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Localization properties of general pseudo-random dimer models

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Abstract. We study localization of states and transmittance of a one-dimensional lattice with incommensurate rapidly varying pseudo-random potential, when site energies are dimerized. The chosen model potential, $V = V_0 \cos(2\pi\alpha n)$, α irrational, $\nu > 1$ and dimerization, is a peculiar generalization of the random-dimer binary model and allows careful control of the localization properties for varying degrees of disorder. We find that insertion of short-range order in the form of adjacent site energy dimerization, causes, in general, a strong increase of the localization lengths and the behaviour of the Lyapunov exponent as a function of the energy is similar to commensurate situations. In particular for $\nu > 2$, the binary alloy situation is reproduced and we confirm the presence of extended states near the two-site energies.

1. Introduction

It is a well established result that a one-dimensional lattice with randomly distributed site energies is characterized by a spectrum which exhibits complete localization of wavefunctions (Anderson 1958, Ishii 1973, Roman *et al* 1986). This is also true, in particular, when the site energies assume only two distinct values (random binary alloy). At first sight, it could appear reasonable to expect that if we systematically assign to each couple of adjacent sites the same random site energy, the random-dimer binary alloy so obtained should obey the localization law mentioned before.

However, it has been recently suggested (Dunlap *et al* 1990) that in a one-dimensional random-dimer binary model some wavefunctions may become extended, corresponding to narrow energy intervals around the two energies E_A and E_B . This fact can be taken as a starting point for the explanation of the insulator–metal transition occurring in polymers such as polyalene with disorder induced by protonation (Wu *et al* 1991, Wu *et al* 1992). The qualitative argument is that by assigning the same random energy to adjacent sites, this is equivalent to inserting short-range order in a globally disordered system and this can ease (for some energies) the propagation of the electron through the lattice. This result appears rather surprising, and for this reason interest in the problem is widespread; however, various numerical and semi-analytic approaches adopted so far have not, until now, unambiguously clarified whether delocalization occurs or not (Gangopadhyay *et al* 1992, Evangelou *et al* 1992, Datta *et al* 1993a, b).

Our purpose is to investigate, in a more general way, the effects of this kind of short-range order, when inserted in an aperiodic potential. For this reason we have found it

useful to apply the operation of 'dimerization' (i.e. doubling of site energy) in situations that generalize the binary distribution. For this aim we have chosen to investigate the rapidly varying incommensurate potentials of the form

$$V_n = V_0 \cos(2\pi\alpha|n|^\nu) \quad \nu > 1 \quad (1)$$

the integer n indicates the site position, α is an irrational number ($0 < \alpha < 1$). This potential has been widely studied in its asymptotically slowly varying version ($0 < \nu < 1$) (Das Sarma *et al* 1988, 1990, Farchioni *et al* 1992, 1993) and in the Aubry model ($\nu = 1$) (Aubry *et al* 1979, Dominguez *et al* 1992). In the case $1 < \nu < 2$, the spectrum shows a complete localization of wavefunctions at any energy except the value $E = 0$ (Thouless 1988); if $\nu \geq 2$, the potential is pseudorandom. Therefore the exponent, ν , allows gradual modification of the degree of disorder of the system and makes it possible to follow the effect of dimerization on the spectrum of (1) for different disorder strengths.

2. Numerical method

In this section we briefly present the numerical method we used for the investigation of the localization properties of the model described above. It is an application of the general renormalization technique (see, for instance, Giannozzi *et al* 1988 and references therein) to the one-dimensional nearest-neighbour tight-binding Schrödinger equation of the form

$$t(u_{n+1} + u_{n-1}) + a_n u_n = E u_n \quad (2)$$

where $a_n = V_n$ given by equation (1) and the energy scale is fixed by $t = 1$. The operation of renormalization consists in removing iteratively the sites $1, 2, \dots, N$ of the lattice, obtaining the effective energies of the extreme sites and the effective hopping interaction between them through the following three iterative equations

$$\varepsilon_0^{(N+1)}(E) = \varepsilon_0^{(N)}(E) + t_{0N}^{(\text{eff})} \frac{1}{E - \varepsilon_N^{(N-1)}(E)} t \quad (3a)$$

$$\varepsilon_{N+1}^{(N)}(E) = a_{N+1} + t \frac{1}{E - \varepsilon_N^{(N-1)}(E)} t \quad (3b)$$

$$t_{0,N+1}^{(\text{eff})}(E) = t_{0N}^{(\text{eff})}(E) \frac{1}{E - \varepsilon_N^{(N-1)}(E)} t = t_{N+1,0}^{(\text{eff})}(E). \quad (3c)$$

