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Simple model for a quantum wire II. Statistically correlated disorder

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Abstract. In a previous paper (Eur. Phys. J. B **30**, 239–251 (2002)) we have presented the main features and properties of a simple model which –in spite of its simplicity– describes quite accurately the qualitative behaviour of a quantum wire. The model was composed of N distinct deltas each one carrying a different coupling. We were able to diagonalize the Hamiltonian in the periodic case and yield a complete and analytic description of the subsequent band structure. Furthermore the random case was also analyzed and we were able to describe Anderson localization and fractal structure of the conductance. In the present paper we go one step further and show how to introduce correlations among the sites of the wire. The presence of a correlated disorder manifests itself by altering the distribution of states and the localization of the electrons within the system.

PACS. 03.65.-w Quantum mechanics – 71.23.An Theories and models; localized states – 73.21.Hb Quantum wires

Introduction

In a previous paper [1], hereafter referred to as I, the authors have developed a simple model describing the main features shown by a Quantum Wire, namely: Band Structure when the structure is periodically arranged, Anderson Localization in the random case and easy calculation of Lyapunov exponents, density of electronic states and electrical conductance endowed with an encouraging fractal behaviour. We address the interested reader to reference [1] for the details of the model and the intrincacies of the computer calculations.

The main drawback of the scheme thereby presented was the lack of a coherent description of the possible correlations which must be present in any realistic model of one dimensional conductance. It is the purpose of the present paper to fill this gap by presenting a surprisingly simple way to incorporate correlations entirely based upon the random nature of the model. This means that in addition to describe correlations with different parameters of the wire (spacing, number and amount of species, ...) the model is flexible enough to be suitable for applying it to different correlation schemes such as the Tight-Binding model, the Anderson model and likely many others correlation prescriptions with sensible physical content.

The paper is organized as follows. In Section 1 we analyze the meaning of the correlations in terms of probabilities of a given atom to be followed by other of a different character. After this analysis we are able to set some limits for the values of these probabilities. The next step is to incorporate those probabilities to the Functional Equation developed in [1]. How this functional equation is modified by the introduction of correlations in the way just described and how it can be used to calculate the correlation-corrected Lyapunov exponent is the subject of Section 2. In Section 3 some results are shown along with a discussion about the effects of the correlations to close finally with a section of Conclusions.

1 Correlations

Let us consider disordered quantum wires with short-range correlations which will be specified by the probability for a certain atomic species to be followed by another type of atom in the chain sequence. In this model, the system will be characterized by the species concentrations $\{c_i\}_{i=1,\ldots,m}$ where m is the number of different species, and the set $\{p_{ij}\}_{i,j=1,\ldots,m}$ where p_{ij} means the probability for i to be followed by j (the prob. of finding j right after i). The correlations introduced in this way must be the consequence of the existence of an atomic interaction (or the effect of some physical parameters such as the size of the atoms) which might choose certain spatial sequences of the atoms modifying subtly the otherwise chain's purely random character. Thus this procedure seems a natural manner to account for correlations which can be present in nature or even those that can be produced inside a manufactured disordered quantum wire in a nonintentional way aside from the fact that of course one can always try to construct a wire exhibiting the desired correlations to recover the theoretical results.

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Let us clarify the meaning of p_{ij}. It is the ratio of the number of -ij- clusters and the number of i atoms (N_i). The probability p_{ij} is not the probability for j to be preceded by i, because the latter would be obtained dividing by the number of j atoms (N_j) instead of N_i. In the limit $N \to \infty$, the system will be determined by $\{c_i\}$ and $\{p_{ij}\}$ and therefore the density of states will be given by a limiting distribution depending only on those quantities. And that distribution is of course the same whether we move from left to right or from right to left along the chain. So, the correlations we measure have to coincide in both directions. Then it is clear that *for the infinite chain* p_{ij} *means the probability for an 'i' species atom to be followed or preceded by a 'j' species atom.*

Once we have understood the meaning of the correlations, let us derive the relations among them. What is the probability of finding at any position of the chain the cluster -iji-? We can write this quantity as,

$$c_i \cdot p_{ij} \cdot p_{ji} \rightarrow \text{prob. of finding } i \cdot \text{ finding } j \text{ after } i \cdot \cdot \text{ finding } i \text{ after } j$$

$$c_j \cdot p_{ji}^2 \rightarrow \text{prob. of finding } j \cdot \text{ finding } i \text{ after } j \cdot \cdot \text{ finding } i \text{ before } j.$$

