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# Explanation of delocalization in the continuous random-dimer model

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We propose an explanation of the bands of extended states appearing in random one-dimensional models with correlated disorder, focusing on the continuous random-dimer model [A. Sánchez, E. Maciá, and F. Domínguez-Adame, Phys. Rev. B **49**, 147 (1994)]. We show exactly that the transmission coefficient at the resonant energy is independent of the number of host sites between two consecutive dimers. This allows us to understand why there are bands of extended states for every realization of the model as well as the dependence of the bandwidths on the concentration. We carry out a perturbative calculation that sheds more light on the above results. In the conclusion we discuss generalizations of our results to other models and possible applications which arise from insight into this problem.

## I. INTRODUCTION

Since the beginning of this decade, a number of disordered one-dimensional (1D) models have been proposed[1–3] which exhibit nontrivial extended states. The key ingredient of those models is *correlation*: The defects or impurities are introduced in the host lattice at random, but always forming pairs, i.e., they never appear isolated. Further research in this and related models supported this unexpected result, including other grouping rules aside from pairing.[4–10] All those results established on firm grounds the existence of bands of extended states in this class of models, at least in finite-size samples. However, the *reasons* for such bands to arise remain unclear: To the best of our knowledge, there are only some perturbative results estimating the number of states,[4,5] and some symmetry conditions for the existence of this kind of resonances.[5] There is no need to stress the importance of achieving a good understanding of this delocalization phenomenon, both from theoretical and applied viewpoints: Such advance will certainly be helpful both to settle down theoretically its relevance and generality, as well as to design devices with specific transmission properties. On the other hand, we concern ourselves with a model which has been much less studied (indeed, we do not know of any perturbative calculation or related result regarding it) and which, on the other hand, has specific properties. We address these issues in this paper. To this end, in Sec. II we present the specific model we study, the continuous random-dimer model,[8,9] and the properties we will be dealing with. In Sec. III we show how those features may be understood in terms of the structure of the transmission coefficients through lattice segments. Finally, in our conclusions we discuss correlated disordered models in general in view of our results, as well as possible applications of this work.

## II. THE CONTINUOUS RANDOM DIMER MODEL

The continuous random-dimer model (CRDM) was introduced in Refs. 8 and 9 and is described by the following Schrödinger equation (we use units such that $\hbar=2m=1$):

$$\left[-\frac{d^2}{dx^2}+\sum_n \lambda_n \delta(x-n)\right]\psi(x)=E\psi(x), \tag{1}$$

where $\lambda_n>0$ (the extension of the results to the $\lambda_n<0$ case is straightforward; besides, the choice of the sign is irrelevant in most applications, e.g., for superlattices[11]). To introduce paired correlated disorder $\lambda_n$ takes only two values at random, namely $\lambda$ and $\lambda'$, with the constraint that $\lambda'$ appears only in pairs of neighboring sites (dimer). This model is related to and inspired by the (tight-binding) random-dimer model (RDM) of Dunlap *et al.*,[2,3] and we believe that our work on the CRDM will provide also relevant ideas for the RDM. However, there are a number of significant differences between both models. First, the CRDM exhibits an infinite number of resonances and their corresponding bands of extended states,[8,9] which makes it interesting from the viewpoint of applications as there are many options to match the Fermi level. Second, the fact that the CRDM is continuous and includes multiple scattering effects gives it a more real-

 

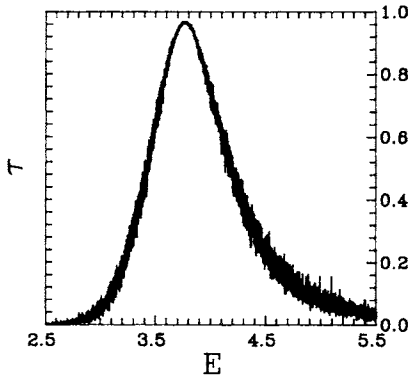


FIG. 1. Transmission coefficient for the CRDM with a dimer concentration $c=0.2$. The $\delta$ function strengths are $\lambda=1$, $\lambda'=1.5$. Shown is an average over 100 realizations. Every realization consists of 15 000 scatterers. The first allowed band in the perfect lattice is [0.921,9.870].

