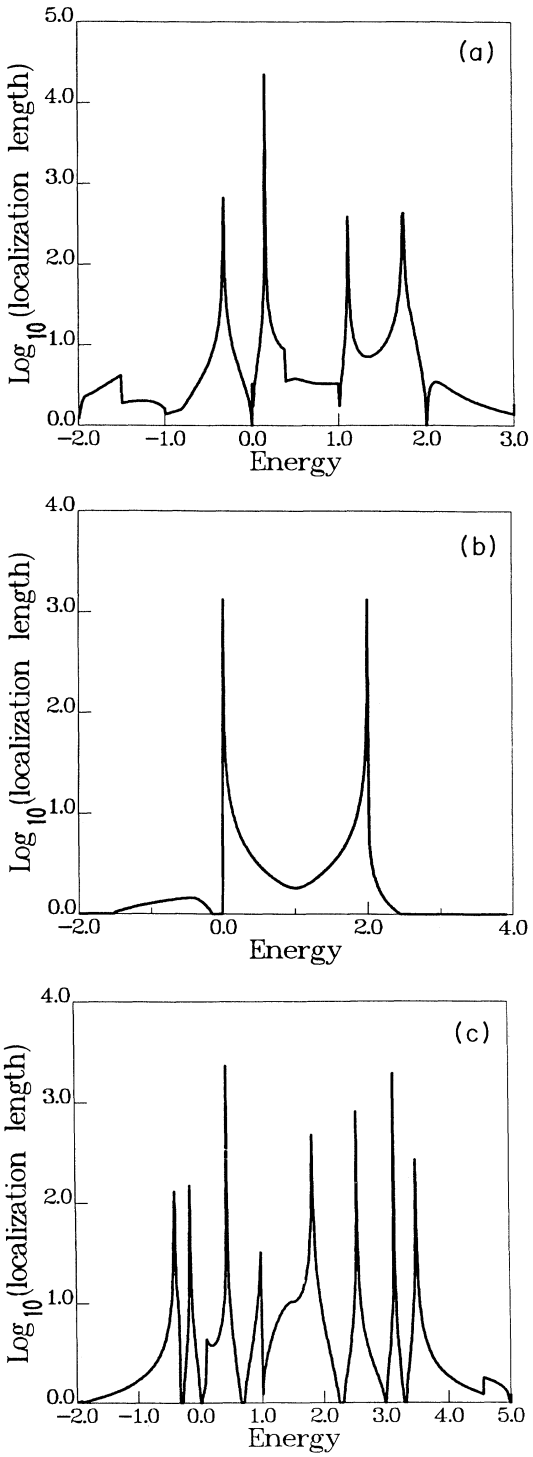

FIG. 3. The analytical results using the microcanonical-ensemble method for the localization length corresponding to Fig. 1.

B. Microcanonical-ensemble method

We have also derived results via the microcanonical method. In Fig. 3 we show results for the localization length corresponding to Fig. 1. It can be seen that they are in good qualitative agreement with Fig. 1. We also show the localization length for different concentrations of the AA's and BB's in Fig. 4. In Fig. 4(a) $\delta=2$, $p=0.1$, and $q=0.9$ and in Fig. 4(b): $\delta=2$, $p=0.9$, and $q=0.1$; the case in Fig. 4(b) corresponds to Fig. 2(b). Again, the agreement is good.

It must be stressed here that the microcanonical method of Ref. 14 is approximate. The authors of Ref. 14, in deriving Eq. (4) for the A,B random binary alloy, have used the following two assumptions: (a) the matrices $\mathbf{M}_A$ and $\mathbf{M}_B$ commute; and (b) the elements of the matrix $\mathbf{D}(x)$ defined by

$$\mathbf{D}(x)\equiv\lambda_1^{-N}(x)(\mathbf{M}_A+x\mathbf{M}_B)^N \tag{9}$$

or

$$\mathbf{D}(x)\equiv\lambda_1^{-N}(x)\mathbf{S}\begin{bmatrix}\lambda_1^N(x) & 0\\ 0 & \lambda_2^N(x)\end{bmatrix}\mathbf{S}^{-1} \tag{10}$$

are of order ~ 1 which implies that the eigenvalues λ_1 and λ_2 are nondegenerate, that is, $|\lambda_1|>|\lambda_2|$. Matrix $\mathbf{S}$ in Eq. (10) is given by

$$\mathbf{M}_A+x\mathbf{M}_B=\mathbf{S}\begin{bmatrix}\lambda_1(x) & 0\\ 0 & \lambda_2(x)\end{bmatrix}\mathbf{S}^{-1}\,. \tag{11}$$

In this paper we access the validity of only the first of the above two assumptions (see also Ref. 18), estimating the corresponding error. An investigation of the second assumption and a more accurate expression for $\tilde{\gamma}(p)$ may be considered elsewhere.