Thus the equations for the correlations are,

$$c_i p_{ij} = c_j p_{ji} \tag{1a}$$

$$\sum_{j=1}^{m} p_{ij} = 1 \tag{1b}$$

$$0 \le p_{ij} \le 1 \quad i, j = 1, \ldots, m. \tag{1c}$$

According to the equations, the correlations matrix (p_{ij}) is completely known from the above diagonal elements, $\frac{m(m-1)}{2}$ where m is the number of different species. However these elements are not completely independent due to (1c), because when one of the correlations is chosen, the maximum allowed value for some of the rest may be affected. This fact can be clearly seen in two simple examples:

2 species: the matrix is completely determined by p_{12},

$$p_{11} = 1 - p_{12}; \quad p_{21} = \frac{c_1}{c_2} p_{12}; \quad p_{22} = 1 - p_{21}$$

but it must be $p_{21} \le 1 \Rightarrow p_{12} \le \frac{c_2}{c_1}$·

Therefore $p_{12} \le \min\left\{1, \frac{c_2}{c_1}\right\}$·

3 species: the matrix is determined by p_{12}, p_{13}, p_{23}. And we choose their values in that order.

$p_{12} \le \min\left\{1, \frac{c_2}{c_1}\right\}$ which implies

$p_{13} \le \min\left\{1 - p_{12}, \frac{c_3}{c_1}\right\}$·

On the other hand it must be,

$$p_{23} \le 1 - p_{21}$$

$$p_{32} \le 1 - p_{31} \Rightarrow p_{23} \le \frac{c_3}{c_2}(1 - p_{31}),$$

therefore $p_{23} \le \min\left\{1 - \frac{c_1}{c_2} p_{12}, \frac{c_3}{c_2} - \frac{c_1}{c_2} p_{13}\right\}$·

An expression for the general form of the maximum values can be obtained for arbitrary m. Choosing the above diagonal elements of the correlations matrix by rows,

$$\mathbf{P} = \begin{pmatrix} p_{11} & p_{12} & \longrightarrow \cdots & \longrightarrow & p_{1m} \\ p_{21} & p_{22} & p_{23} \longrightarrow & \longrightarrow & p_{2m} \\ \vdots & \vdots & \ddots \quad \ddots & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ p_{(m-1)1} & p_{(m-1)2} & \cdots\cdots & p_{(m-1)(m-1)} & p_{(m-1)m} \\ p_{m1} & p_{m2} & \cdots\cdots & p_{m(m-1)} & p_{mm} \end{pmatrix}$$

then

$$p_{ij} \le \min\left\{1 - \frac{1}{c_i}\sum_{k=1}^{i-1} c_k p_{ki} - \sum_{k=i+1}^{j-1} p_{ik}; \ \frac{c_j}{c_i} - \frac{1}{c_i}\sum_{k=1}^{i-1} c_k p_{kj}\right\} \tag{2}$$

where the limits are given by the previous chosen correlations.

Once the concentrations and $\mathbf{P}$ are fixed, the characterization of the quantum wire can be given in a compact form using the matrix

$$\mathbf{Q} = (q_{ij}) \equiv (c_i p_{ij}), \tag{3}$$

which is symmetric ($\mathbf{Q} = \mathbf{Q}^t$) and it determines uniquely the wire and its correlations:

$$\sum_{j=1}^{m} q_{ij} = c_i; \quad \sum_{i=1}^{m} q_{ij} = c_j; \quad p_{ij} = \frac{q_{ij}}{c_i};$$

q_{ij} means the probability of finding the cluster -ij- (-ji-) at any position inside the wire.

This model naturally includes the situation in which the disorder in the wire is completely random[1], that is just defined by the values $p_{ij} = c_j \quad i = 1, \ldots, m$. Figure 1 shows an example of the correlation space for 2 species.

2 The functional equation

We will now obtain the correlation form of the functional equation, which enable us to calculate the density of states. In this process we are using some of the results and expressions obtained in reference [1].

The relations for the phase transmission inside the wire read,

$$\mathcal{T}_j^{-1}(\theta) = \arctan\left(2h_j(\epsilon) - \frac{1}{\tan\theta}\right) \tag{4a}$$

$$\mathcal{T}_j^{-1}(\theta + n\pi) = \mathcal{T}_j^{-1}(\theta) + n\pi \qquad \theta \in [0, \pi) \tag{4b}$$

where $h_j(\epsilon) = \cos(\epsilon) + \frac{(a/a_j)}{\epsilon}\sin(\epsilon)$. To carry out the phase average we rearrange the terms depending on the species

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[1] The case in which the wire is obtained "throwing" the atoms in the given concentrations randomly and there are no mechanisms (interactions) which select some privileged clusters or series of atoms.