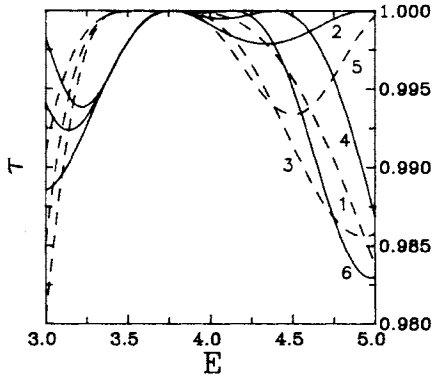


FIG. 2. Transmission coefficient for two dimers with $N$ host sites in between, placed in the middle of an otherwise periodic chain, for $N=1$, 2, 3, 4, 5, and 6 as indicated in the plot (even $N$, solid lines; odd $N$, dashed lines). The $\delta$ function strengths are $\lambda=1$, $\lambda'=1.5$ as in Fig. 1.

istic character, thus supporting the possibility of seeing these effects in a variety of actual physical systems. Finally, the RDM and the CRDM have different parameters: Whereas the RDM depends on the on-site energies $\epsilon_a$ and $\epsilon_b$ and on the hopping term $V$ (see Ref. 2), the CRDM depends on the strengths of the $\delta$ functions and the intersite distance.

We now summarize the main features of the CRDM. In Ref. 9 we developed a generalized Poincaré map formalism that allows us to map exactly general one-dimensional Schrödinger equations onto discrete equations, for any potential allowed in quantum mechanics. In particular, Eq. (1) is equivalent to the discrete map

$$\psi_{n+1}+\psi_{n-1}=2\Omega_n\psi_n, \tag{2}$$

where $\psi_n\equiv\psi(n)$ and $\Omega_n\equiv\cos q+(\lambda_n/2q)\sin q$, with $q=\sqrt{E}$. That formalism allowed us to prove that there are an infinite number of resonant energies for which the reflection coefficient of a *single* dimer vanishes.[12] Resonant energies are given by the conditions $|\Omega|\leq 1$ and $\Omega'=0$, where $\Omega=\cos q+(\lambda/2q)\sin q$ and $\Omega'$ the same but replacing $\lambda$ by $\lambda'$. The same result can be generalized in a different manner by using a technique valid for any equation cast in the form of Eq. (2) as explained in Ref. 13. We further showed that those resonances survive in the presence of a *finite density* of dimers, i.e., in the CRDM, and moreover, that they give rise to bands of finite width of truly extended states. This we established by analyzing several magnitudes, among which we take here the transmission coefficient as an example of the behavior of the model. We choose this magnitude because it will subsequently be the main ingredient for our explanation of delocalization.

An example of the mean behavior of the transmission coefficient around one of the resonant energies is shown in Fig. 1 for a dimer concentration $c=0.2$ ($c$ is defined as the ratio between the number of $\lambda'$ and the total number of $\delta$'s in the lattice); typical realizations behave in the same way, the only effect of averaging being to smooth out particular features of realizations keeping only the main common characteristic, i.e., the wide transmission peak. This is the property we want to highlight: Close to single dimer resonances (in the case of Fig. 1, the first one, which occurs at $E_r=3.7626\ldots$ for the chosen parameters $\lambda=1.0$, $\lambda'=1.5$), there is an interval of energies that shows also very good transmission properties, similar to those of the resonant energy. Most important, such interval has always a finite width, for all values of dimer concentration, $\lambda$ and $\lambda'$ (provided they satisfy the above conditions), or number of sites in the lattice. The peak width depends on the order of the resonance (the higher the resonance, the wider the band of states with transmission coefficient close to unity) and the concentration of dimers (the larger the concentration, the narrower the peak, being always of finite width as already stated). Other magnitudes, such as Landauer resistance or Lyapunov coefficient behave accordingly.[9]

After collecting the main *facts* about the CRDM and its bands of extended states, we state what is it that we want to *explain:* First, why are there intervals of energies for which the transmission is very close to unity *for every realization* of the CRDM? Second, why does the bandwidth decrease with increasing dimer concentration? Third, why does the bandwidth not vanish when the dimer concentration goes to 1? It is clear that if we are able to answer those questions, we would have understood the physical reasons for the appearance of the extended bands we are concerned with. This we discuss in detail in the next section.