The quantity which gives information on the localization of states is the effective interaction $t_{0N}^{(\text{eff})}(E)$ which presents oscillating behaviour in the case of extended states, and rapidly decreasing behaviour in the case of exponentially localized states. The Lyapunov coefficient $\gamma(E)$ (inverse localization length) is directly available from the effective interaction $t_{0N}^{(\text{eff})}(E)$ through the following asymptotical relation (Farchioni *et al* 1992)

$$\gamma(E) = - \lim_{N \rightarrow \infty} \frac{1}{N} \ln |t_{0N}^{(\text{eff})}(E)| \quad (4)$$

We underline that this technique is numerically very stable; the logarithmic form of equation (4) allows to process as many sites as necessary (more than 10^9 when useful) without occurrence of underflow errors that one generally encounters when dealing with vanishingly small quantities.

3. Results

In this section we discuss our results concerning the effects of the dimerization on two models of pseudo-random incommensurate potentials. Dimerization in this case means that each energy of the pseudo-random law is repeated in the following site. Firstly, we will treat a potential model which can assume just two values, reproducing a binary model. Then we will discuss the more general case of a cosinusoidal rapidly varying law with various degree of pseudo randomness. Finally, we will show the transmission properties of the system.

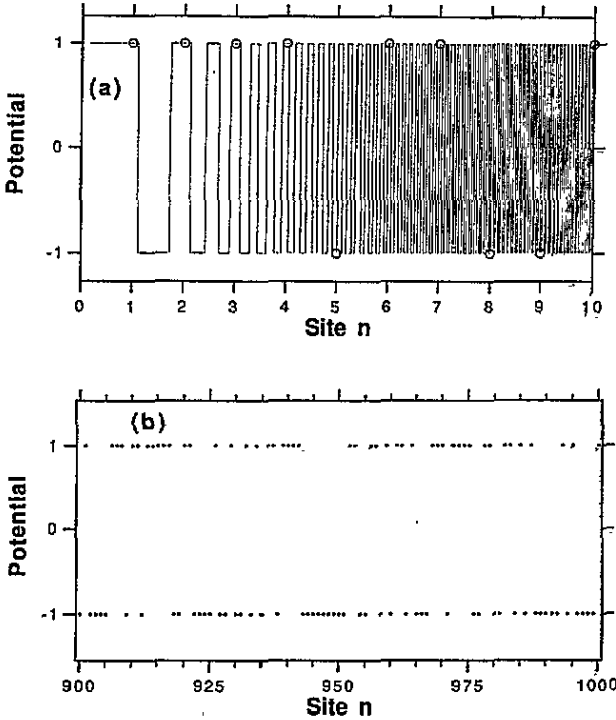


Figure 1. Pictorial view of the potential $V_n = V_0 \cos(2\pi \alpha n^\nu)$ ($2\pi \alpha = 1.2$, $\nu = 2.5$) in its 'rectified' version (see text) in the cases: (a) low site number n (the site energies are represented with circles) and (b) high site number n .