The error due to assumption (a) is simply the difference given by the commutator between the two transfer matrices involved. For the paired AA,BB model this difference $\Delta\equiv\mathbf{M}_A\mathbf{M}_B-\mathbf{M}_B\mathbf{M}_A$ becomes

$$\Delta=(\epsilon_A-\epsilon_B)(E-\epsilon_A)(E-\epsilon_B)\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}. \tag{12}$$

Then Δ is small when δ is small or the energy E is close to ϵ_A or ϵ_B. These conditions are not always satisfied when the dependence of $\tilde{\gamma}(p)$ on the full energy spectrum is considered. Our results, using the microcanonical approach (Figs. 3 and 4) for low δ and near the band center rather than close to the band edges, should be in better agreement with the corresponding accurate values of Figs. 1 and 2, due to the lower values for the matrix elements of Δ there. From the results displayed in this section it can be concluded that the microcanonical-ensemble method can be regarded as a useful working approximation in most cases. Using the microcanonical method we show in Fig. 5 the expected $1/E$ localization-length singularity for the AA,BB random alloy when $\delta=2$.

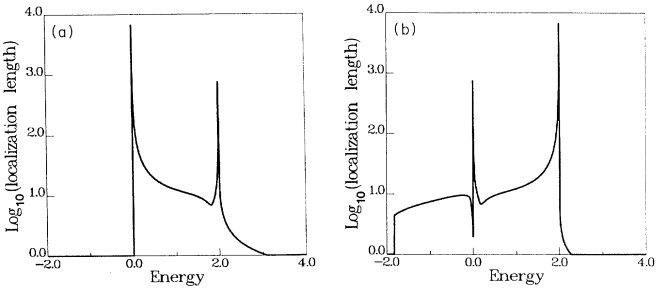

FIG. 4. (a) $P_{AA}=0.1$ and $P_{BB}=0.9$ and (b) $P_{AA}=0.9$ and $P_{BB}=0.1$; (b) corresponds to Fig. 2(b).

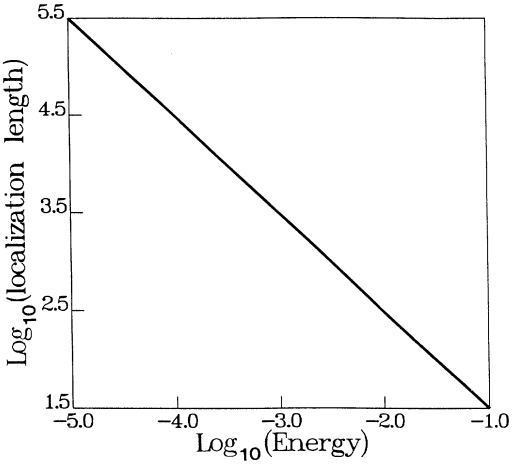

FIG. 5. The singularity of the localization length $\xi(E)\sim 1/E$ for $\delta=2$ and E close to zero, obtained by the microcanonical-ensemble method, is demonstrated in a $\log_{10}$-$\log_{10}$ plot as a straight line with slope 1.

IV. ANTICORRELATED AB,BA AND THE GENERAL AA, AB,BA,BB RANDOM ALLOYS

In this section we report results for the general four-component correlated random binary alloy, employing the usual canonical-ensemble method. We start in Fig. 6 with the strongly anticorrelated AB,BA alloy case ($P_{AA}=P_{BB}=0.0$, $P_{AB}=P_{BA}=0.5$). The corresponding DOS displays a two-band structure with a band gap of width which increases proportionally to δ. From the low localization-length values seen in Fig. 6 the localization of all the states is depicted. At the special energies ϵ_A and $\epsilon_B=\delta$ the localization-length distribution shows peaks indicating weak singularities always expected in alloys[16] but unable to produce transmitting wave modes, such as those of Figs. 1(a) and 1(b).

