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Simple model for a quantum wire III. Transmission in finite samples with correlated disorder

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Abstract. The effect of a continuous model of correlations upon one-dimensional finite disordered quantum wires modeled by an array of delta-potentials, is analyzed. Although the model proposed is not able to include new truly extended states in the spectrum, the transport properties of a finite sample are noticeably improved due to the existence of states whose localization length is larger than the system size. This enhancement of transmission is maximized for relatively short chains.

PACS. 03.65.-w Quantum mechanics – 72.15.Rn Localization effects (Anderson or weak localization) – 73.63.Nm Quantum wires

Introduction

In a previous series of papers [1,2], the authors have analyzed in detail a simple model describing the main features shown by a one-dimensional quantum wire. The potential consists of an array of delta potentials, a pattern which has been extensively considered (and indeed it is nowadays) in the literature [3]. In reference [1] the band structure was fully analytically solved when the structure is periodically arranged and the density of states together with the localization properties were described in the random case, for which several novel features such as the fractal structure of the DOS were reported. In reference [2] the random model was extended to include statistically correlated disorder in a very natural manner. The effects of the correlations upon the properties of the system in the thermodynamic limit were studied, however the question of whether that type of correlations changes or not the transport properties of real finite structures was left open, and this is the subject of the present work. The presence of a correlated disorder in a one-dimensional random system can strongly change its physical properties, by including new resonant extended states in the case of short-range correlations [4], or with the emergence of mobility edges for the carriers when long-range correlations appear [6]. The importance of these correlation phenomena has also been established for two-dimensional structures [7].

The paper is organized as follows. In Section 1, we briefly review the model focusing on the description of the binary disordered chain and the techniques used to analyze the transport properties. In Section 2 a large amount of results is presented together with a discussion about the effects observed, to close finally with a section of Conclusions.

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1 Review of the model

Let us briefly review the basic features of the 1D model proposed. For a detailed description see references [1,2]. The wire is modeled by a linear array of equally spaced delta potentials with different couplings following a random sequence. In the completely random case, the properties of the system are then determined by the couplings (a/a_i) of the species composing the chain and their concentrations $\{c_i\}$. The density of states and the localization of the electrons can be studied in the thermodynamic limit by making use of the functional equation formalism. It is also possible to introduce short-range correlations in the structure, modifying the probability of different atomic clusters to appear in the wire sequence. This can be done by considering an additional set of probabilities $\{p_{ij}\}$ obeying certain equations, where p_{ij} means the probability for an i-atom to be followed or preceded by a j-atom. Thus the frequency of appearance of binary atomic clusters can be altered by this quantities. The probability of finding at any position the couple $-ij-(-ji-)$ would be c_ip_{ij} or equivalently c_jp_{ji}. Then in the thermodynamic limit the physical properties of such a system will depend upon the couplings of the species, the concentrations, and the probabilities $\{p_{ij}\}$. This correlated model naturally includes the situation when the disorder in the wire is completely random, that is just defined by the values $p_{ij} = c_j$.

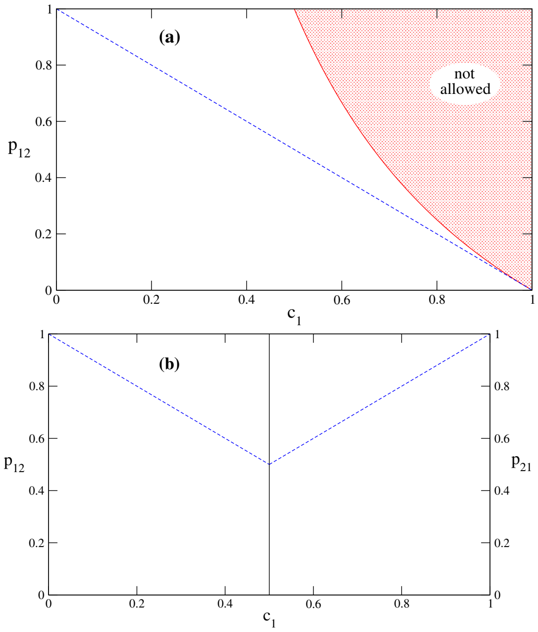

Fig. 1. (color online) Correlation space for 2 species as a function of the concentration. (a) p_{12} vs. c_1, (b) optimal representation: if $c_1 \leq 0.5$ then p_{12} vs. c_1, if $c_1 > 0.5$ then p_{21} vs. c_1. The blue dashed line corresponds to the completely random configurations.