## III. TRANSMISSION COEFFICIENT THROUGH LATTICE SEGMENTS

Pursuing answers to the above questions, we have computed the transmission coefficient of structures formed by $N$ sites of type $\lambda$ sandwiched either between two dimers or two single impurities, with all that group embedded in a perfect infinite chain of $\lambda$ sites. The calculation is once again a transfer matrix one, which yields an expression that can be evaluated with the help of a computer. The results, obtained by numerical evaluation of those exact analytical expressions, are plotted in Fig. 2 for the two dimer case and in Fig. 3 for the two single impurities case. Let us begin discussing the dimer results. It is apparent from Fig. 2 that in all cases considered, the transmission coefficient is very close to unity

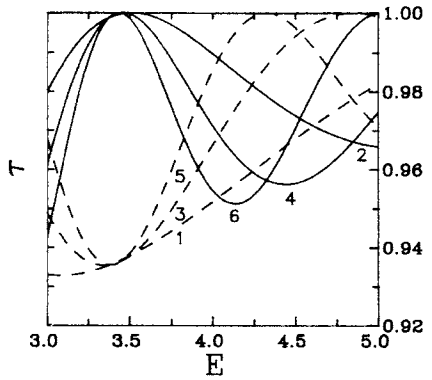


FIG. 3. Transmission coefficient for two single impurities with $N$ host sites in between, placed in the middle of an otherwise periodic chain, for $N=1$, 2, 3, 4, 5, and 6 as indicated in the plot (even $N$, solid lines; odd $N$, dashed lines). The $\delta$ function strengths are $\lambda=1$, $\lambda'=1.5$ as in Fig. 1.

for energies in the neighborhood of the resonant one. This must be related to the fact that eigenfunctions corresponding to those energies acquire an extra phase which will be different from the resonant energy condition (the change of phase has to be $\pi$), but very close to $\pi$ anyway. The key point is that for any value of $N$ considered, this interval is *always* located around the resonant energy. This must be compared to Fig. 3, where it can be seen that for different $N$ values the position of the perfectly transmitted energies is also different. Therefore, we can conclude that the physical reason underlying the existence of bands of extended states is this overlap of good transmission properties that happens in the CRDM *forced by the resonant energies* of the dimers.

The above results allow us also to understand why the width of the bands decreases with increasing concentration but being always finite: Note for the case with $N=1$ in Fig. 2 that even in this case, the band shows a nonzero extent. It is quite clear that in the high density limit most occurrences of the $\lambda$ sites will be of that type, i.e., one $\lambda$ between two dimers. This is the case that will then govern the total transmission coefficient of the chain (obviously, groups of dimers will be perfectly transparent around the resonant energy as this is placed in the $\lambda'$ band). We thus see that even in the case when the dimer concentration tends to unity, the structure of the transmission coefficient for $N=1$ will preserve the band. Upon decreasing the concentration, those cases will be more and more rare, and the dominant ones will have larger $N$. Figure 2 shows the dramatic increase of the band with increasing $N$, and this is in perfect agreement with the observations for the dilute chain.[8,9]

It is also possible to carry out a power expansion in $E-E_r$ of the transmission coefficient $\tau$ close to the resonant energy, starting from the above-mentioned transfer-matrix results. Importantly, the approach is general for any 1D model, because it can be first cast in the form of Eq. (2) (see Ref. 9) and then treated within the formalism we describe now. For the sake of brevity, we skip the general formulas and particularize Eq. (2) for the system $\lambda_1=\lambda_2=\lambda_{N+3}=\lambda_{N+4}=\lambda'$ and $\lambda_n=\lambda$ otherwise. We introduce reflection $r$ and transmission $t$ amplitudes through the relationships

$$\psi_n=\begin{cases} e^{ikn}+re^{-ikn}, & \text{if } n\leq 1, \\ te^{ikn}, & \text{if } n\geq N+4, \end{cases} \tag{3}$$

where $\cos k=\Omega$, and we define the promotion matrices

$$P=\begin{pmatrix} 2\Omega & -1 \\ 1 & 0 \end{pmatrix}, \quad P'=\begin{pmatrix} 2\Omega' & -1 \\ 1 & 0 \end{pmatrix}. \tag{4}$$

Notice that $P$ and $P'$ are unimodular. The reflection amplitude can be found as follows:

$$r=e^{ik}\frac{T_{11}-T_{22}+T_{12}e^{-ik}-T_{21}e^{ik}}{T_{21}-T_{12}+T_{22}e^{ik}-T_{11}e^{-ik}}, \tag{5}$$

where $T=(P')^2P^N(P')^2$. Taking into account that $P^N=U_{N-1}(\Omega)P-U_{N-2}(\Omega)I_2$, $I_2$ and $U_n$ being the $2\times 2$ unity matrix and the Chebyshev polynomial of second kind, respectively. Thus, the matrix elements $T_{ij}$ can be easily written down. So far, this result is exact for all energies; since we are interested in those values of $E$ close to $E_r$, a power expansion leads us after lengthy but straighforward calculations to the result $\tau=1-|r|^2\sim 1-f(N)(E-E_r)^2$, where $f(N)$ is a positive, energy-independent function written as $f(N)=A(E_r)\tilde{f}(N)$ with