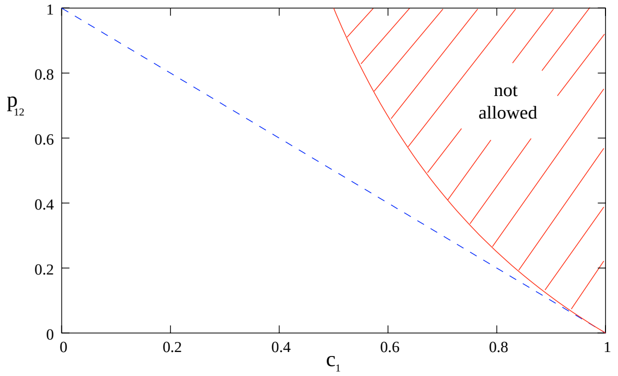


Fig. 1. Correlation space for 2 species as a function of the concentration. The blue dashed line corresponds to the completely random configurations.

of the last atom we have passed,

$$\langle\Delta\theta\rangle = c_1\frac{1}{N_1}\sum_{j_1}\{\mathcal{T}_j(\theta_j)-\theta_j\}+\ldots$$

$$\ldots + c_m\frac{1}{N_m}\sum_{j_m}\{\mathcal{T}_j(\theta_j)-\theta_j\} \quad (5)$$

where N_i is the number of atoms of species i and the sumatory over j_i means we are summing over all the positions j such that the atom at $(j-1)$ is of i-kind:

$$\langle\Delta\theta\rangle = c_1\langle\Delta\theta\rangle_1+\ldots+c_m\langle\Delta\theta\rangle_m=\sum_\gamma c_\gamma\langle\Delta\theta\rangle_\gamma. \quad (6)$$

From now on the greek indices will refer to species while the latin indices mean the sites of the chain. In this case there exist correlations in the sequence of atoms, that is the probability for one species to be a neighbour of another type can be different for all of them. This implies that each species will give rise to a particular distribution function for the phase.

$$\langle\Delta\theta\rangle_\gamma = \frac{1}{N_\gamma}\sum_{j_\gamma}\int_0^\pi\frac{\mathrm{d}W_j^\gamma(\theta)}{\mathrm{d}\theta}\{\mathcal{T}_j(\theta)-\theta\}\,\mathrm{d}\theta \quad (7)$$

where $W_j^\gamma(\theta)$ is the distribution function of the phase at the position j generated by the species γ. The equations for the distributions ((B.14) in [1]) become here,

$$W_j^\gamma(\theta) = W_{j-1}^{(*)}\left(\mathcal{T}_\gamma^{-1}(\theta)\right)-W_{j-1}^{(*)}\left(\frac{\pi}{2}\right)+1 \quad (8a)$$

$$W_j^\gamma(\theta+r\pi) = W_j^\gamma(\theta)+r \quad \theta\in[0,\pi) \quad r\in\mathbb{Z} \quad (8b)$$

for all species and positions, where the superscript "$(*)$" means that we do not know the species of the atom preceding the γ atom, placed at position $(j-1)$; we only know the probability for a certain species to be there. Let us introduce now the average over all possible sequences with the given concentrations.

$$\langle\Delta\theta\rangle_\gamma = \frac{1}{N_\gamma}\sum_{j_\gamma}\int_0^\pi\frac{\mathrm{d}W_j^\gamma(\theta)}{\mathrm{d}\theta}\sum_\beta p_{\gamma\beta}\{\mathcal{T}_\beta(\theta)-\theta\}\,\mathrm{d}\theta \quad (9)$$

and,

$$W_j^\gamma(\theta) = \sum_\beta p_{\gamma\beta}\left\{W_{j-1}^\beta\left(\mathcal{T}_\gamma^{-1}(\theta)\right)-W_{j-1}^\beta\left(\frac{\pi}{2}\right)\right\}+1. \quad (10)$$

The next step consists in taking the limit $N\rightarrow\infty$ to approach the limiting distribution.