In this work only binary chains are considered, so let us study in detailed the correlation scheme for this case. Our wire will be determined by one of the concentrations $\{c_1, c_2\}$ and one the probabilities $\{p_{11}, p_{12}, p_{21}, p_{22}\}$, that satisfy the relations $p_{11} + p_{12} = p_{22} + p_{21} = 1$ and $c_1 p_{12} = c_2 p_{21}$. One usually takes as configuration parameters $c_1 \leq 1$ and $p_{12} \leq \min\{1, c_2/c_1\}$. The allowed configuration space with these parameters is shown in Figure 1a. However one can optimize the representation of this space by choosing the parameters $\{c_1, p_{12}\}$ when $c_1 \leq 0.5$ and $\{c_1, p_{21}\}$ when $c_1 > 0.5$, so that the configuration space is expanded and the spatial points can be better differentiated, as shown in Figure 1b. Therefore, for a given concentration different values for $p_{12}(p_{21})$ can be chosen, and only one of them corresponds to the completely random chain. When the configuration of the binary chain lies on the dashed lines of Figure 1, we have a completely random chain whereas if the configuration lies anywhere else we have a correlated chain.

The main aim of this work is to elucidate whether or not this type of short-range correlations can improve the transport properties of real finite systems. With this purpose the following techniques are used, in contrast with the ones used in [1,2] for treating infinite systems.

1.1 Transmission matrix formalism

The time-independent scattering process in one-dimension can be described using the well-known continuous transfer matrix method [8]. The transmission matrix for a delta potential preceded by a zero potential zone of length a can be easily calculated yielding,

$$\mathbf{M}_j(k) = \begin{pmatrix} \left(1 - \frac{\mathrm{i}}{ka_j}\right) \mathrm{e}^{\mathrm{i}ka} & -\frac{\mathrm{i}}{ka_j}\mathrm{e}^{-\mathrm{i}ka} \\ \frac{\mathrm{i}}{ka_j}\mathrm{e}^{\mathrm{i}ka} & \left(1 + \frac{\mathrm{i}}{ka_j}\right) \mathrm{e}^{-\mathrm{i}ka} \end{pmatrix} \quad (1)$$

where $a_j = \hbar^2/(m\alpha_j)$ means the "effective range" of the jth delta, being α_j its coupling. The composition of N potentials can then be considered through the product of matrices,

$$\mathbb{M} = \mathbf{M}_N \ldots \mathbf{M}_2 \mathbf{M}_1 \quad (2)$$

to obtain the global transmission from $T(k) = |\mathbb{M}_{22}|^{-2}$. This formalism can be numerically applied to consider large chains but one finds also that for delta potentials it is possible to write analytical closed expressions for the scattering amplitudes of a chain composed of N different units [9].

Once the transmission of the finite sample has been calculated, the inverse of the localization length of the electronic states can be characterized by the Lyapunov exponent via the expression [10,11]

$$\lambda(k) = -\frac{1}{2N} \log T(k). \quad (3)$$

2 Results

The effects of the correlations upon the system at the thermodynamic limit were extensively analyzed in reference [2]. The authors concluded that the density of states is drastically changed by the effect of correlations. For a wire with fixed concentrations, the correlations can be tuned to open or close gaps in the spectrum, and they alter the number of available states at a certain energy as well as the smooth or irregular evolution of the DOS. Concerning the spatial extension of the electron wave functions, the influence of the correlations on the localization properties was established. An important change on the localization length was observed for all energies. The value of the Lyapunov exponent could be greatly decreased for some energies at the expense of an increasing behaviour in other ranges. However this type of correlations does not cause the appearance of neither new resonant energies nor mobility edges for the carriers. The question of whether these correlations might change the transport properties of a finite system was left open.

