Abstract

We consider a one-dimensional continuous (Kronig-Penney) extension of the (tight-binding) Random Dimer model of Dunlap et al. [Phys. Rev. Lett. 65, 88 (1990)]. We predict that the continuous model has infinitely many resonances (zeroes of the reflection coefficient) giving rise to extended states instead of the one resonance arising in the discrete version. We present exact, transfer-matrix numerical calculations supporting, both realizationwise and on the average, the conclusion that the model has a very large number of extended states.
The question as to whether Anderson localization occurs for any one-dimensional, disordered system, has been considered solved for many years. However, a number of recent papers strongly suggest that the widely held view that disorder prevents long-range transport in one-dimension is not always true. This is the case with the work by Dunlap, Wu, and Phillips (see for a review). These authors studied a tight-binding model (so called Random Dimer model, RDM) in which each on-site energy can have only one of two possible values, one of these values being assigned at random to pairs of lattice sites. They showed that for a certain energy the reflection coefficient of a single defect vanished, and that this resonance was preserved when a finite concentration of defects were randomly placed in the chain. This gave rise to a set of delocalized states proportional to the square root of the number of sites. As a consequence, in such a system electronic transport can take place almost balistically. Similar results have been also shown to hold true for dilute binary alloys by Flores. Besides, the arguments of Dunlap et al. to conclude that such a large number of states were not localized have been further confirmed by perturbative calculations by Bovier. The RDM has been generalized recently by Wu, Goff, and Phillips to include more complex arrangements of defects. In this work, they also considered the continuum limit of their model, given by square barriers and wells randomly placed on a line, and it appeared to exhibit the same kind of localization-delocalization transition.

In this letter, we concern ourselves with an even simpler continuous model, which we call continuous Random Dimer model (henceafter, CRDM). This system is the natural continuum version of the RDM of Dunlap et al., although it is not its continuum limit as studied in. We build our model in the following way: We start from a usual Kronig-Penney model, given by a potential of the form

\[ V(x) = \sum_{n=1}^{N} \lambda_n \delta(x - x_n). \] (1)

We choose \( \lambda_n > 0 \); the extension of our computations below to the \( \lambda_n < 0 \) case is straightforward although a bit involved. To mimic the RDM, we now take the positions of the delta functions to be regularly spaced, i.e., \( x_n = na \), \( a \) being the lattice spacing; moreover, we
allow only two values for \(\lambda_n, \lambda\) and \(\lambda',\) with the additional constraint that \(\lambda'\) appears only in pairs of neighbouring deltas. In this fashion, we have defined what comes naturally as a continuous version of the tight-binding Random Dimer model. The corresponding Schrödinger equation is then

\[
\left[-\frac{d^2}{dx^2} + \sum_{n=1}^{N} \lambda_n \delta(x - x_n)\right] \Psi(x) = E \Psi(x).
\] (2)

We believe that Eq. (2) represents a more realistic model than the RDM since no tight-binding approach is involved. In addition, it is well known that the \(\delta\)-function potential is a good candidate to model more structured and more sophisticated interaction potentials [9]. We will see in the following that there exists a number of energies for which the reflection coefficient at a single dimer vanishes. Because interference effects are quite more complex in a continuous model than in a tight binding approach, it is a nontrivial task to elucidate whether these resonances will survive when several dimers are located at random along the lattice.

We can now use the techniques of dynamical systems theory, as first used by Bellissard et al. [10] (see also [11]) to construct the Poincaré map associated with Eq. (2). It is important to stress that, by doing this reduction to an equivalent tight-binding set of equations, we are not losing any information at all, and the calculations remain exact. The resulting equations are

\[
\Psi_{n+1} + \Psi_{n-1} = \left[2 \cos \sqrt{E} + \lambda_n \frac{\sin \sqrt{E}}{\sqrt{E}} \right] \Psi_n,
\] (3)