We define $\mathbf{W}_\gamma(\theta)=\lim\limits_{N_\gamma\rightarrow\infty}\frac{1}{N_\gamma}\sum\limits_{j_\gamma}W_j^\gamma(\theta)$ which is the solution of:

$$\mathbf{W}_\gamma(\theta) = \sum_\beta p_{\gamma\beta}\left\{\mathbf{W}_\beta\left(\mathcal{T}_\gamma^{-1}(\theta)\right)-\mathbf{W}_\beta\left(\frac{\pi}{2}\right)\right\}+1 \quad (11a)$$

$$\mathbf{W}_\gamma(\theta+r\pi)=\mathbf{W}_\gamma(\theta)+r \quad \theta\in[0,\pi) \quad r\in\mathbb{Z}. \quad (11b)$$

And finally we have to calculate,

$$\langle\Delta\theta\rangle = \sum_{\gamma,\beta}c_\gamma p_{\gamma\beta}\int_0^\pi\frac{\mathrm{d}\mathbf{W}_\gamma(\theta)}{\mathrm{d}\theta}\{\mathcal{T}_\beta(\theta)-\theta\}\,\mathrm{d}\theta. \quad (12)$$

To carry out the integral we shall make use of the existence of a value θ_0 such that $\mathcal{T}_\gamma(\theta_0)=\theta_1 \quad \forall\,\gamma$, and proceeding by parts,

$$\langle\Delta\theta\rangle = (\theta_1-\theta_0)-\overbrace{\sum_{\gamma,\beta}c_\gamma p_{\gamma\beta}\int_{\theta_0}^{\theta_0+\pi}\mathbf{W}_\gamma(\theta)\frac{\mathrm{d}\mathcal{T}_\beta(\theta)}{\mathrm{d}\theta}\mathrm{d}\theta}^{\text{①}}$$

$$+\sum_\gamma c_\gamma\int_{\theta_0}^{\theta_0+\pi}\mathbf{W}_\gamma(\theta)\mathrm{d}\theta. \quad (13)$$

To evaluate the middle term we use the average of equations (11a) which is

$$\sum_\gamma c_\gamma\mathbf{W}_\gamma(\theta)+\sum_\beta c_\beta\mathbf{W}_\beta\left(\frac{\pi}{2}\right)-1=$$

$$\sum_{\gamma,\beta}c_\gamma p_{\gamma\beta}\mathbf{W}_\beta\left(\mathcal{T}_\gamma^{-1}(\theta)\right). \quad (14)$$

With a simple change of variable, the use of (14) and the equations for the correlations we can write,

$$\text{①} = \sum_{\gamma,\beta}c_\beta p_{\beta\gamma}\int_{\theta_1}^{\theta_1+\pi}\mathbf{W}_\gamma\left(\mathcal{T}_\beta^{-1}(\theta)\right)\mathrm{d}\theta$$

$$=\sum_\gamma c_\gamma\int_{\theta_1}^{\theta_1+\pi}\mathbf{W}_\gamma(\theta)\mathrm{d}\theta+\pi\sum_\beta c_\beta\mathbf{W}_\beta\left(\frac{\pi}{2}\right)-\pi, \quad (15)$$

and going back to (13),

$$\langle\Delta\theta\rangle = (\theta_1-\theta_0)+\pi-\pi\sum_\beta c_\beta\mathbf{W}_\beta\left(\frac{\pi}{2}\right)$$

$$+\sum_\gamma c_\gamma\left\{\int_{\theta_0}^{\theta_0+\pi}\mathbf{W}_\gamma(\theta)\mathrm{d}\theta-\int_{\theta_1}^{\theta_1+\pi}\mathbf{W}_\gamma(\theta)\mathrm{d}\theta\right\}. \quad (16)$$

It is not hard to see with the help of (11b) that the last term is $\theta_0 - \theta_1$. Therefore,

$$\frac{\langle \Delta\theta\rangle(\epsilon)}{\pi} = 1 - \sum_{\gamma} c_\gamma \mathbf{W}_\gamma\left(\frac{\pi}{2}\right)\cdot \tag{17}$$

Thus the density of states reads ((B.8) in [1]),

$$g(\epsilon) = \left|\sum_{\gamma} c_\gamma \frac{d\mathbf{W}_\gamma\left(\frac{\pi}{2}\right)}{d\epsilon}\right| \tag{18}$$

which can be calculated numerically solving equation (11a) for several values of the energy.

2.1 The Lyapunov exponent

The quantity that provides information about the degree of spatial localization of the electronic states is the Lyapunov exponent, which gives the exponential growth rate of the wave function, and thus its inverse is a measure of the localization length of a state exponentially localized inside the wire. The Lyapunov coefficient can be written for the infinite wire as

$$\Lambda = \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N} \log\left|\frac{\Psi_{j+1}}{\Psi_j}\right| \tag{19}$$