Let us have a look at the transmission patterns of finite binary chains for different configurations of concentrations and correlations. In Figures 2 and 3 the transmission is shown for several chains composed of 1000 atoms, for different values of the couplings and concentrations. In these cases the worst transmission corresponds to the completely random configurations, for which the transmission probability only raises near the multiples of π due to the well known resonances of the model at these energies. However as we move away from the completely random configuration (above or below the dashed line) the

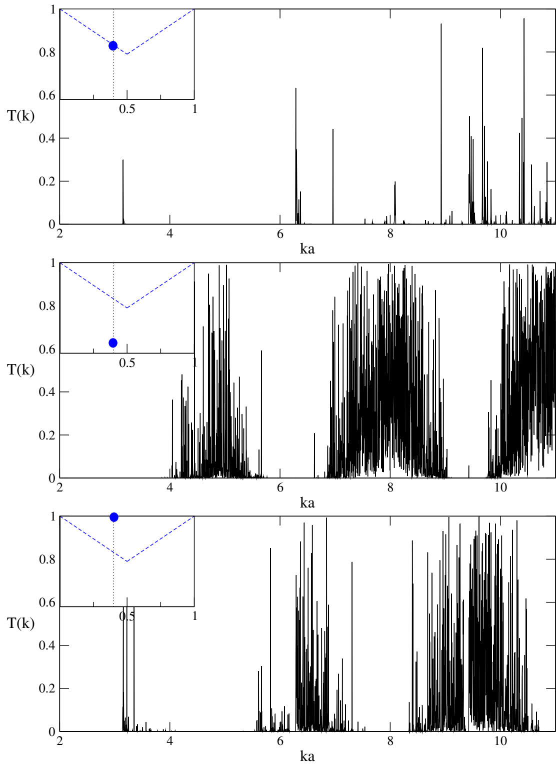

Fig. 2. Transmission probabilities vs. energy for 1000 atoms binary disordered chains with couplings $(a/a_1) = 1$, $(a/a_2) = -1$ and concentrations $c_1 = 0.4$, $c_2 = 0.6$ for different correlation configurations. From top to bottom $p_{12} = 0.6, 0.1, 1.0$. The circular point inside the insets mark the configuration on the correlation space. Only one realization of the disorder has been considered for each case.

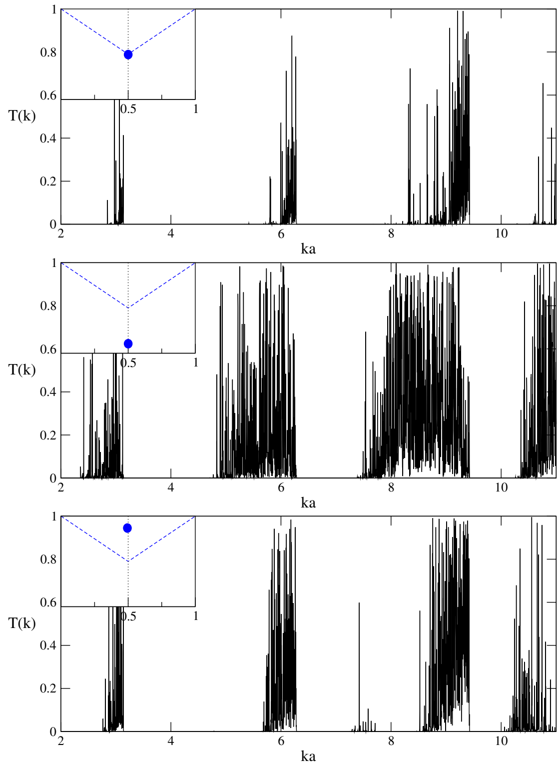

Fig. 3. Transmission probabilities vs. energy for 1000 atoms binary disordered chains with couplings $(a/a_1) = 2$, $(a/a_2) = 4$ and concentrations $c_1 = c_2 = 0.5$ for different correlation configurations. From top to bottom $p_{12} = 0.5, 0.1, 0.85$. The circular point inside the insets mark the configuration on the correlation space. Only one realization of the disorder has been considered for each case.

transmission is noticeably improved. Notice that this improvement is not necessary localized around the multiples of π. Although quantitatively this enhancement depends on the values of the couplings, qualitatively it seems a generic behaviour. In order to check whether this effect can be extended over the whole correlation space, we characterize each of its points by an efficiency of transmission defined as,

$$T_{\rm eff} = \frac{1}{k_2 - k_1} \int_{k_1}^{k_2} T(k) \mathrm{d}k \qquad (4)$$

which is the area enclosed by the transmission coefficient per energy unit. This definition depends on the integration interval, but qualitatively the results will not be affected as long as a reasonable interval is chosen, generally one of the form $[0, k_2]$. Notice that for very high energies the transmission will saturate for all configurations, thus the contribution to the integral in (4) will be the same independently of the c_1, p_{12} values. We are interested in establishing a qualitative comparison of this efficiencies for different correlations.