In Fig. 7 the numerically computed average DOS and the localization length with $P_{AA}=P_{BB}=0.475$ and $P_{AB}=P_{BA}=0.025$ is shown. This case is close to the AA,BB correlated case of Fig. 1. In Fig. 8 results for the opposite limit $P_{AA}=P_{BB}=0.025$ and $P_{AB}=P_{BA}=0.475$ are shown, a case closer to the anticorrelation of Fig. 6. In comparing Fig. 8 with Fig. 6 we see that by introducing a percentage of AA,BB sites states are distributed inside the gap. For completeness, in Fig. 9 an intermediate

asymmetric distribution with $P_{AA}=0.5$ and $P_{AB}=P_{BA}=0.25$ is demonstrated.

V. SCATTERING FROM SINGLE-IMPURITY PAIRS

We found that most of our results can be explained by considering a single-impurity pair between two semi-infinite pure chains of the dominant pair type. The difference equation, also responsible for Eq. (1), is

$$(E-\epsilon_n)c_n=V(c_{n-1}+c_{n+1}) , \tag{13}$$

and was studied in Ref. 10 when two consecutive B impurities are contained in sites $n=0$ and 1, the rest of the sites being only of kind A. Using the initial conditions

$$c_n=\begin{cases} Te^{ikn} & \text{for } n\geq 1 \\ e^{ikn}+Re^{-ikn} & \text{for } n\leq -1 , \end{cases} \tag{14}$$

where T and R are the transmission and reflection coefficients, respectively, the expression

$$|R|^2=\frac{\delta_-^2(\delta_-+2V\cos k)^2}{\delta_-^2(\delta_-+2V\cos k)^2+4V^4\sin^2 k} , \tag{15}$$

was obtained.[10] The energy dispersion without the impurity BB is simply $E=\epsilon_A+2V\cos k$. From Eq. (15) we obtain zero reflection at $E=\epsilon_B$.

The behavior of the transmission probability $|R|^2$ with $\epsilon_A=0$, $\epsilon_B\geq 0$, $\delta=|\epsilon_A-\epsilon_B|=|\delta_-|$ and for the three cases (a) $\delta=1$, (b) $\delta=2$, and (c) $\delta=3$ is shown in Fig. 10. If we expand $|R|^{-2}$ near ϵ_B we obtain

$$\frac{1}{|R|^2}\simeq\frac{V^2(4V^2-\delta_-^2)/\delta_-^2}{(E-\epsilon_B)^2}+\frac{2V^2/\delta_-}{(E-\epsilon_B)}+\frac{\delta_-^2-V^2}{\delta_-^2} . \tag{16}$$