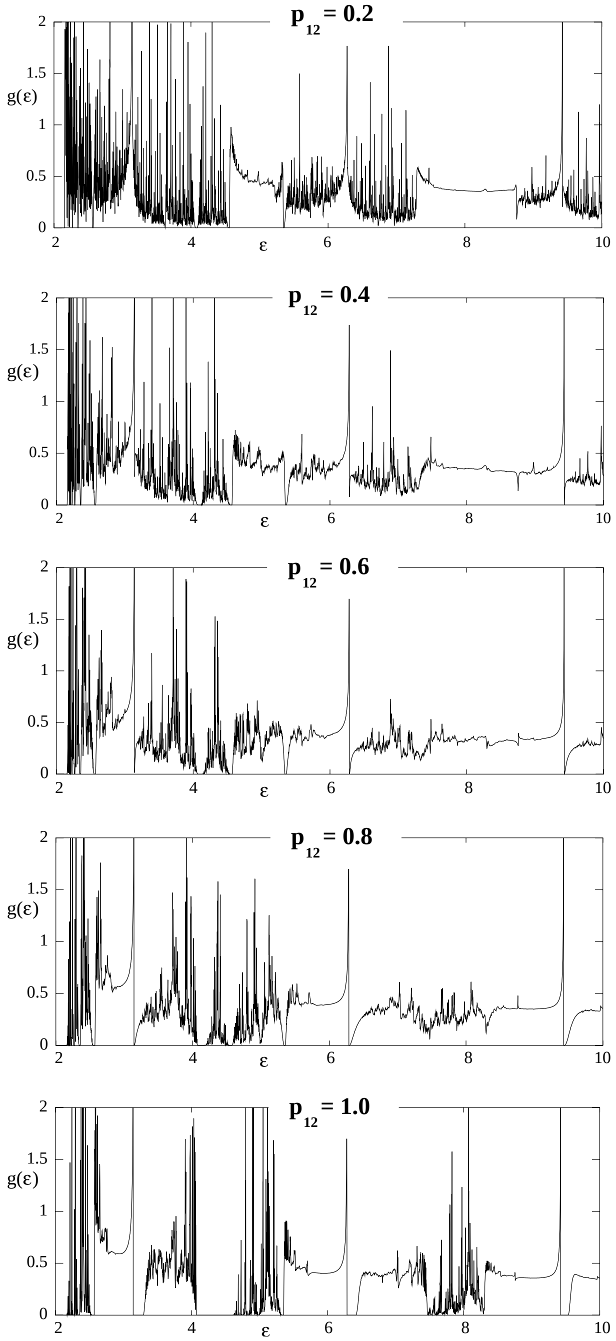
where Ψ_j is the amplitude of the wave function at the jth atomic site. Using a mapping technique originally proposed in reference [2] we are able to write Λ as a function of the phase (Appendix A),

$$\Lambda = \frac{1}{2} \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N} \log F_{\gamma_j}(\theta_j) \tag{20}$$

where $F_{\gamma_j}(\theta) = 1 - 2h_{\gamma_j}(\epsilon)\sin(2\theta) + 4h^2_{\gamma_j}(\epsilon)\cos^2\theta$ and γ_j stands for the species of the jth atom. Due to the periodicity of $F(\theta)$ we can use the distribution functions of the phase to calculate the average (20):

$$\begin{aligned}\Lambda &= \frac{1}{2}\sum_{\gamma,\beta} c_\gamma p_{\gamma\beta} \int_0^\pi \frac{\mathrm{d}\mathbf{W}_\gamma(\theta)}{\mathrm{d}\theta} \log F_\beta(\theta)\mathrm{d}\theta \\ &= \frac{1}{2}\sum_{\gamma} c_\gamma \log F_\gamma(\pi) - \frac{1}{2}\sum_{\gamma,\beta} c_\gamma p_{\gamma\beta} \int_0^\pi \mathbf{W}_\gamma(\theta)\frac{F'_\beta(\theta)}{F_\beta(\theta)}\mathrm{d}\theta.\end{aligned} \tag{21}$$

From this last expression one can obtain numerically the Lyapunov exponent as a function of the energy.


$p_{12} = 0.2$

$p_{12} = 0.4$

$p_{12} = 0.6$

$p_{12} = 0.8$

$p_{12} = 1.0$

Fig. 2. Density of states for a disordered wire of two species with different correlations. $\left(\frac{a}{a_1}\right) = -3$ and $\left(\frac{a}{a_2}\right) = 4$ with $c_1 = 0.4$.