3.1. Binary model

Before studying directly the potential model (1) we can take into consideration its 'rectified' version: $V = V_0$ when $V_n > 0$, $V = -V_0$ when $V_n < 0$ (see figure 1(a) for low n values and figure 1(b) for large n values) for $2\pi \alpha = 1.2$ and for $\nu = 2.5$ (the results, if $\nu \neq 1$, are independent from the value of α). As can be seen from figure 1(b), this type of potential with $\nu > 2$ can be considered the pseudorandom version of the random binary model studied by Dunlap *et al* (1990). When the pseudorandom energies are repeated at adjacent sites (dimerization), we can see that in two narrow energy intervals around the values $\pm V_0$, the Lyapunov coefficient $\gamma(E)$ approaches zero following a quadratic law; as is so for the random model (Evangelou *et al* 1993, Bovier 1992). In figure 2(a) we show the sharp peaks of the localization length in the case of $V_0 = 0.5$ and in figure 2(b) the

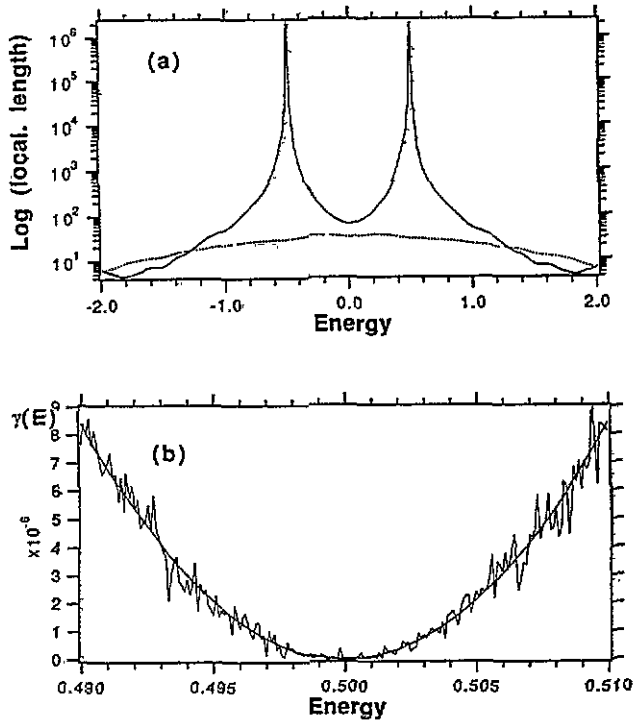


Figure 2. (a) Behaviour of localization length (in a logarithmic scale) for the pseudorandom potential $V_n = V_0 \cos(2\pi\alpha n^\nu)$ ($2\pi\alpha = 1.2$, $\nu = 2.5$) in its 'rectified' version of figure 1; dimerized case (full lines) and not-dimerized case (dashed line). Here $V_0 = 0.5$, and the sharp peaks at $E = \pm V_0$ are visible. (b) Behaviour of the Lyapunov coefficient as a function of the energy near $E = V_0$. Even if the value of $\gamma(E)$ is very low it is clear that it vanishes in a quadratic way around $E = V_0$. A similar behaviour is present for $E = -V_0$.

quadratic behaviour of $\gamma(E)$ near $E = V_0$. We also confirm that this behaviour is observed if the differences, Δ , between the two dimer binary energies are less than the critical value $\Delta_c = 2t$, where t is the nearest neighbour interaction. For $\Delta = \Delta_c$, $\gamma(E)$ approaches zero linearly, and for $\Delta > \Delta_c$ extended states disappear. Therefore, within our rapidly varying 'rectified' incommensurate potential model, we confirm the delocalization of the states near the two energies assigned to the sites of the chain. To stress this result more clearly, we can consider, for instance, the case of exponent $\nu = 2.5$, potential amplitude $V_0 = 0.5$, and the state of the spectrum with energy corresponding to V_0 . We show in figure 3 the behaviour of the effective interaction $t_{0N}^{(\text{eff})}(E)$ as a function of N : its oscillatory and regular behaviour beyond 10^8 renormalizations is an unambiguous sign of the presence of an extended state.

