Nonlinearity Effect on 1D Periodic and Disordered Lattices

K. Senouci\textsuperscript{1}, N. Zekri \textsuperscript{1}, H. Bahlouli\textsuperscript{2} and A.K. Sen \textsuperscript{3}

AS-ICTP, 34100 Trieste Italy

\textsuperscript{1}Laboratoire d’Etude Physique des Materiaux, Departement de Physique, UST Oran, B. P. 1505, Oran El-M’naouer, Algerie.

\textsuperscript{2}Physics Department, KFUPM, Dhahran 31261, Saudi-Arabia.

\textsuperscript{3}LTP Division, Saha Institute for Nuclear Physics, 1/AF Bidhannagar, Calcutta 700 064, India

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Abstract

The Kronig-Penney model is used to study the effect of nonlinear interaction on the transmissive properties of both ordered and disordered chains. In the ordered case, the nonlinearity can either localize or delocalize the electronic states depending on both its sign and strength but there is a critical strength above which all states are localized. In the disordered case, however, we found that the transmission decays as $T \sim L^{-\gamma}$ around the band edge of the corresponding periodic system. The exponent $\gamma$ is independent of the strength of the nonlinearity in the case of disordered barrier potentials, while it varies with this strength for mixed potentials.

Keyword: Band spectrum, non-linearity, interaction, disorder.
1 Introduction

Wave propagation in nonlinear media is a subject of recent intensive research [1]. The study of this phenomenon is of great practical importance in the understanding of transport properties of superlattices [2], electronic behavior in mesoscopic devices and optical phenomena in general. 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 might correspond to different physical phenomena. In electronic systems it would correspond to Coulomb interaction between confined electrons while in a superfluid it corresponds to the Gross-Pitaevsky equation which attracted much interest in recent years in the area of Bose-Einstein condensation of trapped bosonic atoms [3]. One then uses the usual technique, as in linear systems, to deduce transmission and related properties of interest. However, there are differences though with the linear problem. Most important for us is the fact that the transmission is not uniquely defined. In contrast to the linear case it is no longer equivalent to study the transmission for a fixed input (normalized incident wave) or fixed output (normalized transmitted wave). This non-equivalence originates from the fact that for a given output, there is one and only one solution to the given problem. In contrast, for a fixed input, there is at least one solution to the problem but, because of the nonlinearity, there might be more than one solution for a given system length [4]. In particular, it is believed that this non-uniqueness gives rise to multistability and noise and might originate a chaotic behavior in certain systems [5, 6].

From the theoretical point of view we expect new effects to arise due to the competition between the well known localizing effects of the disorder and the delocalizing effect due to the nonlinear interaction in an appropriate regime. Anderson’s theory predicts that the wave function of a non-interacting electron moving in a one dimensional lattice with on-site energetic disorder is localized even for an infinitesimal amount of disor-
Thus in the linear regime but in the presence of disorder, for a given incident wave with wavenumber $k$ (or an electron with energy $E$), the transmission coefficient decays exponentially with the system length. On the other hand, the decay of the transmission is much slower in nonlinear systems. Actually a power-law decay of the transmission was already obtained in nonlinear systems with on-site disorder [4, 8]. However, Kivshar et al. [9], while studying the propagation of an envelope soliton in a 1D disordered system, have found that the decay is actually not a power-law type and that strong nonlinearity washes out localization effects. This means that above a certain critical value of the nonlinearity strength we can have wave propagation in nonlinear disordered media, which is a situation of great practical interest. Molina et al. [10], on the other hand, studied the transport properties of a nonlinear disordered binary alloy using a tight binding Hamiltonian. They have confirmed the power law behavior of the transmission but concluded that the decay exponent does not depend on the degree of nonlinearity and that delocalization disappears for large nonlinearities.