For certain values of the couplings and a length of 1000 atoms the evolution of this transmission efficiency over the configuration space is shown in Figure 4. It is clearly shown that the lowest values for the transmission efficiency are distributed around the completely random configurations, specially when the participation of the species is homogenized ($c_1 \sim 0.5$). High efficiencies can be observed for low and high concentrations of one of the species (and therefore approaching a pure chain) and around the point $\{c_1 = 0.5, p_{12} = 1.0\}$ which corresponds to the periodic binary chain. Nevertheless by looking at the evolution of $T_{\rm eff}$ as a function of p_{12} for

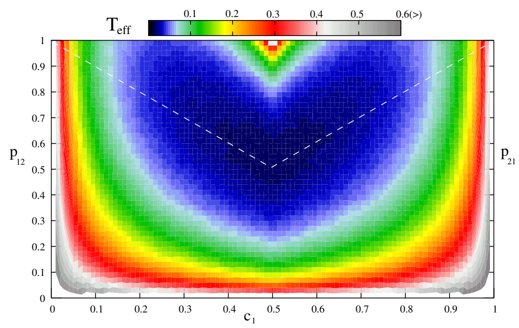

Fig. 4. (color online) Transmission efficiency for different configurations of a binary chain with 1000 atoms and couplings $(a/a_1) = 1$, $(a/a_2) = -1$. For each configuration only one realization of the disorder has been considered. The integration interval for $T_{\rm eff}$ was $[0, 15]$.

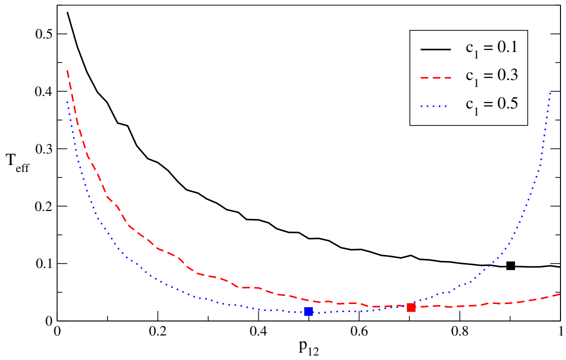

Fig. 5. (color online) $T_{\rm eff}$ vs. p_{12} for 1000 atoms binary chains with couplings $(a/a_1) = 1$, $(a/a_2) = -1$ and different concentrations. The squares on the lines mark the position of the completely random configuration.

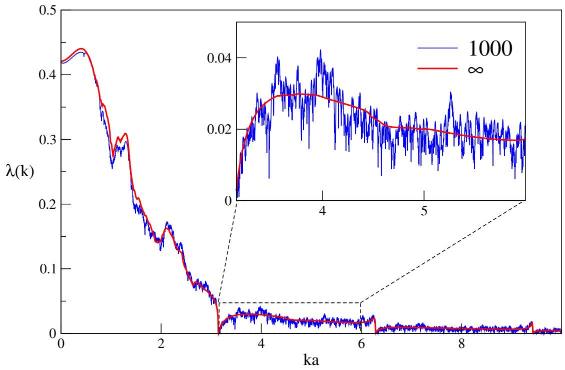

Fig. 6. (color online) Lyapunov exponent vs. energy for a binary chain with parameters $(a/a_1) = 1$, $(a/a_2) = -1$, $c_1 = 0.4$, $p_{12} = 0.6$. The blue line corresponds to a 1000 atoms realization and the red line to the infinite chain.