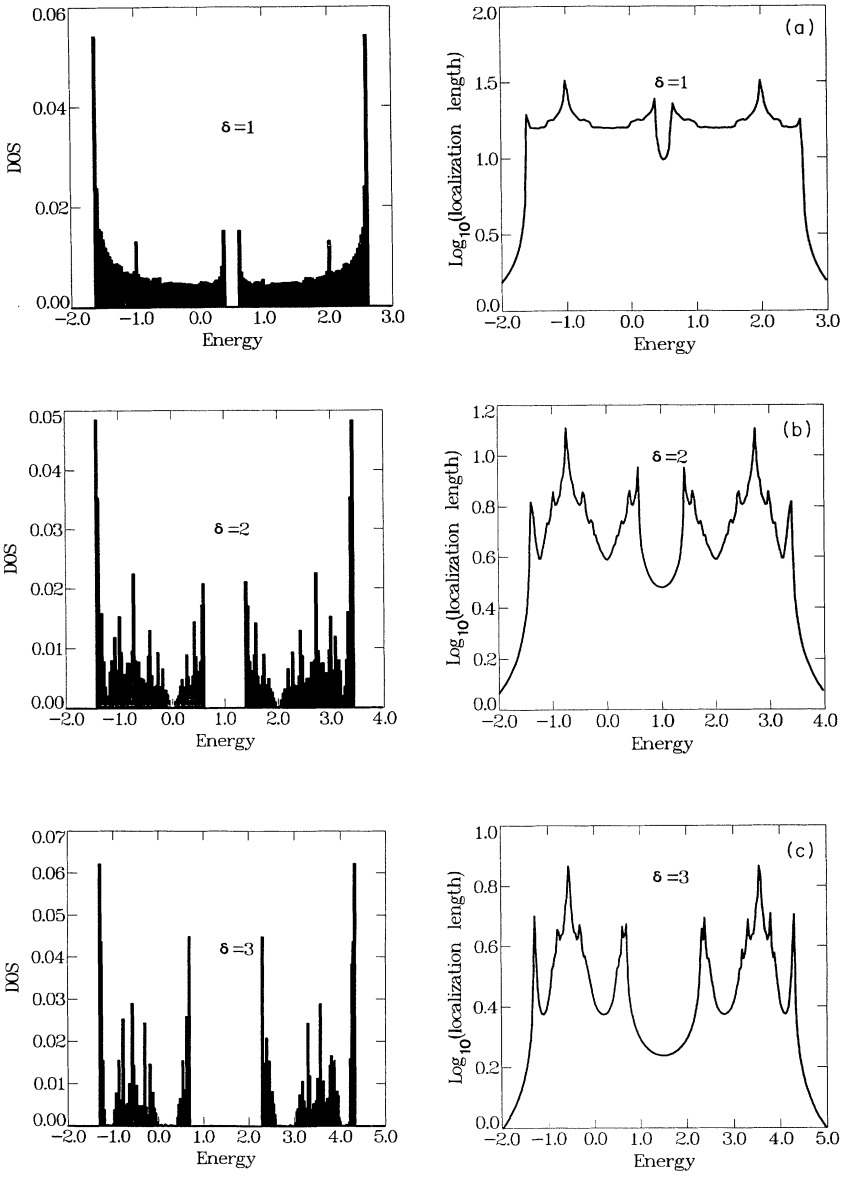

FIG. 6. The numerically computed averaged DOS and the localization length for the anticorrelated AB,BA alloy case of $P_{AA}=P_{BB}=0.0$ and $P_{AB}=P_{BA}=0.5$.

Moreover, from the behavior of $|R|^{-2}$ in the vicinity of this special zero reflection energy the localization length ξ for the AA,BB random binary alloy at $E=\epsilon_A,\epsilon_B$ can be determined. It is expected that ξ should be proportional to $[\frac{1}{2}\ln(1-|R|^2)]^{-1}$, which for small $|R|^2$ becomes

$$\xi=\frac{4}{|R|^2}\ , \tag{17}$$

using also an extra factor of 2 because of the pair correlation. From Eqs. (16) and (17) it can be seen that the first term responsible for the $1/E^2$ singularity dominates only for $\delta<2$. Precisely at $\delta=2$ the first term of Eq. (16) vanishes and the singularity is of the form $1/E$. We have verified these exact singular forms for the AA,BB random alloy by multiplying 10^8 transfer matrices (see also the demonstration of Fig. 5 for $\delta=2$).

We have also studied the anticorrelated AB,BA case discussed in the preceding section. In the limit of the ordered AB chain with just a single paired impurity BA in the middle, the initial conditions become

$$c_{2n}=\begin{cases} T_A e^{ik2n} & \text{for } n\geq 1 \\ e^{ik2n}+R_A e^{-ik2n} & \text{for } n\leq -1 \end{cases} \tag{18}$$

and

$$c_{2n+1}=\begin{cases} T_B e^{ik(2n+1)} & \text{for } n\geq 1 \\ e^{ik(2n+1)}+R_B e^{-ik(2n+1)} & \text{for } n\leq -1\ . \end{cases} \tag{19}$$