It is the purpose of this work to study how the decay of the transmission is affected by nonlinear interactions in general for disordered systems and its effect in periodic systems. In particular, in a recent work on nonlinearity effect on periodic systems [11], we found that the bandwidth decreases when the lattice potential has the same sign as the nonlinear interaction coefficient while in the case of opposite signs the bandwidth increases and some states appear in the bandgap of the corresponding linear periodic system. We study here the scaling properties of the transmission at these gap-states in order to know how the nature of the eigenstates behave with nonlinearity.

2 Model description

Due to the above mentioned non-uniqueness problem we will restrict ourselves to a uniquely defined situation where the output is fixed and one is interested in finding
the necessary input. Leaving this issue aside we would like to investigate the effect of nonlinearity on the transmission of an ordered and disordered Kronig-Penney lattice model. We use the following standard model to describe this system [12]

\[
\left\{-\frac{d^2}{dx^2} + \sum_n (\beta_n + \alpha |\Psi(x)|^2) \delta(x-n)\right\}\Psi(x) = E\Psi(x)
\] (1)

Here \(\Psi(x)\) is the single particle wavefunction at \(x\), \(\beta_n\) the potential strength of the \(n-th\) site, \(\alpha\) the nonlinearity strength and \(E\) the single particle energy in units of \(\hbar^2/2m\) with \(m\) being the electronic effective mass. For simplicity the lattice spacing is taken to be unity in all this work. The potential strength \(\beta_n\) is picked up from a random distribution with \(-W/2 < \beta_n < W/2\) for the mixed potentials case and \(0 < \beta_n < W\) for the potential barriers case (\(W\) being the degree of disorder). The local nature of the nonlinear interaction in (1) does not stem only from its simplicity in numerical computation, but also from a physical point of view that many of the interactions leading to nonlinearity are of local nature such as an on-site Coulomb interaction. From the computational point of view it is more useful to consider the discrete version of this equation which is called the generalized Poincaré map and can be derived without any approximation from equation (1). It reads [13]

\[
\Psi_{n+1} = \left[2 \cos k + \frac{\sin k}{k} (\beta_n + \alpha |\Psi_n|^2)\right] \Psi_n - \Psi_{n-1}
\] (2)

where \(\Psi_n\) is the value of the wavefunction at site \(n\) and \(k = \sqrt{E}\). This representation relates the values of the wavefunction at three successive discrete locations along the x-axis without restriction on the potential shape at those points and is very suitable for numerical computations. The solution of equation (2) is done iteratively by taking for our initial conditions the following values at sites 1 and 2: \(\Psi_1 = \exp(-ik)\) and \(\Psi_2 = \exp(-2ik)\). We consider here an electron having a wave vector \(k\) incident at site \(N+3\) from the right (by taking the chain length \(L = N\), i.e. \(N+1\) scatterers). The transmission coefficient \((T)\) can then be expressed as
\[ T = \frac{4 \sin^2 k}{|\Psi_{N+2} - \Psi_{N+3} \exp(-ik)|^2} \]  

(3)

Thus \( T \) depends only on the values of the wavefunction at the end sites, \( \Psi_{N+2}, \Psi_{N+3} \) which are evaluated from the iterative equation (2).

### 3 Results

First let us examine how the allowed bands and band gaps in the periodic systems get affected by the nonlinear interaction. The nonlinearity is expected under certain conditions to delocalize the electronic wavefunction\[4, 12\]. Therefore, in the framework of the transmission spectrum a decrease of the width of the bandgap will signal delocalization while an increase in the bandgap will signal localization effect. To explain qualitatively the behavior of the transmission for different signs of the nonlinear interaction, we first start with a simple double barrier structure. In a recent work we examined the transmission spectrum for this structure but we restricted ourselves to small nonlinearity strengths. In Figure 1, we show the effect of nonlinearity on the first two resonances of both double barrier and double potential well systems. In the case of barriers Fig.1a shows that for positive \( \alpha \) the resonances get displaced to higher energies and become sharper. As we increase \( \alpha \) the valleys deepen which is a signature of confinement within the well between the two barriers. For negative \( \alpha \), Figure 1b shows that for small values \( |\alpha| < \beta \), the resonances get displaced to lower energies while the valleys increase and get more and more suppressed as we increase \( \alpha \) in magnitude. Thus one can conclude that for small values of \( \alpha \), the gap gets suppressed with increasing values of \( \alpha \) provided that \( |\alpha| < |\beta| \). On the other hand for larger values of the nonlinearity, \( |\alpha| > |\beta| \), the effect is reversed, that is the gap gets larger and larger.

