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# Effect of nonlinear interactions on resonant states of the random dimer model

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#### Abstract

A simple Kronig–Penney model for 1D mesoscopic systems with  $\delta$  peak potentials is used to study numerically the effect of non-linear interaction on the resonant states of the random dimer model. It is shown that the nonlinear interaction increases or decreases the width of the resonances depending on both its sign and strength. The resonance width  $\Delta E$  is a power law decaying with the system size as  $L^{-\gamma}$ . The exponent  $\gamma$  decreases linearly with the nonlinear interaction strength when the dimer impurity concentration increases. The resonance energy states, in these systems, are shifted depending on the kind of interaction. Further investigations are provided on the effect of nonlinearity on conductance fluctuations near the resonances.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

It is well established that almost all eigenstates of one-dimensional disordered systems are localized for any amount of disorder [1]. The electronic transmission coefficient was shown to have an exponential decay [2, 3] leading to the absence of transport in an infinite system. However, recently some models of disorder introducing correlation [4, 5] and nonlinearity [6, 7] have been found to exhibit a number of extended states at particular energies. These discrete extended states have been observed recently in the experiment with  $GaAs-Al_xGa_{1-x}As$  random superlattices [8] and in nonlinear disordered media [9].

Several one-dimensional models with correlated disorder have been proposed which exhibit delocalized states. The typical one is the random dimer model (RDM) introduced by Dunlap *et al* [10]. In the RDM, where the impurities are randomly embedded in nearest-neighbour pairs in an originally pure host chain,  $\sqrt{N}$  extended electronic states were found of length N [10, 11]. A discrete number of extended eigenstates was found numerically [12, 13]

in RDM and experimentally examined using transmission measurements on semiconductor superlattices [8]. These results have been confirmed by microwave transmission spectra of single-mode waveguides with inserted correlated scatterers [14]. Delocalization has also been reported to occur in disordered chains with correlated off-diagonal interactions [15, 16]. Short-range correlation was found to be responsible for a metal-insulator transition in one-dimensional lattices [17]. In these 1D systems, the metallic phase is well characterized by a Gaussian conductance distribution. Furthermore, the existence of a mobility edge separating extended and localized states was confirmed for 1D random systems with weak long-range correlated disorder [18–20]. The bandwidth of extended states was found to behave as  $1/\sqrt{L}$  (*L* being the system size) [21]. This means that this phase has a zero measure in the thermodynamic limit.

On the other hand, nonlinear interactions are often present in a real system. The nonlinear Schrödinger equation has been studied extensively in recent years and served as a prototype for studying nonlinear phenomena. The origin of the nonlinearity in the Schrödinger equation corresponds to different physical phenomena. In electronic systems, it would correspond to Coulomb interaction while in a superfluid it corresponds to Gross–Pitaevsky equation. In a previous paper [22], we found that the nonlinearity can either localize or delocalize the electronic states depending on the strength and the sign of the nonlinear potential. Physically, a repulsive nonlinear (NL) potential represents the electron–electron interactions are important in various systems such as quantum dots, superlattices, etc [23]. It is also found that the nonlinearity can suppress the Wannier–Stark effect caused by the electric field in the case of ordered potentials and can give rise to a transition from superlocalized to weakly localized states in disordered systems [24].

The aim of this paper is to investigate the effect of nonlinear interactions in a system with correlated disorder and particularly their effects on resonant transmission induced by correlation. It is also important to study the effect of nonlinear interaction on resonance band width, which is important for conduction. Interplay between the delocalization effect induced by the correlated disorder and the localization (delocalization) effect caused by the non-linear interaction is our interest.