where \(\Psi_n \equiv \Psi(x = na).\) Notice that the energy enters in the equations in a rather complicated fashion. To proceed, we have to take into account in the first place the condition for an electron to be able to move in the perfect \((\lambda' = \lambda)\) lattice, namely

\[
\left| \cos \sqrt{E} + \frac{\lambda}{2} \frac{\sin \sqrt{E}}{\sqrt{E}} \right| \leq 1; \tag{4}
\]

this constraint gives the allowed energy values once \(\lambda\) is fixed. On the other hand, we follow Dunlap et al. and study the problem of a single pair defect on an otherwise perfect chain. In
our case, a straightforward application of the results in [2] leads to the following condition for the vanishing of the reflection coefficient:

\[ \cos \sqrt{E} + \frac{\lambda'}{2} \frac{\sin \sqrt{E}}{\sqrt{E}} = 0. \]  

(5)

It is a matter of simple algebra to transform the two equations (4) and (5) into these other, more useful two:

\[ -\frac{2}{\lambda'} = \tan \sqrt{E} \sqrt{E}, \]  

(6a)

\[ |\cos \sqrt{E}| \leq \frac{\lambda}{|\lambda - \lambda'|}. \]  

(6b)

Restricting ourselves to the range \(0 \leq \lambda' \leq 2\lambda\), Eq. (6a) is trivially verified, and therefore it poses no restrictions on the allowed energy values, aside from the fact that they must be positive. Hence, we are left only with Eq. (6a) to select the energy values for which the reflection coefficient of a single defect becomes exactly zero. As the \(\tan \sqrt{E}\) is a \(\pi\)-periodic function and it takes all values in \([-\infty, +\infty]\), for any \(\lambda'\) we choose we will find energies solving (6b) in each interval \([n \pi/2, (n + 1) \pi/2]\), i.e., we will have an infinite countable set of energies for which the single defect reflection coefficient vanishes. This is to be compared with the result of Dunlap et al., who found a unique energy for which the same perfect transmission took place in the RDM.

We now proceed to the problem of the disordered lattice, containing a certain number of pair defects. To this end, we go back to Eq. (2) and introduce the reflection and transmission amplitudes through the relationships:

\[ \Psi(x) = \begin{cases} 
    e^{iqx} + R_N e^{-iqx}, & \text{if } x < 1, \\
    T_N e^{iqx}, & \text{if } x > N,
\end{cases} \]  

(7)

where \(T_N\) and \(R_N\) are the transmission and the reflection amplitudes of a system with \(N\) scatterers respectively, \(q \equiv \sqrt{E}\), and we have put the lattice spacing \(a = 1\) without loss of generality. It is not difficult to compute recursively both amplitudes using well-known transfer matrix procedures (see, e.g., [12]). In particular, the transmission amplitude can be written as
\[ A_N = \left( \alpha_N + \frac{\alpha_{N-1}^* \beta_N}{\beta_{N-1}} \right) A_{N-1} - \left( \frac{\beta_N}{\beta_{N-1}} \right) A_{N-2}, \] (8)

where \( A_N \equiv 1/T_N^2 \), and

\[ \alpha_j \equiv \left[ 1 - i \left( \frac{1}{2q} \right) \lambda_j \right] e^{iq}, \quad \beta_j \equiv -i \left( \frac{1}{2q} \right) \lambda_j e^{-iq}. \] (9)

Finally, Eq. (8) must be supplemented by the initial condition \( A_0 = 1, A_1 = \alpha_1 \) to completely determine the amplitudes.

Once we have computed the transmission amplitude, some physically relevant magnitudes can be readily obtained from it. Thus, the transmission coefficient is given by

\[ \tau_N = |T_N|^2, \] (10)

whereas the resistivity, according to the Landauer formula [13], is simply

\[ \rho_N = \frac{1}{|T_N|^2} - 1. \] (11)

Aside from these two quantities, there are others that can also be obtained from the transmission amplitude, although somewhat less naturally. Indeed, the Lyapunov coefficient (which is nothing but the inverse of the localization length) depends on this amplitude through the expression [12]

\[ \gamma_N = \frac{1}{2N} \log |T_N|^2 = -\frac{1}{2N} \log \tau_N, \] (12)

and it can be also shown [12] that the integrated density of states (IDOS) is related to \( T_N \) by

\[ \Gamma_N = -\frac{i}{2\pi N} \log \frac{T_N^*}{T_N}; \] (13)

from this last expression, the density of states (DOS) can be obtained by simple derivation with respect to the energy.