3 Results

Once we have built the mathematical framework lying under the model, one can try to answer the physical questions that obviously arise from this new configuration of the disordered quantum wire: how strong is the effect of this short-range correlations, does it produce a measurable change in the density of states or in the localization of the electrons? As in reference [1], we solve the functional equation numerically to obtain the density of states and to calculate the Lyapunov exponent. It seems really hard to find analytical solutions for equations (11) if they exist at all. Let us analyze in the first place the density of states (DOS) for our quantum wires. In Figure 2 the evolution of

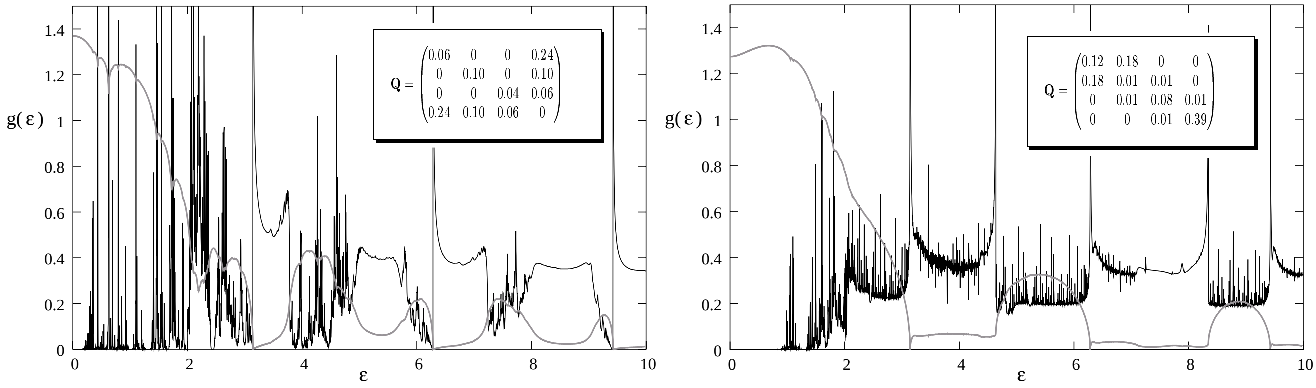
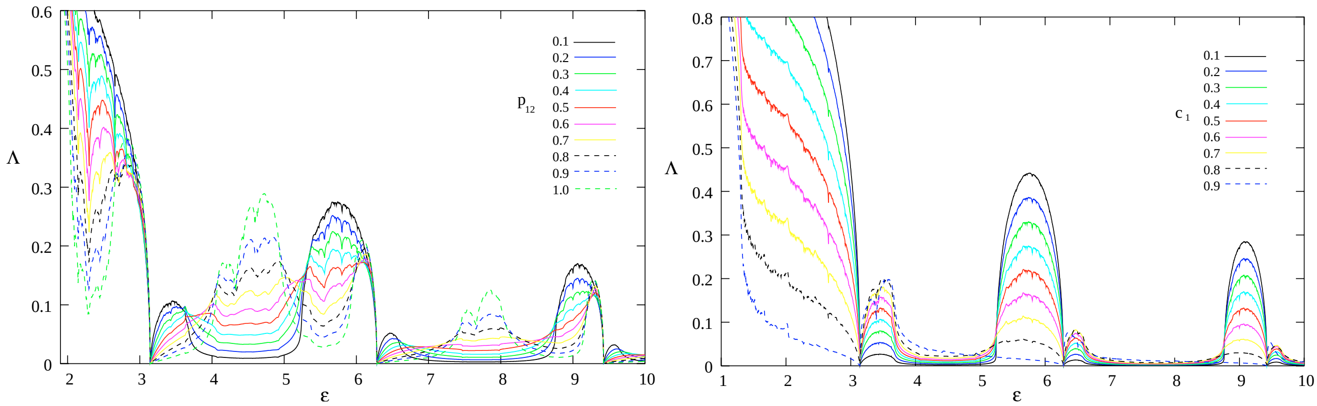


Fig. 3. DOS and Lyapunov exponent (grey line) for a 4 species quantum wire: $\left(\frac{a}{a_i}\right) = 1, -1, 3, -5$. Notice that the concentrations are the same for the two configurations.