### 2. Model description

The model considered here is of an electron with energy *E* moving along a one-dimensional periodic lattice of *N*  $\delta$ -peak potentials plus nonlinear interaction of strength  $\alpha$  on each site. The corresponding Schrödinger equation is [25]

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{n=1}^N (\beta_n + \alpha |\Psi(x)|^2) \delta(x - na)\right] \Psi(x) = E \Psi(x) \tag{1}$$

where  $\Psi(x)$  is the single-particle wavefunction at site x. The *n*th site potential strength  $\beta_n$  takes either the value  $\beta_{cr}$  or  $\beta_{dm}$  corresponding to the crystal host and the dimer respectively. The potential  $\beta_{dm}$  is randomly distributed along the chain and appears in pairs. The nonlinear interaction is of  $\delta$ -function type and with constant strength  $\alpha$ . This means that the electron propagates freely between lattice sites and interacts only at x = n. The electron energy E is expressed here in units of  $\hbar^2/2m$ . All the nonlinear physics is contained in the coefficient  $\alpha$ . The positive  $\alpha$  corresponds to repulsive (electron–electron) interaction while negative  $\alpha$  models attractive (electron–phonon or ion) interactions. The lattice parameter is taken for commodity to be unity (L = N). The two ends of the chain are assumed to be connected to perfect leads where the wavefunctions are plane waves. The wavefunctions between lattice sites are of the

form  $\Psi_n = A_n e^{ikx} + B_n e^{-ikx}$  where the momentum is given by  $k = \sqrt{E}$ . The differential equation (1) can be mapped by the Poincaré map representation into the following recursive equation [25]:

$$\Psi_{n+1} + \Psi_{n-1} = \left[ 2\cos\sqrt{E} + \frac{\sin\sqrt{E}}{\sqrt{E}} (\beta_n + \alpha |\Psi_n|^2) \right] \Psi_n.$$
<sup>(2)</sup>

The solution of equation (2) is carried out iteratively by taking the two initial wavefunctions at sites 1 and 2:  $\Psi_1 = e^{-ik}$  and  $\Psi_2 = e^{-2ik}$ .

The transmission problem considers an incident wave at x = L with  $\Psi(x) = r_0 e^{-ik(x-L)} + r_1 e^{ik(x-L)}$  for  $x \ge L$  and a transmitted wave  $\Psi(x) = t^{-ikx}$  for  $x \le 0$ . In order to have a uniquely defined problem the output is fixed  $|t^2| = 1$  and then the corresponding input  $r_0$  is calculated. The coefficient  $r_0$  is given by

$$r_0 = t \frac{(\Psi_N - e^{-i\sqrt{E}}\Psi_{N+1})}{(e^{2i\sqrt{E}} - 1)}.$$
(3)

The transmission coefficient  $(T = |t/r_0|^2)$  reads [26]

$$T = \frac{|e^{2i\sqrt{E}} - 1|^2}{\left|\Psi_{N+2} - e^{-i\sqrt{E}}\Psi_{N+3}\right|^2}.$$
(4)

Thus the transmission coefficient depends only on the values of the wavefunction at the end sites,  $\Psi_{N+2}$  and  $\Psi_{N+3}$ , which are evaluated from the iterative equation (2). In order to study the nature of the electronic states around the resonance of the dimer, we use the dimensionless conductance *g* which is related to the transmission coefficient via the Landauer formula for 1D systems [27]:

$$g = \frac{2T}{1 - T} \tag{5}$$

where the factor of two arises from the two possible states of the electron spin and the variance of the logarithm of the conductance (Ln(g)) reads

$$\operatorname{var}(\operatorname{Ln}(g)) = \langle \operatorname{Ln}(g)^2 \rangle - \langle \operatorname{Ln}(g) \rangle^2 \tag{6}$$

where  $\langle \cdots \rangle$  denotes an average over different realizations of the random potential.

#### 3. Results and discussion

We choose for convenience in the rest of the paper  $\beta_{cr} = 1$  and  $\beta_{dm} = 1.5$ . The chain length is 5000 and we take dimer concentration c = 2%. We define the concentration c as the ratio between the number of single scatterers with potential strength  $\beta_{dm}$  and the total number of scatterers of the system. The transmission coefficient is averaged over 1000 samples. The nonlinear interaction is present in the dimer impurities. We first examine the NL interaction effect on the resonance width of dimer within the first allowed band of the host. In a second step, we study the conductance and its fluctuations around and away from the resonance energy to explain the transition induced by nonlinearity.