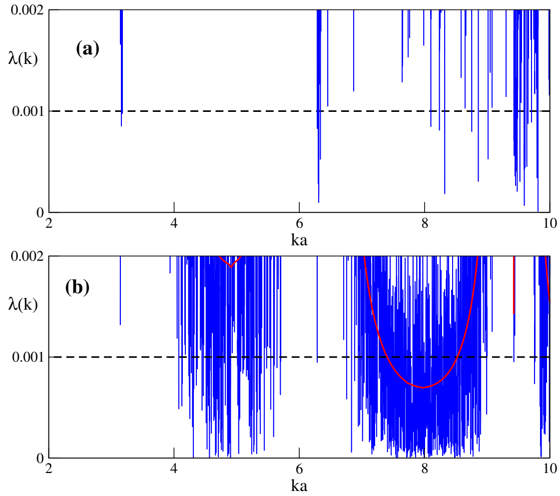

Fig. 7. (color online) Lyapunov exponent vs. energy for a 1000 atoms binary chain with couplings $(a/a_1) = 1$, $(a/a_2) = -1$ and concentration $c_1 = 0.4$ for (a) completely random configuration $p_{12} = 0.6$ and (b) correlated configuration $p_{12} = 0.1$. The dashed line marks the inverse of the length of the sample. The red line shows the Lyapunov exponent for the infinite chain.

a fixed concentration (Fig. 5) we conclude that the minimum efficiency is reached near the completely random configuration and the correlated situations show noticeably higher values. Therefore the electronic transmission through a finite wire is improved by this type of correlations although truly extended states do not appear in the system. The reason for the improvement then must be the existence of states behaving as extended states, that is their localization length being larger than the system size. Let us analyze the behaviour of the Lyapunov exponent. In Figure 6 the Lyapunov exponent as a function of the energy is shown for a random chain. We can see a very good agreement between the thermodynamic limit and the finite realization of the disorder, that shows a characteristic fluctuating behaviour around the values of the former one. These fluctuations are responsible for the enhancement of transmission. A fine observation of the Lyapunov exponent, in Figure 7, reveals that for a chain with fixed concentrations the number of states whose localization length exceeds the sample length increases dramatically in a correlated configuration with respect to the completely random situation. The correlations induce a decrease of the limiting distribution of the Lyapunov exponent in certain energy ranges, so that for a finite system the fluctuations of this quantity around its mean value make the appearance of such states possible. Let us notice that the decreasing of the limiting value of the Lyapunov exponent does occur in different energy ranges depending on the parameters of the chain so that the improvement of the transmission can take place in different energy intervals because the appearance of states whose localization length ($L_{\rm loc}$) is larger than the length of the system (L) is not restricted to the vicinity of the resonances located at the multiples of π. This is in sharp contrast to other short-range correlated models such as the random dimer [4,5], which is able to improve the transport in finite systems [12] in a similar manner but the states with $L_{\rm loc} > L$ always appear around a resonant extended state ($L_{\rm loc} = \infty$). Let us remark that although the fluctuating pattern is a fingerprint of the particular realization of the disorder, the amplitude of these oscillations does only depend upon the length of the system. Therefore the results are not due to particular bizarre realizations of the disorder for a given length. The behaviour described can be clearly observed in all realizations of a certain configuration. The fluctuations of the Lyapunov exponent for finite chains are quantified through the variance var(λ) that according to the central limit theorem must decrease asymptotically with the length of the system as L^{-1} [13]. This asymptotic behaviour of the Lyapunov exponent can be checked in Figure 8 where the evolution of the variance with the length of the system is analyzed for different localization lengths corresponding to different configurations. For a certain value of the energy and the correlations the localization length is obtained from the Lyapunov exponent in the thermodynamic limit λ_∞ (calculated with the method described in Ref. [2]). Then, different realizations of the disorder for different lengths are considered for calculating

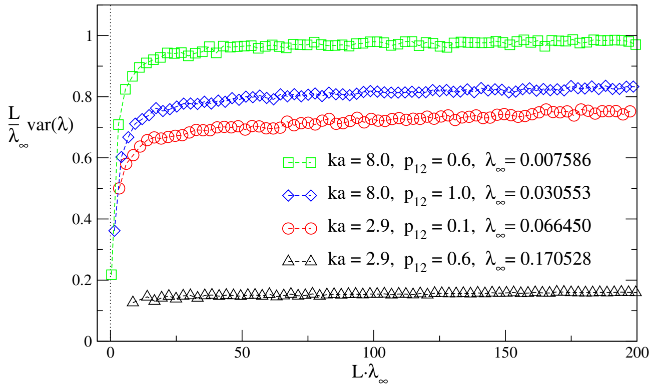

Fig. 8. (color online) Evolution of the fluctuations of the Lyapunov exponent versus the length of the system for a binary chain with parameters $(a/a_1) = 1$, $(a/a_2) = -1$ and concentration $c_1 = 0.4$. The variance times the length of the system divided by the value of the Lyapunov in the thermodynamic limit (λ_∞) is plotted for different energies and correlations. For each length the variance is obtained after averaging over 5×10^4 realizations of the disorder.