T_A,R_A and T_B,R_B are the transmission and reflection

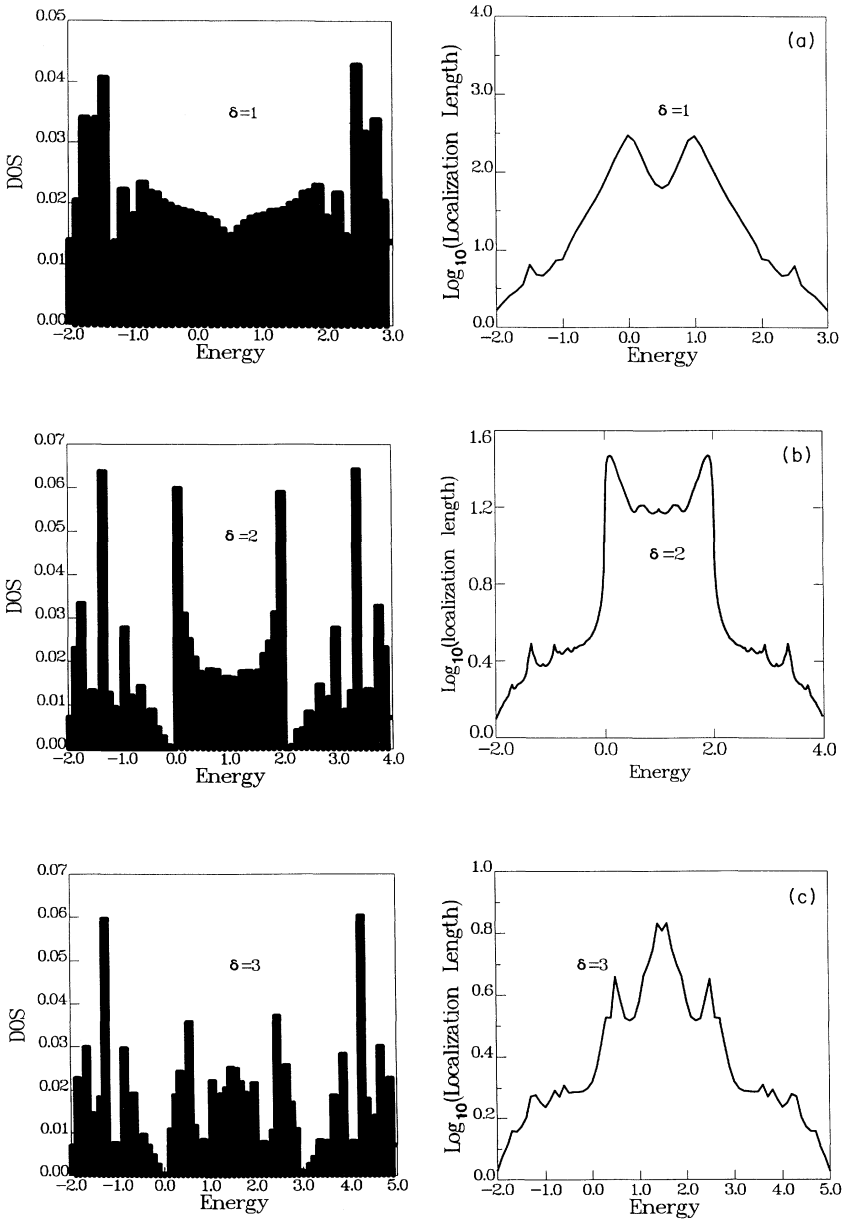

FIG. 7. The numerically computed averaged DOS and the localization length for the general AA,BB,AB,BB alloy with $P_{AA}=P_{BB}=0.475$ and $P_{AB}=P_{BA}=0.025$.

amplitudes on A and B sites, respectively. The impurity pair, consisting of B and A, is located at sites 0 and 1 and in the rest the periodic chain consists of alternatingly placed A's and B's. Inserting Eqs. (18) and (19) into the appropriate difference equations for the sites $-2,-1,0,1,2,3$, we can eliminate c_0 and c_1. After a rather tedious calculation we finally obtain for the reflection probabilities

$$R_A=\frac{A}{B}e^{-i2k}\ , \tag{20}$$

$$R_B=\frac{1}{2V\cos k}\{(E-\epsilon_A)R_A - e^{-i4k}[2V\cos k-(E-\epsilon_A)]\}\ , \tag{21}$$

$$T_A=\frac{V(E-\epsilon_B)(e^{-ik}+R_Be^{ik})}{C}e^{-i2k}\ , \tag{22}$$

$$T_B=\frac{2V\cos k}{E-\epsilon_B}T_A\ , \tag{23}$$

where

$$A\equiv 2V\cos k(4\cos^2k-1)[(E-\epsilon_B)-Ve^{-ik}]C-2V\cos k[(E-\epsilon_A)C+V^2(E-\epsilon_B)] - [2V\cos k-(E-\epsilon_A)][(4\cos k^2-1)(E-\epsilon_B)C-(E-\epsilon_A)C-V^2(E-\epsilon_B)]e^{-2ik}\ , \tag{24}$$

$$B\equiv 2V^2\cos k(4\cos^2k-1)Ce^{ik}-(E-\epsilon_A)[(4\cos^2k-1)(E-\epsilon_B)C-(E-\epsilon_A)C-V^2(E-\epsilon_B)]\ , \tag{25}$$