3.2. Generalized model

Let us now investigate of the more general case of the potential (1). The mechanism of dimerization we described before when applied to potential (1) can be formally expressed as follows

$$V_n = V_0 \cos(2\pi\alpha|(n/2)|^\nu) \quad (5)$$

where $(n/2)$ indicates the integer part of $n/2$. A pictorial view of this potential is reproduced in figures 4 for low and high values of site n , in the case $2\pi\alpha = 1.2$ and $\nu = 2.5$. We

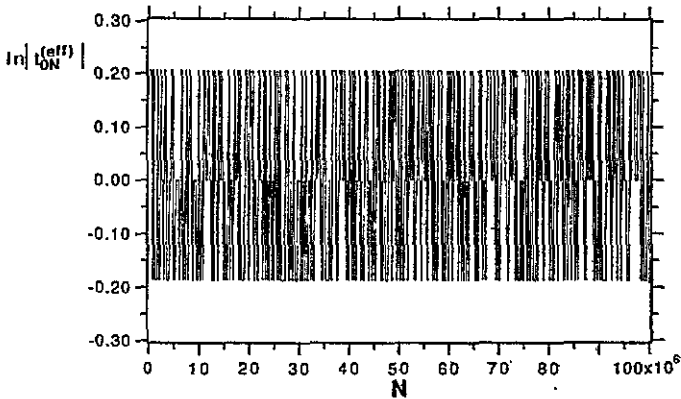


Figure 3. Behaviour of the logarithm of absolute value of effective hopping interaction $t_{0N}^{(eff)}(E)$ for the potential of figure 1 as a function of the number of renormalized lattice sites, at the energy $E = 0.5$, equal to the value of V_0 . It is clearly visible the oscillatory behaviour of $t_{0N}^{(eff)}(E)$ up to $N = 10^8$ renormalizations, indicating the extended nature of the state.

have found that the operation of 'doubling' the site energies produces a deep change in the behaviour of the inverse localization length. As another important point, we have observed that when the system has a moderate degree of disorder ($1 < \nu < 2$), the above dimerization does not determine complete delocalization of the states, even if our results in general show a strong decrease of the inverse localization length $\gamma(E)$ in narrow energy regions around the site energies of the lattice. We have verified that the general behaviour of $\gamma(E)$, around $E = 0$, for the potential (5), is very similar to the behaviour it assumes in the case of low-order rational approximations of the number α , even if the distribution of eigenstates and their spatial localization properties in the spectrum are quite different. For this reason, before showing our results on a pseudo-random incommensurate potential, we investigate what happens for its periodic approximants, i.e. when we dimerize according to the law (5) the site energies in periodic cases ($\nu = 1$ and $\alpha = 1/N$). In the periodic case we have a unit cell of $2N$ sites; the resulting spectrum is composed by $2N$ bands disposed around $E = 0$, the centre of the spectrum, which lies in an energy gap. The effect of dimerization of the periodic case is to open a gap around $E = 0$ when N is odd; if N is even (and $N > 2$), the width of the gap pre-existent in the non-dimerized case increases. We can recall the fact that the presence of a gap in the centre of the spectrum is a common feature in the case of a doubling the elementary cell dimension, as suggested for one dimensional lattices (Peierls 1955).

With these few points in mind, let us now consider the results for the Lyapunov coefficient $\gamma(E)$ for the incommensurate asymptotically rapidly varying potential (1) in the case $\nu = 1.5$ and dimerization (5). In figure 5 we have reproduced the plots for $\gamma(E)$ (solid lines) for $V_0 = 0.1$, $V_0 = 0.2$ and $V_0 = 0.3$. They are compared with $\gamma(E)$ in a simple periodic dimerized case ($\alpha = 1/4$, dashed line). As said before, the most surprising fact is that in the incommensurate case the behaviour of $\gamma(E)$ near $E = 0$ is very regular and very similar to the periodic case where the gap is recovered. After this regular part for the incommensurate potential, the plot of $\gamma(E)$ shows a tail fluctuating around very low values, ($\sim 10^{-6}$ for low values of V_0) indicating a strong delocalization effect but not a transition toward genuine extended states. This behaviour of $\gamma(E)$ has been verified for energies up to V_0 ; for energies $E \gtrsim V_0$, the Lyapunov coefficient starts increasing, as can