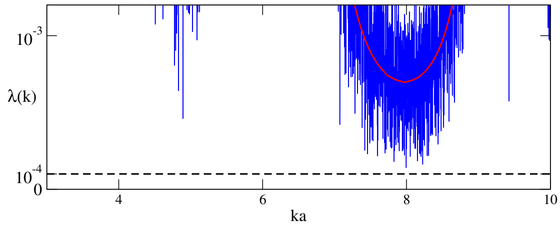

Fig. 9. (color online) Lyapunov exponent vs. energy for a binary chain with couplings $(a/a_1) = 1$, $(a/a_2) = -1$ in a correlated configuration $c_1 = 0.4$, $p_{12} = 0.1$ for 10^4 atoms. The dashed line marks the inverse of the length of the sample. The red line corresponds to the infinite chain. To be compared with Figure 7b.

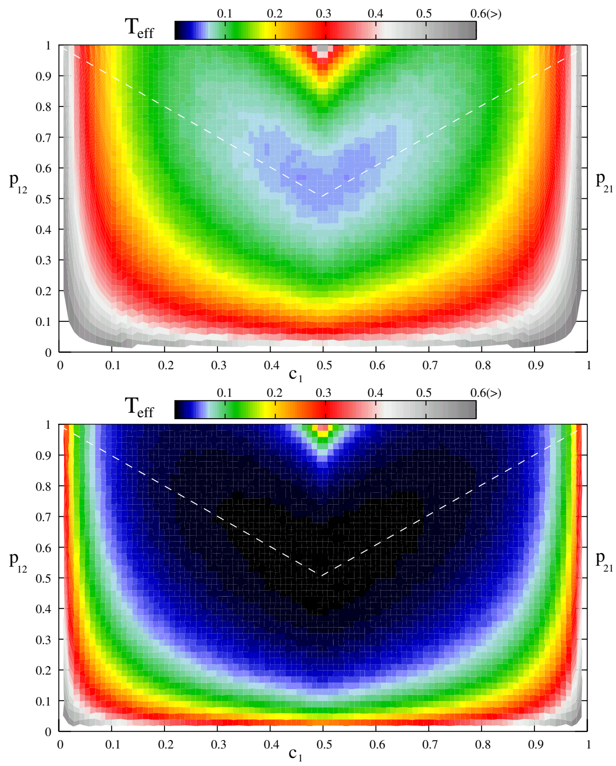

Fig. 10. (color online) Transmission efficiency over configuration space for a binary chain with couplings $(a/a_1) = 1$, $(a/a_2) = -1$ for different lengths: $L = 500$ (top) and $L = 2000$ (bottom).

the variance of the Lyapunov $\mathrm{var}(\lambda) = \langle \lambda^2 \rangle - \lambda_\infty^2$ where the average is taken over 5×10^4 realizations for each length. The plot $\mathrm{var}(\lambda) L/\lambda_\infty$ versus $L/L_{\rm loc} \equiv L\lambda_\infty$ clearly shows a saturation when $L \gg L_{\rm loc}$ in all the cases considered. The asymptotic value reached depends of course on λ_∞ and the distribution of these asymptotic values for different λ_∞ must necessarily be related to the single parameter scaling theory [14]. This theory originally establishes that in the localized regime ($L\lambda_\infty \gg 1$) the variance of the Lyapunov exponent (LE) scales with the length of the system according to the limiting value of the LE itself, so that the distribution of the variance for different values of the LE (i.e. different values of the energy) satisfies $\tau \equiv \mathrm{var}(\lambda) L/\lambda_\infty \sim 1$. However the regime in which the single parameter scaling works is still controversial and new expressions for τ and new scales for the validity of SPS have recently appeared [15]. Also the exact value of τ seems to depend on the model and the type of distributions considered. It would be very interesting to check the applicability of SPS for this correlated model. However this task deserves a thorough and deep analysis [16].

It must then be clear that taking averages of the Lyapunov exponent over several realizations kills its fluctuating behaviour since that procedure is intended to approach the thermodynamic limit. And on the other hand averaging the values of the efficiency of transmission over several realizations for a given length will not have any effect on the results presented, according to the previous discussion.