$$A(E_r)=\frac{\Omega_r^2[\lambda'(\cos q_r-\sin q_r/q_r)-2q_r\sin q_r]^2}{E_r^2(1-\Omega_r^2)}, \tag{6a}$$

$$\tilde{f}(N)=\frac{1}{1+(1-\Omega_r^2)\left(\dfrac{U_{N-1}}{\Omega_r U_{N-1}-U_{N-2}}\right)^2}, \tag{6b}$$

and the dependence of the Chebyshev polynomials on $\Omega_r$ is understood. Here the subscript $r$ means that all expressions must be evaluated at the resonant energy $E_r$. Taking into account that $\tilde{f}(N)\leq 1$ we obtain a very important result, namely that $f(N)$ is bounded above. The upper bound is $A(E_r)=0.0247\ldots$ with our chosen parameters [$f(N)$ equals this value whenever $N$ satisfys $U_{N-1}(\Omega_r)=0$]. Hence, the transmission in the vicinity of the resonant energy is very close to unity. In addition, the above perturbative treatment yields a divergence of the localization length of the form $\sim(E-E_r)^{-2}$, as found in the RDM,[4] as well as by different means.[13]

## IV. CONCLUSIONS

In summary, we have explained the existence of bands of extended states in the CRDM as arising from the property that transmission is almost perfect for all kinds of segments in the lattice around the resonant energy, which is not the case if the impurities are not paired. It is crucial to notice that this holds for *every realization* of the model. This explanation also accounts for the dependence of the bandwidth on the dimer concentration and its finiteness for any such concentration. We have been able to estimate perturbatively the transmission coefficient and the divergence of the localization length in that energy interval. The relevance of this perturbative calculation increases if one realizes that it is possible to compute the mean transmission coefficient around the resonance by integrating $f(N)$ with the probability of

finding a segment of $N$ host sites in the infinite lattice. Furthermore, we believe that this explanation applies to all models in the same kind of disordered systems with defect grouping, because the calculations on those models will be formally very similar, as shown in Ref. 13.

We note in closing that the structure of the transmission coefficient as depicted in Fig. 2 suggests that it is possible to build devices with tailored properties by designing an *ordered* structure made up of unit cells formed by dimers with the appropriate number $N$ of host monomers between them. In this context, quantum well superlattices can be a perfect example of such devices, as it has been shown[11] that the CRDM can be realized in practice as a GaAs/AlGaAs system. On the other hand, there has been recently a significant increase of interest in nanotechnological applications of monomolecular assemblies on solid surfaces.[14] Such self-assembled monolayers (SAM) can build up complicated quasi-1D and 2D structures. One of the important properties of SAM's is that they can show very different electron conductivity depending on their composition and structure. We hope that the above resonant mechanism of appearance of the extended states in correlated disordered models will be relevant to understand and design SAM's with the desired conduction properties.

## ACKNOWLEDGMENTS

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

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

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

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

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

[6] P. K. Datta, D. Giri, and K. Kundu, Phys. Rev. B **47**, 10 727 (1993).

[7] J. C. Flores and M. Hilke, J. Phys. A **26**, L1255 (1993).

[8] A. Sánchez and F. Domínguez-Adame, J. Phys. A **27**, 3725 (1994).

[9] A. Sánchez, E. Maciá, and F. Domínguez-Adame, Phys. Rev. B **49**, 147 (1994); **49**, 15 428(E) (1994).

[10] A. Chakrabarti, S. N. Karmakar, and R. K. Moitra, Phys. Rev. B **50**, 13 276 (1994).

[11] E. Diez, A. Sánchez, and F. Domínguez-Adame, Phys. Rev. B **50**, 14 359 (1994). F. Domínguez-Adame, A. Sánchez, and E. Diez, *ibid.* **50**, 17 736 (1994).

[12] In addition, this calculation pinpoints another difference between RDM and CRDM. In the RDM, the energy is $E=q^2$, $q$ being the corresponding wave vector, where in the CRDM its role is played by $2\cos q$, thus giving rise to more than one band.

[13] F. Izrailev, T. Kottos, and G. P. Tsironis (unpublished).

[14] N. L. Abbott, J. P. Folkers, G. M. Whitesides, Science **257**, 1380 (1992); R. C. Tiberio, H. G. Craighead, M. Lercel, and T. Lau, Appl. Phys. Lett. **62**, 476 (1993); G. P. Berman, E. N. Bulgakov, and A. F. Sadreev (unpublished).