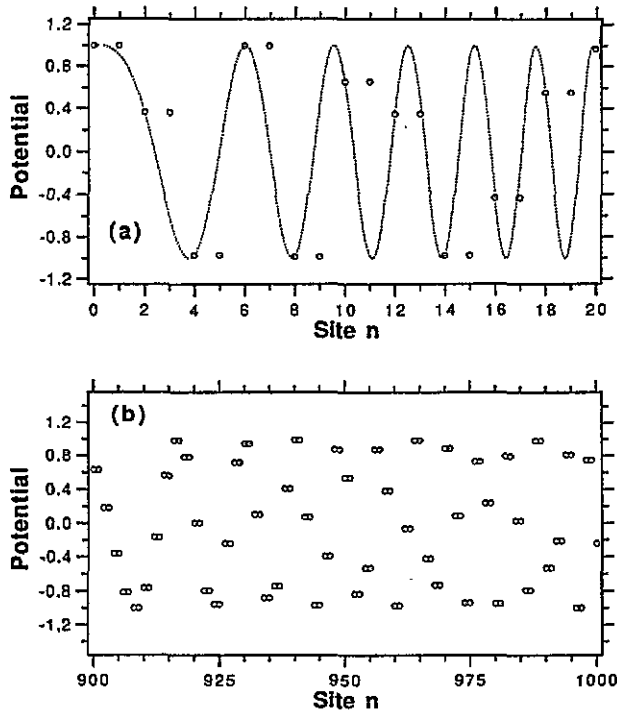


Figure 4. Pictorial view of the potential $V_n = V_0 \cos(2\pi\alpha(n/2)^\nu)$ ($2\pi\alpha = 1.2$, $\nu = 1.5$); (a) low site number n (the site energies are represented with circles) and; (b) high site number.

be seen from figure 6, which represent the plots of $\gamma(E)$ in the cases $V_0 = 0.5$ and $V_0 = 1$ both for the dimerized potential (5) and for the not-dimerized potential (1). We can remark on the fact that if in the random binary model the dimerization of the lattice is decisive for the transition of some electronic states toward an extended nature, in the more general case of potential (1) the propagation of the electron is strongly enhanced if its energy coincides with one of the values assumed by V_n ; however, this condition stops at $E \sim V_0$, and this explains the increase of Lyapunov coefficient.

We can observe in figure 6 that insertion of short-range order modifies the behaviour of the wavefunction localization lengths making it very similar to a simple periodic case, where dimerization causes opening of a gap around $E = 0$. In spite of the similarity of the plots of $\gamma(E)$ in figure 5, we stress the fact that in the aperiodic case no gap is present, and we have explicitly verified this fact by means of calculations of density of states. Dimerization tends to assign to the eigenstates of the part of the spectrum near $E = 0$ an inverse localization length very close to the Lyapunov exponents corresponding to the gap of the ordered system (see figure 5). As a consequence, near $E = 0$, the Lyapunov coefficient in the case of dimerization is greater than for the not-dimerized system (see figure 6). This fact can appear rather surprising because it means that in this energy interval the states are more localized in the more ordered system than in the less ordered one.

3.3. Consequences on the transmittivity

As a confirmation of these results, we have made some calculations of the transmittivity of the system using the transfer matrix technique (see, for instance, Douglas Stone *et al* 1981).

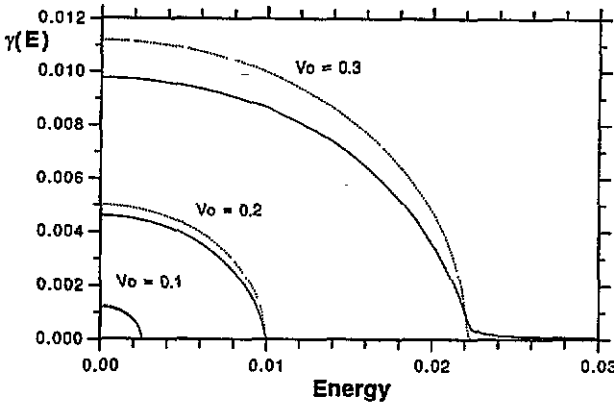


Figure 5. Comparison of Lyapunov coefficient for the aperiodic ($2\pi\alpha = 1.2$, $\nu = 1.5$) dimerized case (full lines) and for its commensurate rational approximation dimerized case with $\alpha = 1/4$ (dashed lines) in the cases $V_0 = 0.1$, $V_0 = 0.2$ and $V_0 = 0.3$. In the aperiodic case, $\gamma(E)$ assumes always non-zero value.