$$C\equiv 2V^2\cos k(4\cos^2k-1)e^{-ik}-(E-\epsilon_B)^2\ . \tag{26}$$

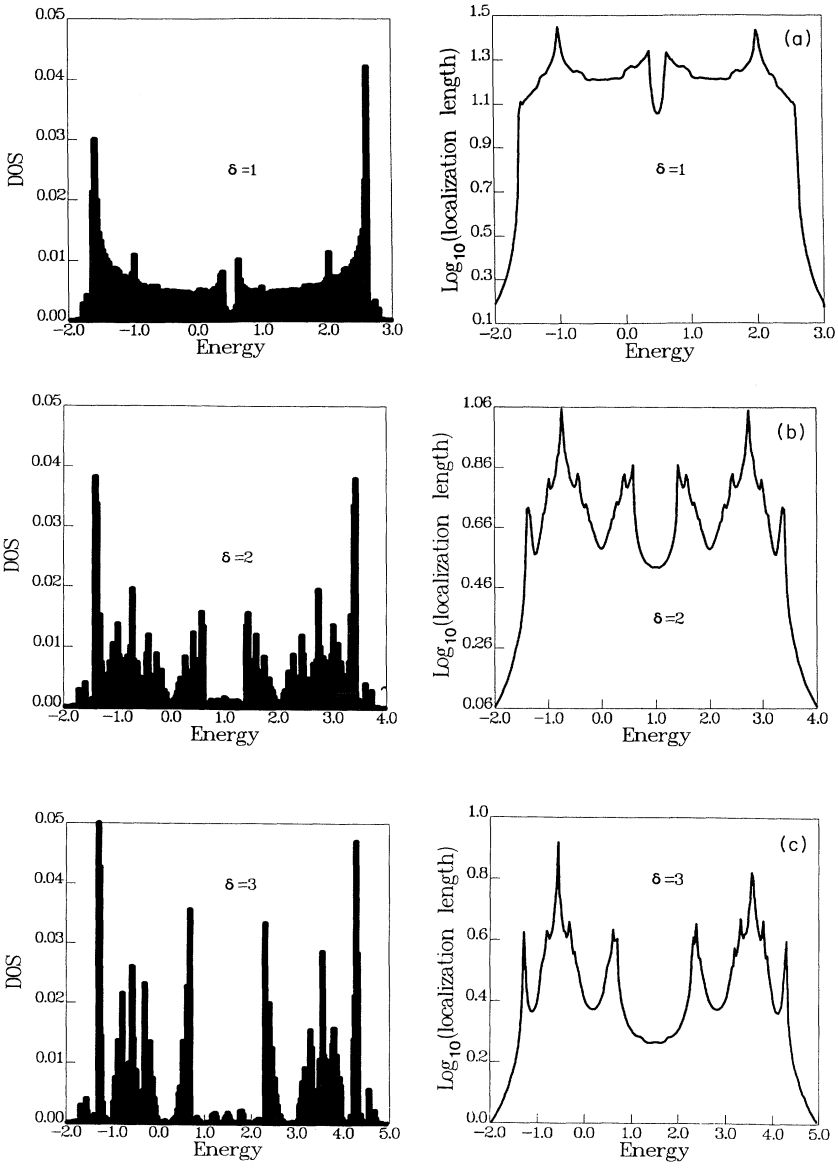

FIG. 8. The numerically computed averaged DOS and the localization length for the general AA,BB,AB,BB alloy with $P_{AA}=P_{BB}=0.025$ and $P_{AB}=P_{BA}=0.475$.

The energy dispersion is

$$E_{\pm}=\tfrac{1}{2}[\delta_{+}\pm(\delta_{-}^{2}+16V^{2}\cos^{2}k)^{1/2}]\ . \tag{27}$$

The expressions for $|R_A|^2$ and $|R_B|^2$ are displayed in Figs. 11 and 12. It can be seen that although they have minima they never go to zero, which implies the absence of delocalization in this case.

VI. DISCUSSION

A one-dimensional tight-binding model with binary-alloy-type site (diagonal) disorder assigned randomly every two sites in succession was recently shown to exhibit superdiffusion at long times[10] when the difference between the two energy values is below a critical value. We have studied the localization length and the DOS for this model and its extensions, where all different pairs of A and B sites are distributed at random. We have used the usual transfer-matrix techniques as well as a new analytical method.

The obtained numerical results are displayed as both a function of the energy and the degree of disorder, which is expressed by the difference $\delta=|\epsilon_A-\epsilon_B|$. We find that the DOS for the AA,BB random alloy exhibits, if $\delta=1$, a pure nonfluctuating smooth part near the band center having exactly the same form as that of the pure chain, and the localization length shows two $1/E^2$ singularity peaks. This singular behavior corresponds to delocalized states, the rest of the states being localized, as can be seen from the fluctuating DOS near the band edges. For the other cases involving the distribution of AA, AB, BA, and BB considered, localization is always found, with the most prominent case being when the AB,BA are distributed at random. It must be mentioned that the strong