As expected for a model of short-range correlations, all the effects disappear unavoidably in the thermodynamic limit. Thus as the length of the chain grows the fluctuations of the Lyapunov exponent decrease and the localized character of the electronic states naturally manifests itself for all energies (Fig. 9). The lost of the enhancement of transmission can also be shown as a function of the evolution of $T_{\rm eff}$ over the configuration space for different lengths. The higher the number of atoms the more the black zones spread from the completely random lines (Fig. 10). However the decay of the transmission efficiency with the length of the system depends upon the correlations. In Figure 11 it can be seen how the fastest decreasing corresponds to the completely random situation, whereas the correlated chains show always higher efficiencies for all lengths. Plotting for different configurations $\Delta T_{\rm eff} = T_{\rm eff} - T_{\rm eff}(R)$ as a function of the length, where (R) means the completely random situation, we see how the effect of the correlations reaches a maximum which is roughly contained in the region $L \sim 200 - 500$, apparently independent of the values of the species couplings.

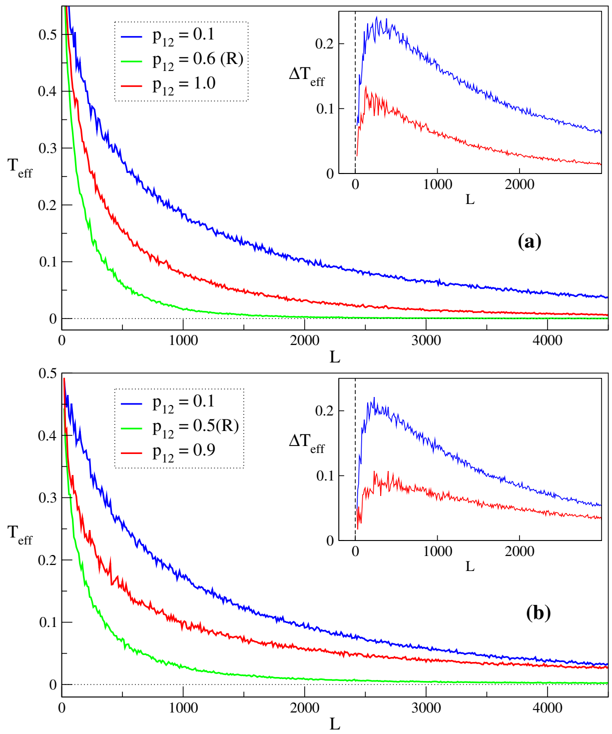

Fig. 11. (color online) Transmission efficiency vs. length for different configurations of a 1000 atoms binary chain with parameters (a) $(a/a_1) = 1$, $(a/a_2) = -1$, $c_1 = 0.4$ and (b) $(a/a_1) = 2$, $(a/a_2) = 4$, $c_1 = 0.5$. (R) marks the completely random situation. The inset shows the relative differences $\Delta T_{\text{eff}} = T_{\text{eff}} - T_{\text{eff}}(R)$.

3 Conclusions

To summarize, we have analyzed in detail the effect of a model of correlations proposed in [2], on finite disordered wires. The improvement of the transport properties has been established, not only by looking at the transmission coefficient of particular chains, but also in the whole correlation space of a binary array through the transmission efficiency. For fixed concentrations the electronic transport reaches its minimum intensity near the completely random configuration, whereas the correlated situations show noticeably higher transmission efficiencies. The enhancement of the transport properties is due to the appearance of states with a localization length larger that the system size that effectively behave as extended states. As the length of the system grows the effect of these short-range correlations disappears, and the transmission decreases. The fastest decay corresponds to the completely random situation. The effect of the correlations as a function of the length reaches a maximum for relatively short chains $L \sim 200 - 500$.

We believe that the behaviour described is essentially independent of the potential model and that the same effects could be observed for other models such as the tight-binding scheme or for square barriers, as well as for the case where more species are included in the wire. Let us finally remark that although the correlation model considered is not able to include any new truly extended state in the spectrum, its effects upon the transport of real finite samples are absolutely non-negligible and they may be significant in certain experimental devices such as for example superlattices, which have already been used to observe the effect of other models of short-range correlations [12].

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