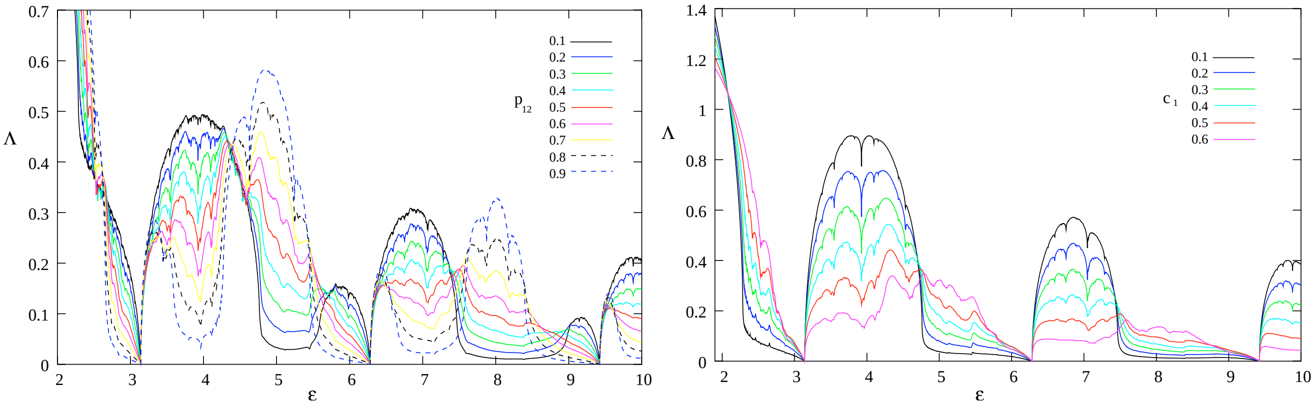
(a) $c_1 = 0.4$

(b) $p_{12} = 0.1$

Fig. 4. Variation of the Lyapunov exponent for a binary wire composed of $\left(\frac{a}{a_1}\right) = 1$ and $\left(\frac{a}{a_2}\right) = -3$, as a function of the correlation and as a function of the concentration.

the DOS for a binary wire as a function of the correlation p_{12} is shown for a certain value of the concentrations. This distribution of states is drastically changed from the initial situation in which the probability to find the cluster -12- is low to the final stage when we impose the atoms of species 1 to appear always isolated. Note however that the concentrations are the same in both cases! Another example can be seen in Figure 3 for a wire composed of 4 species. As the number of species increases, the number of correlations grows as $\frac{m(m-1)}{2}$, and the distribution of states can adopt a lot of different shapes: the exploration of the whole correlations and concentrations space for $m > 2$ can take a long time. From these graphics we conclude that the correlations can unbalance the spectra of the disorder system quite far from the completely random configuration. In fact the correlation can be tuned to open (close) an energy gap or to increase (decrease) the number of available states in a certain energy interval without changing the concentrations of the atomic components. The variation of the DOS with the correlations is of course a function of the concentrations being the chain with homogenized participation the one whose distribution has the strongest dependence on **P**. Let us also remark that the fractal behaviour of the density of states in certain energy ranges, reported in reference [1], still manifests itself for the different correlations regimes.

Let us have a look at the localization of the electronic states. In Figures 4 and 5 the behaviour of the Lyapunov exponent for a binary chain changing the correlations and the concentrations is shown. In Figure 3 the different shapes of the degree of localization for different correlations can also be noticed for a 4-species wire. The effective influence of the correlations on the localization of the electrons inside the quantum wires is established. In the study of correlated disorder two main kinds of correlations have been taken into account namely short-range and long-range. The former, mainly represented by the random dimer model [3], has been widely accepted to be the reason for the emergence of resonant energies and a set of states close to the resonant one for which



(a) $c_1 = 0.5$ (b) $p_{12} = 0.5$

Fig. 5. Variation of the Lyapunov exponent for a binary wire composed of $\left(\frac{a}{a_1}\right) = -2$ and $\left(\frac{a}{a_2}\right) = 5$, as a function of the correlation and as a function of the concentration.

the localization length becomes larger that the system size [4], improving greatly the transport properties [5]. The long-range correlations seem to be able to include in the spectrum mobility edges [6], that can be entirely controlled by the correlators [7], yielding an energy interval of a complete transparency. In our type of wires we have not observed mobility edges nor resonant energies. However an important effect on the localization of the states is shown that seems to act globally in the whole energy range in contrast to the more restricted effect of others short-range correlated disorder models. In fact for certain energies the Lyapunov exponent can be decreased an 80–90% of its maximum value changing the correlations at the expense of an increasing behaviour for other energies. Whether these correlations might cause Λ to go below the inverse of the length of a finite sample for some energy intervals is not certainly clear but it could be a point for future discussions. One can now argue if this influence of the correlations on the localization as well as on the DOS will be a measurable effect on short finite wires that represent a simple practical implementation, or on the contrary is just theoretically achievable only in infinite unreal systems. In order to answer that question and ascertain ourselves of the importance of the results we learn to generate finite sequences showing this kind of correlations. In Figure 6 we show the Lyapunov exponent of an infinite wire for a certain concentration and correlation calculated using the functional equation, and the one obtained numerically from equation (19) for a correlated disordered chain of 1000 atoms. The convergence is excellent with only one realization of the correlated disorder using one thousand of atoms, and we have also checked it for others couplings of the species and other correlations obtaining a high degree of agreement. Thus it means that the described results are real effects with some practical importance on experimental realizations and on the other hand that the method of the functional equation, although designed for an infinite wire, can reproduce quite well the tendency in finite samples.