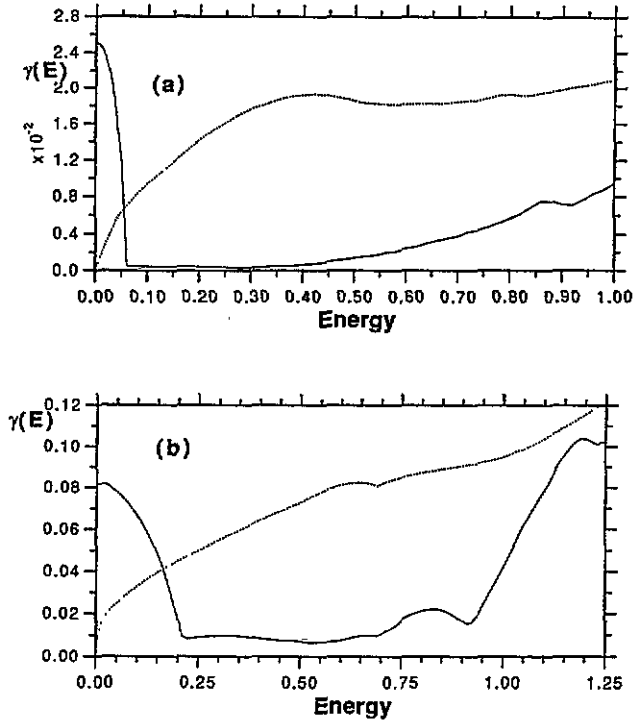


Figure 6. Comparison of Lyapunov coefficient in the dimerized (full lines) and not dimerized (dashed lines) aperiodic cases ($2\pi\alpha = 1.2$, $\nu = 1.5$) for $V_0 = 0.5$ (a) and $V_0 = 1$ (b). Near $E = 0$, $\gamma(E)$ in the dimerized case is greater than in the not-dimerized case, indicating a stronger localization in a more ordered system. Beyond this zone, $\gamma(E)$ for dimerized potential decreases, showing a tendency to delocalization. This tendency stops at $E \sim V_0$, where $\gamma(E)$ begins to increase.

While in order to clarify the extended or localized nature of eigenstates, we performed typically 10^7 , 10^8 renormalizations so as to guarantee the control of a practically infinite system, now we want to emphasize the surprising effects of local order on more spatially limited samples, for instance composed by 10^3 sites. In this case, the system is shorter than the typical values of the localization length for the dimerized case, except in the energy interval around $E = 0$. We have therefore, to expect from the system, a good transmittivity in the interval $-V_0 \lesssim E \lesssim V_0$ with the exception of the zones mentioned before where the transmittivity has to be near zero. This is confirmed by figure 7 where we have compared the dimerized and not dimerized case near $E = 0$. We can see that the enhancement of the Lyapunov coefficient in this part of the spectrum has as the consequence that the dimerized (and more ordered system) has a lower transmittivity than the not-dimerized case. This conclusion is valid also for the conductance.

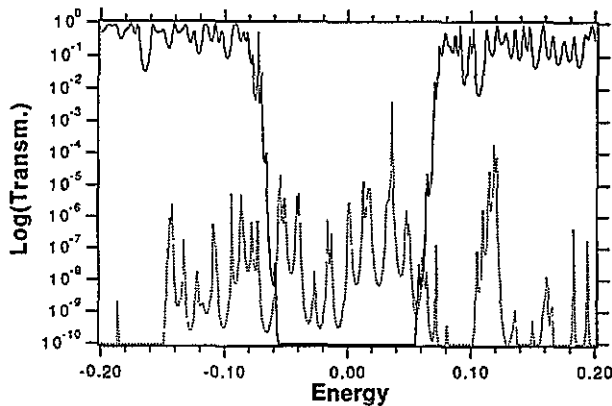


Figure 7. Comparison of the logarithm of transmittance in the aperiodic ($V_0 = 0.5$, $2\pi\alpha = 1.2$, $\nu = 1.5$) dimerized case (full line) and not-dimerized case (dashed line) for a sample of 10^3 sites. The transmittivity is in general higher in the dimerized system, because the localization lengths are comparable with the length of the sample. It is interesting to observe, however, that near $E = 0$ (corresponding to the arc in the plot of Lyapunov coefficient) the dimerized system has transmittivity lower than the less ordered not-dimerized one.