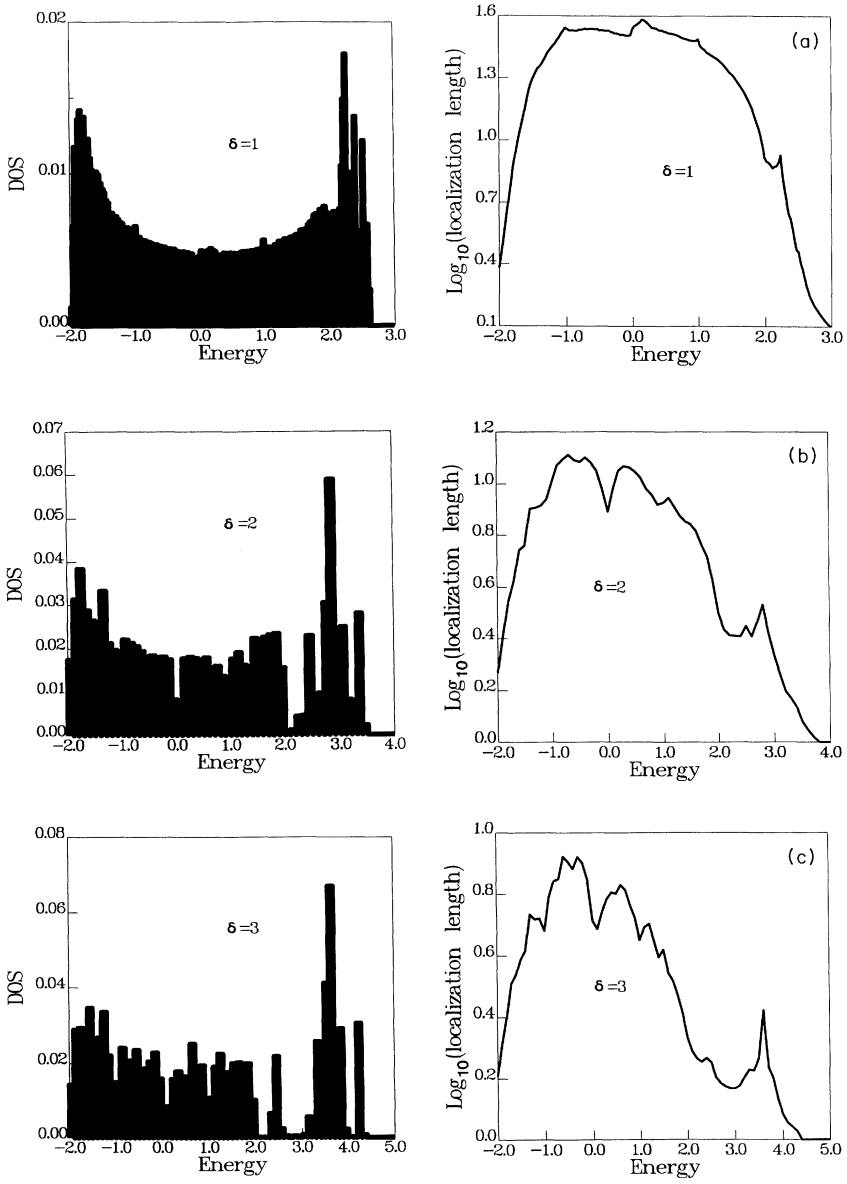

FIG. 9. The numerically computed averaged DOS and the localization length for the general AA,BB,AB,BB alloy with $P_{AA}=0.5$ and $P_{AB}=P_{BA}=0.25$.

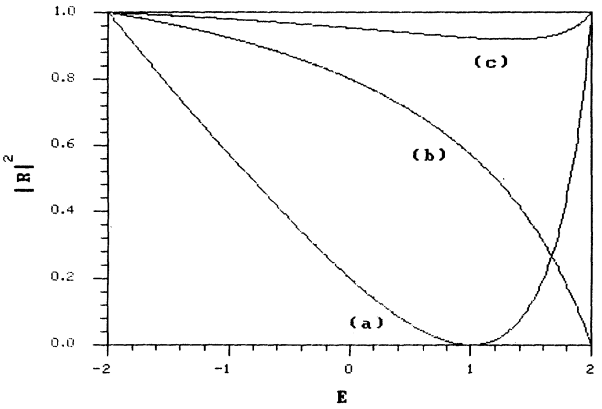

FIG. 10. The reflection probability amplitude $|R|^2$ vs energy E [Eq. (15)] for a BB impurity in a periodic ... $AAAAAAAAAAAAAA$ ... chain.