The results we have obtained so far provide an exact, although non closed analytical description of any one-dimensional, disordered KP model. With them, we can compute the
magnitudes we mentioned above for any given model and, in particular, for the CRDM. All expressions are very simple and suitable for an efficient numerical treatment of any specific case. We will now evaluate them for several of these cases to check whether there is any relevant feature of the transmission coefficient and related quantities that may be the fingerprint of extended states. We have to notice that there are several parameters that can be varied in the CRDM: the strengths of the two kinds of scatterers, $\lambda$ and $\lambda'$, the defect concentration, and the length of the system, $N$. As to the first two of them, it can be checked that the factor $\lambda$ can be rescaled and subsequently suppressed in Eq. (2), and therefore, the relevant quantity is just the ratio $\lambda'/\lambda$, which allows us to fix $\lambda = 1$ from now on.

We first describe our results realizationwise, because we believe that these are the most physically relevant; we briefly deal with the average properties of the model below. In Fig. 1, we show the transmission coefficient for a system with $\lambda' = 1.5$, 5 000 scatterers, and a probability of having a dimer $q = 0.5$ [14]. In this plot, it is clearly appreciated the peak in the transmission coefficient very close to the predicted value for the first resonance ($E \approx 3.7626$ for this parameter set). Moreover, neighbouring states have a transmission coefficient close too unity, that decreases as we move away from the resonance. In Fig. 2, the Lyapunov exponent is plotted vs the energy for the same system; again, we appreciate that there is a deep minimum around the resonance value, which implies a very large localization length, much larger than the system size. The other magnitude we study, the resistivity, confirms the existence of an energy interval for which a typical realization of our model shows transport properties similar to those of perfect lattices.

The IDOS, which is plotted in Fig. 3, deserves some separate comments. Due to the presence of the multivalued arctan function in the defining relationship (13), this magnitude is very sensitive to the resolution in energies: if there is a jump in the arctan between two points for which the IDOS is computed, this jump will be missed and the IDOS will be subsequently underestimated. However, we checked several cases computing the IDOS with tiny energy steps ($5 \times 10^{-6}$) which is very time consuming; with this accuracy, we recover
the agreement between systems of different sizes (notice that the magnitude we discuss is in fact the IDOS per volume) as regards the total number of states and the IDOS structure. As to this last feature, we want to stress that the IDOS is well behaved (smooth) over all the studied range of energies. This implies that the same argument used by Dunlap et al. [2] to show that $\sqrt{N}$ states were extended holds in this case too, because the reasoning depends crucially on the DOS structure (see [7]).

It is most important to report on how the above picture is modified when the system parameters are changed. First of all, the main characteristic of our model, i.e., that it has an infinite number of resonances, is confirmed by our calculations; besides, the higher the resonant energy (meaning the higher $n$ in $[n \pi/2, (n + 1) \pi/2]$), the wider the peak in the transmission coefficient and the other transport magnitudes. The peak width increases also when decreasing $\lambda'$ towards $\lambda = 1$, and decreases when increasing $\lambda'$ up to its maximum $\lambda' = 2$. This is to be expected, because when $\lambda' = \lambda$ we recover the perfect lattice. With respect to the other parameters, the number of scatterers and the concentration of dimers, both cause a narrowing of the set of extended states when they are increased in the studied range ($100 \leq N \leq 50000$, $0.1 \leq q \leq 0.5$), although it is important to stress that this set always has nonzero width. Interestingly, when the number of scatterers increases, the IDOS steepens (i.e., the DOS exhibits a sensitive increment) around the resonant energy; consequently, the number of extended states may be constant in spite of the decreasing of the width of the transmission peak.