In figures 8 we show the corresponding results concerning Lyapunov coefficient and transmittance for the pseudo-random potential (1) and $\nu = 2.1$ (strong disorder). All the considerations made for the case $1 < \nu < 2$ remain valid, even if in a weaker sense. In this case the behaviours of $\gamma(E)$ for dimerized potential (figure 8(a)) are not so regular, however, the same 'bell' feature of the plots is visible near $E = 0$ and it is followed by a general decrease of $\gamma(E)$ until $E \sim V_0$. Beyond this value the electronic propagation is not favoured because of the dimerization of the system. In this case the Lyapunov exponent around $E = 0$ remains smaller than in the not-dimerized case and then, as usual, longer localization length in the more ordered system is found. The reduction of the inverse localization length has its counterpart in an enhancement of the transmittivity (figure 8(b)), with the exclusion of the region around $E = 0$ where instead transmission is suppressed.

4. Conclusions

By means of calculations of inverse localization length $\gamma(E)$ and transmissivity of a dimerized lattice with rapidly varying incommensurate and pseudo-random site energies,

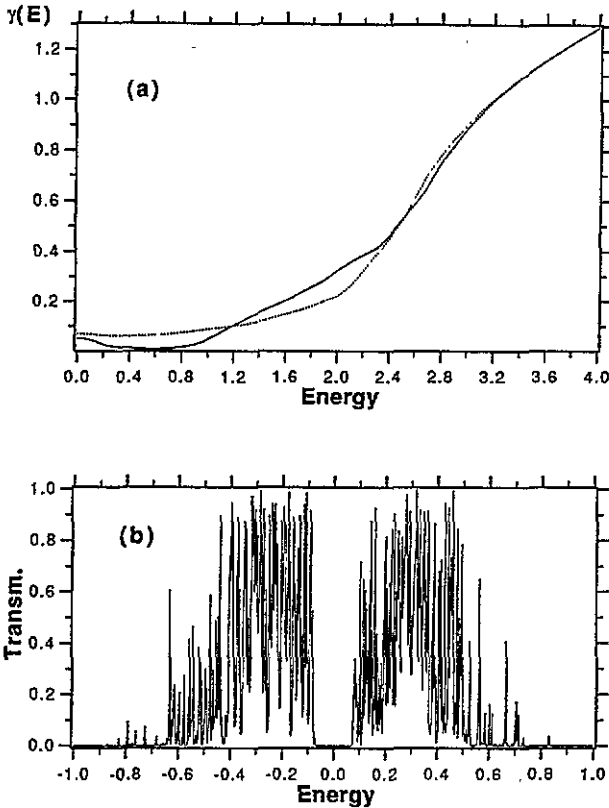


Figure 8. (a) Comparison of Lyapunov coefficient in the case of aperiodic strongly disordered ($V_0 = 1$, $2\pi\alpha = 1.2$, $\nu = 2.1$) dimerized case (full line) and not-dimerized case (dashed line). (b) Transmittivity of the system in the aperiodic strongly disordered case ($V_0 = 1$, $2\pi\alpha = 1.2$, $\nu = 2.1$).

we have found that the behaviour of $\gamma(E)$ changes greatly if compared with the not-dimerized system. In particular, near $E = 0$ it becomes surprisingly more similar to that of a simple periodic approximation than to that of the not-dimerized potential. This is a sign of the strong effect of the local order that we impose with the operation of dimerization. In agreement with this fact, in the binary potential, we confirm delocalization of electronic states near site energies.

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