Let us examine how the resonance width is affected by the NL interaction. The transmission coefficient of the random dimer model is plotted, in figure 1, for three values of NL strength  $\alpha$ . For negative nonlinear interaction  $\alpha$ , it is seen that the energy resonance is slightly shifted to the lower energies while it width increases in comparison with the linear case ( $\alpha = 0$ , dotted curve). For positive  $\alpha$ , the resonances get displaced to higher energies and

1,0

0,8

 $\alpha = -0.2$ 





Figure 1. Transmission coefficient versus the energy averaged over 1000 realizations of the same system for different NL strengths for  $\alpha = 0$ ,  $\alpha = +0.2$  and  $\alpha = -0.2$ .

become sharper. The energy resonant shift is due to the variation of the effective potential of the dimer. From figure 1 we can measure the resonance width for different values of nonlinear interaction strength. The behaviour of the band width is clearly shown in figure 2, where the width of the resonance  $\Delta E$  is plotted as a function of the nonlinear interaction both for positive and negative  $\alpha$ .

It is shown from this figure that a positive non-linearity decreases the width of the resonance, indicating a localization phenomenon. Therefore, for negative nonlinearity, the width starts to increase for  $|\alpha| < |\beta_{dm} - \beta_{cr}|$  which is a signature of delocalization of the electron eigenstates. The resonance width becomes maximum for  $|\alpha| = |\beta_{dm} - \beta_{cr}|$  and beyond this critical value the behaviour is then reversed, that is the resonance width decreases with  $|\alpha|$ . For the critical value  $|\alpha|_c = |\beta_{dm} - \beta_{cr}|$  the system seems to be transparent and the electron moves freely.

The delocalization (the increase of the resonance width) can be explained by the fact that when the nonlinear interaction strength  $|\alpha|$  ( $\alpha < 0$ ) is increased the effective potential of the dimer component in equation (1) given by

$$\beta_{\rm dm}^* = \beta_{\rm dm} + \alpha |\Psi_n|^2 \tag{7}$$

tends to approach the crystal component potential  $\beta_{cr}$ . For the critical value  $|\alpha|_c = |\beta_{dm} - \beta_{cr}|$ , the effective potential in equation (7)  $\beta_{dm}^* \approx \beta_{cr}$  and the system becomes periodic.

It was shown in the random dimer model and in the linear case ( $\alpha = 0$ ) that the width of the resonance behaves with the system size as  $1/\sqrt{L}$  [21]. This means that in the thermodynamic limit the resonance width vanishes. To understand the behaviour of the band width with the nonlinear interaction, we plotted the resonance width as a function of the system size (log–log scale) for different values of  $\alpha < 0$ . All the curves show a power-law decrease of  $\Delta E$  with the system size. The inset in figure 2 is an example for  $\alpha = -0.4$ . The curve is compared



**Figure 2.** The resonance width as a function of the nonlinear interaction  $|\alpha|$ . The solid lines are a guide for the eye. Inset: the resonance width versus the system size (log–log scale) for  $\alpha = -0.4$ ; the slope of the fitted line is -0.30.



**Figure 3.** Power-law exponent  $\gamma$  as a function of nonlinear interaction  $|\alpha|(\alpha < 0)$  for dimer concentration c = 0.2 (diamond), c = 0.5 (squares) and c = 0.7 (triangles). The straight lines are the result of numerical fitting.

with a linear fit of a slope equal to -0.3. This means that  $\Delta E$  behaves as  $L^{-0.3}$ . In figure 3 is plotted the power-law exponent  $\gamma$  ( $\Delta E = L^{-\gamma}$ ) as a function of NL strength  $|\alpha|$  ( $\alpha < 0$ ) for



**Figure 4.** Mean of the logarithm of conductance (Ln(g)) versus the system size at resonant energy  $E_r$  for different NL strengths  $\alpha > 0$ .