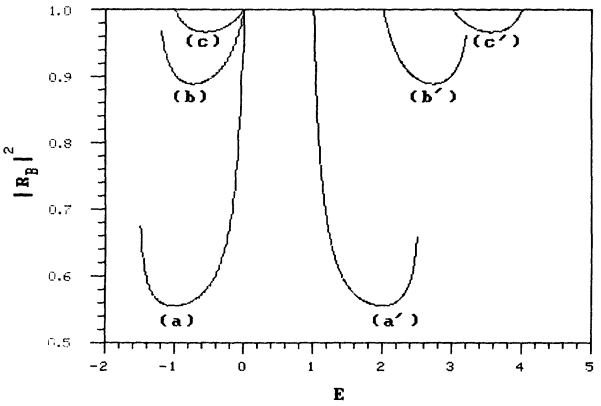

FIG. 12. The same as in Fig. 11 but the $|R|_B^2$ [Eq. (21)].

singular behavior found in this paper is unrelated to that occurring at other energies where the DOS vanishes and the localization length is weakly singular.[16]

The reason for the partial delocalization in the case of AA,BB random alloy and the absence of delocalization in all other correlated cases considered is related to the presence of short-range order. The underlying lattice structure for the mostly disordered AA,BB random alloy implies a mean cluster size of about 4 A or 4 B atoms in a row, while the anticorrelated case assumes the much lower value of 1.33 such atoms. These mean values measure the extent of correlations and for the other cases studied we obtain values intermediate between these extremes.

Our paired correlated model is also suitable for the microcanonical-ensemble approach of Deutsch and Paladin,[14] although it is a rather unfavorable application. This is due to the fact that we are considering the full energy-dependent Lyapunov exponent, for different values of the disorder strength, which is a singular measure. Despite this fact we are able, nevertheless, to obtain useful results. However, the method, although it gives a quite reasonable description, still remains approximate. A complete understanding of our results is obtained, however, by studying scattering in the presence of single-impurity pairs. Such results should be valid in the limit where the impurity concentration is close to zero but we find that they remain essentially valid at any concentration.

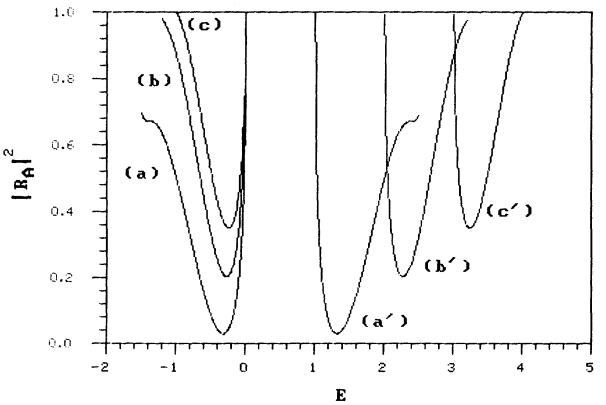

FIG. 11. The reflection probability amplitude on the A sites $|R|_A^2$ vs energy E for a BA impurity in a periodic ... $ABABABABABABABAB$ ... chain [Eq. (20)]. (a), (b), and (c) involve the three δ values 1, 2, and 3, respectively, and for the energy band E_-. The (a'), (b'), and (c') are for the E_+.

Although the present study has been limited to the binary distribution of the pairs, we expect similar results for any arbitrary discrete distribution. We have also briefly considered the case of distributing AAA,BBB or even arbitrary lengths of A's and B's at random in order to represent more realistically a binary medium. Our preliminary results favor the presence of delocalization via similar strong singularities whose number increases and we also find that they persist for even larger values of the disorder. In that case superfast diffusion is expected even for $\delta=2$.

In summary, we focused on the conditions under which partial delocalization occurs in the band for weakly disorder paired-correlated random binary alloys via dominant $1/E^2$ and in critical cases $1/E$ singularities of the localization length. In the present study, by combining an analytical method with very accurate numerical results, we demonstrate that if $\delta<2$ and $\delta=2$ partial delocalization and a critical situation occurs, respectively, while ordinary localization is obtained in the whole band only if $\delta>2$. We are also able to unravel the behavior of the averaged DOS, having in the case of localization a pure-like smooth part and a fluctuating measure in the case of localization. Many interesting questions still remain in this area; the most important concerns extension of our correlated-alloy results to higher dimensions and involves more sites than just pairs. Then we expect to be able to mimic scattering from objects in continuous media regarded as finite impurities.

ACKNOWLEDGMENTS

This work was supported in part by EEC through Contract No. SCC-CT90-0020 and by a PENED Research Grant of the Greek Secretariat of Science and Technology.

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