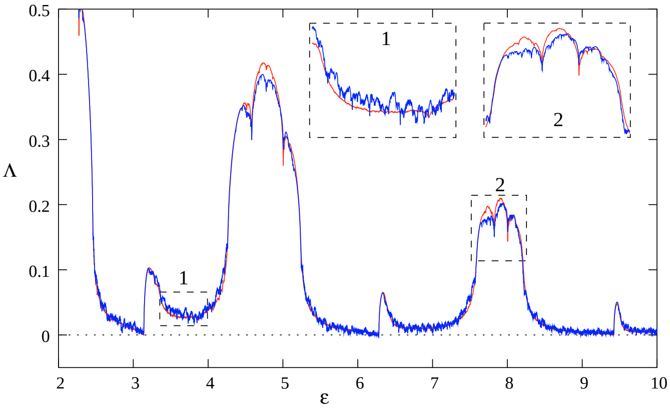


Fig. 6. Lyapunov exponent for a binary wire with $\left(\frac{a}{a_1}\right) = -2$, $\left(\frac{a}{a_2}\right) = 3$, $c_1 = 0.5$ and $p_{12} = 0.9$. The red line corresponds to the infinite wire. The blue line shown Λ numerically calculated for a sequence of 1000 atoms.

4 Concluding remarks

To summarize, we have extended the model proposed in reference [1] and completed the formalism introduced there including the possible correlations which must be present in any realistic model of one dimensional conductance. The method described here is the most natural manner to account for correlations that can manifest in nature or even inside a manufactured quantum wire in a nonintentional way.

It has been established how due to the correlated disorder the density of states is essentially modified and the localization of the electronic states changes in a non negligible proportion which might alter some macroscopic properties of these structures.

In addition to the obtained results we are preparing a future report in which we will construct the functional equation formalism in a more coherent way relating it to others methods currently used. There it will be shown how this mathematical framework is flexible enough to be suitable for applying it to different disorder models such as the Tight-Binding model as well as other correlation schemes such as the random dimer.

Finally we would like to point out that the software we have built to solve numerically the functional equation with correlations and to calculate the density of states and the Lyapunov exponent is freely available to the public at `http://sonia.usal.es/qwires/` so everyone can use it to reproduce the results hereby presented and to explore new configurations.

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Appendix A: Lyapunov exponent

It can be shown that the electronic wave function satisfies,

$$2h_{\gamma_j}(\epsilon)\Psi_j = \Psi_{j+1} + \Psi_{j-1} \tag{22}$$

where Ψ_j is the amplitude of the wave function at the jth atomic site of the chain. This equation can be visualized as a two dimensional mapping in polar coordinates with the identification $\Psi_{j+1} = r_{j+1}\cos\theta_{j+1}$ and $\Psi_j = r_{j+1}\sin\theta_{j+1}$,

$$\begin{pmatrix} r_{j+1}\cos\theta_{j+1} \\ r_{j+1}\sin\theta_{j+1} \end{pmatrix} = \begin{pmatrix} 2h_{\gamma_j}(\epsilon) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} r_j\cos\theta_j \\ r_j\sin\theta_j \end{pmatrix} \tag{23}$$

which yields the known transmission relationship for the phase and the following for the moduli r,

$$\frac{r_{j+1}^2}{r_j^2} \equiv F_{\gamma_j}(\theta_j) = 1 - 2h_{\gamma_j}(\epsilon)\sin(2\theta_j) + 4h_{\gamma_j}^2(\epsilon)\cos^2\theta_j. \tag{24}$$

If now we introduce the polar coordinates into the definition of the Lyapunov exponent we obtain:

$$\begin{aligned} \Lambda &= \lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N}\log\left|\frac{\Psi_{j+1}}{\Psi_j}\right| \\ &= \lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N}\log\left(\frac{r_{j+1}}{r_j}\right) + \lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N}\log\left|\frac{\cos\theta_{j+1}}{\cos\theta_j}\right| \\ &= \lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N}\log\left(\frac{r_{j+1}}{r_j}\right) \end{aligned} \tag{25}$$

because according to the meaning of Λ the cosinus term must be zero. And using (24) we can calculate the Lyapunov coefficient as a function of the phase, as:

$$\Lambda = \frac{1}{2}\lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N}\log F_{\gamma_j}(\theta_j) \tag{26}$$

which is our expression (20).

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