three values of dimer concentration c = 0.2, 0.5 and 0.7. For small concentration (c = 0.2), it is clearly seen that the power-law exponent  $\gamma$  is invariant as in the linear case ( $\alpha = 0$ ). The behaviour is preserved for any amount of NL interaction, that is  $\Delta E = 1/\sqrt{L}$ . When the concentration is increased,  $\gamma$  seems to decrease linearly following the equation

$$\gamma = A|\alpha| + B$$

(8)

where A = -0.48 (-0.6) and B = 0.48 (0.44) for c = 0.5 (0.7).

It is also shown, from figure 3, that even in the linear case ( $\alpha = 0$ )  $\gamma$  depends slightly on the dimer concentration *c*.

To investigate the nature of the electronic states at and around the resonance, we have studied the scaling of the conductance at resonant energy. Figure 4 shows the mean of the logarithm of conductance  $\langle Ln(g) \rangle$  as a function of system size for different values of  $\alpha > 0$ . Each curve is built by averaging over 1000 realizations of the disorder. For  $\alpha = 0$ , the conductance is essentially constant up to system size N = 5000, indicating the extended nature of the eigenstates. When increasing  $\alpha$ , the conductance drops exponentially towards zero as the system size increases, indicating a clear-cut transition. This behaviour confirms that a positive NL interaction localizes the electronic eigenstates.

In figure 5, we show the variance of Ln(g) as a function of the electron energy for different values of the NL interaction  $\alpha$ . Notice the strong decrease of the fluctuations close to the resonant energy  $E_r$  (figure 5(a)). Away from the energy resonance  $E < E_r$ , these fluctuations increase with the strength of the NL interaction  $|\alpha| (\alpha > 0)$ , indicating the strong localization of the eigenstates. We can also observe from this figure that the conductance fluctuations are smaller at the right side of the resonance  $(E > E_r)$  in comparison to those at the left side  $(E < E_r)$ . The correlations induce an increase of the conductance in certain energy ranges so that for a finite system the fluctuations of this quantity around its mean value become small. The delocalization transition is different on each side of the resonance.



**Figure 5.** Variance of Ln(g) versus the energy for different NL strengths for L = 1000 and (a) repulsive NL potentials, (b) attractive NL potentials.

For a negative NL interaction, the magnitude of the conductance fluctuations becomes smaller on increasing the NL intensity  $|\alpha|$  (figure 5(b)), which is an indication of delocalization of the electron eigenstates.

In summary, the non-linear interaction seems to delocalize the electronic states when it is attractive ( $\alpha < 0$ ) and provided that  $|\alpha| < |\beta_{dm} - \beta_{cr}|$ . For the other cases ( $|\alpha| > |\beta_{dm} - \beta_{cr}|$ ) or for a repulsive nonlinear interaction ( $\alpha > 0$ ), it seems to localize the electronic states.

## 4. Conclusion

We investigated in this paper the effect of non-linearity on the resonant states of the random dimer model using a simple Kronig–Penney Hamiltonian. We found that the nonlinear interaction increases or decreases the width of the resonance depending on both its sign and strength. We also found that the resonance width  $\Delta E$  is a power-law decaying with the system size as  $L^{-\gamma}$ . The exponent  $\gamma$  depends on the concentration of the dimer impurities. It decreases linearly with the nonlinear interaction strength when the concentration increases. This means that the conduction is enhanced when the NL interaction increases provided that  $|\alpha| < |\beta_{\rm dm} - \beta_{\rm cr}|$ . At energy resonance, we found that increasing repulsive interaction leads to localization while an attractive one reduces the conductance fluctuations near the resonance energy, indicating a delocalization transition. It is important to study the whole conductance distribution near the resonance to know more on this transition. The difference in the behaviour of the conductance fluctuations, on both sides of the resonant energy, suggests more investigations using the Lyapunov exponent statistics. This will be a subject for a forthcoming paper.

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