We now comment on the averaged results. When computing averages, they were taken over a number of realizations varying from 100 to 10000 to check the convergence of the computed mean values. The convergence was always satisfactory, with discrepancies of less than 1% between all the ensembles. Once more, however, to get accurate results for the IDOS is quite time consuming due to the necessary resolution in energies. The averaged results for the transmission coefficient, the Lyapunov exponent, the resistivity, and the density of states are basically the same as those for a typical realization we commented on above. This is a crucial point because it supports our claim that those are the main features of our model.
irrespective of the particular realization of the disorder.

In summary, we have studied a Kronig-Penney model with two kinds of $\delta$-functions, one of them constrained to appear only pairwise. This is a continuous extension of the RDM of Dunlap et al. [2]. We find an infinite number of energies for which the reflection coefficient of a single defect vanishes. We have shown, through numerical evaluation of exact expressions, that these resonances give rise to a very large number of extended states, that can be much larger than that of the RDM where a unique resonance exists. These extended states are characterized by a transmission coefficient close to unity and a localization length much larger than the system one. The basis for the existence of a extended states as relevant as to affect the transport properties, the smooth character of the DOS around the resonance [2,7], holds, supporting our conclusions. The increasing of the DOS around the resonant for large systems helps keep relevant the number of extended states. We believe that similar results will arise in related continuous models. Work currently in progress regarding the structure of the wavefunctions, as well as the development of better, more accurate methods to compute the DOS, will be reported elsewhere.

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REFERENCES

[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).

[2] D. H. Dunlap, H.-L. Wu, and P. Phillips, Phys. Rev. Lett. **65**, 88 (1990).

[3] H.-L. Wu and P. Phillips, J. Chem. Phys. **93**, 7369 (1990).

[4] H.-L. Wu and P. Phillips, Phys. Rev. Lett. **66**, 1366 (1991).

[5] P. Phillips and H.-L. Wu, Science **252**, 1805 (1991).

[6] J. C. Flores, J. Phys. Condensed Matter **1**, 8471 (1989).

[7] A. Bovier, J. Phys. A **25**, 1021 (1992).

[8] H.-L. Wu, W. Goff, and P. Phillips, Phys. Rev. B **45**, 1623 (1992).

[9] P. Erdős and R. C. Herndon, Helv. Phys. Acta **50**, 513 (1977).

[10] J. Bellissard, A. Formoso, R. Lima, and D. Testard, Phys. Rev. B **26**, 3024 (1982).

[11] J. B. Sokoloff and J. V. José, Phys. Rev. Lett. **49**, 334 (1982).

[12] P. D. Kirkman and J. B. Pendry, J. Phys. C **17**, 4327 (1984).

[13] R. Landauer, Phil. Mag. **21**, 863 (1970).

[14] The probability of having a dimer is used when building up the system; each site is assigned a value \( \lambda \) or \( \lambda' \) according to it. It does not coincide with the concentration, however, because if a site happens to be part of a dimer, the next one is automatically part of a dimer too, so the value of the delta function at that point is deterministic.
FIGURES

FIG. 1. Transmission coefficient vs energy for a system with $\lambda' = 1.5$, 5 000 scatterers, and a probability of having a dimer of 0.5 [14]. The arrow marks the predicted resonance.

FIG. 2. Lyapunov exponent vs energy for a system with $\lambda' = 1.5$, 5 000 scatterers, and a probability of having a dimer of 0.5 [14]. The dashed line marks the inverse of the system length: Energies with a lower exponent will have a localization length larger than the system one. The arrow marks the predicted resonance.

FIG. 3. Integrated density of states for systems with $\lambda' = 1.5$ and a probability of having a dimer of 0.5 [14], of sizes 1 000, 5 000, and 10 000 scatterers from top to bottom. The arrow marks the predicted resonance.