If we consider a double potential wells instead (Figs.2) this behavior is reversed. Thus for negative nonlinearity (Fig.2a) the valleys become deeper while they become more
and more suppressed for positive nonlinearity as shown in Fig2b and similarly to the case of the barriers the valleys start becoming deeper for $|\alpha| > |\beta|$. In summary, the nonlinear interaction seems to delocalize the electronic states when it is repulsive (attractive) for potential barriers (potential wells) and the nonlinearity strength satisfies $|\alpha| < |\beta|$. For all the other cases it seems to localize the eigenstates. In fact the delocalization can be simply explained by the fact that the effective potential in (1) tends to vanish. Thus when the on-site potential and the interaction potential (represented by nonlinearity) have opposite signs the effective potential decreases in Eq.(1) and vanishes for $|\alpha| = |\beta|$. Therefore, the electron tends to become free in this case. When the nonlinear strength increases the effective potential starts increasing and the electron will 'see' the effective potential.

However, we found in the previous work [11] that the delocalization (narrowing of the bandgap) in periodic systems appears as resonant transmission states (sometimes not overlapping) in the gap. We try to examine the nature of these states in the gap of the corresponding linear periodic system in the presence of nonlinearity. To this end, we choose an energy ($E = 11$) in the bandgap of the periodic potential barriers and another one ($E = 9$) in that of the potential wells. Obviously, in the absence of nonlinearity and for finite systems the transmission coefficient decreases exponentially with the length scale at these energies (as shown in Figure 3). If we switch on the nonlinear interaction (with the sign chosen so as to have a delocalization following the above discussion) we find that the transmission coefficient (or equivalently the wavefunction) becomes Bloch like both for potential barriers (Figure 4a) and potential wells (Figure 4b). It is shown in these figures that when the nonlinear strength (in absolute value) increases but remains smaller than the absolute value of the potential strength ($|\alpha| < |\beta|$) the amplitude of the transmission oscillations becomes larger (while its period increases) reaching a constant unity transmission at the critical strength ($|\alpha_c| = |\beta|$) while for larger nonlinearity strengths ($|\alpha| > |\beta|$) the amplitude of these oscillations keeps increasing and its period decreases. This behavior means that the eigenstates in the gap region of the corresponding linear
systems become extended even for a small amount of nonlinearity but the transmission is maximum at the critical nonlinear strength $\alpha_c$ (or in other words the resistance vanishes at this critical strength).

In order to explain qualitatively this delocalization, we note that the nonlinear term in Eq.(1) contains $|\Psi|^2$ which behaves as the inverse of the transmission coefficient from Eq.(3). Thus for decreasing transmission this modulus increases while if the transmission is close to unity it decreases. Therefore, in the gap region, since the transmission coefficient decreases with the length scale, $|\Psi|^2$ increases and consequently the effective potential decreases which leads to the increase of the transmission and so on. The transmission oscillates then with the length scale and its period depends on the speed of the variation of $|\Psi|^2$ which depends on the nonlinearity strength. If this strength increases, we reach rapidly the condition of vanishing effective potential and the variation of $|\Psi|^2$ is slow (and the period of oscillations is large) while for very small strengths this modulus starts increasing rapidly up to the condition of vanishing effective potential where it becomes very large, and then this effective potential increases rapidly leading to smaller periods of the transmission oscillations. We note here that the transmission never decays with the length even for high nonlinearity strength.

Let us now examine the effect of disorder on the nonlinear Schrödinger equation. We consider here two kinds of disorder as discussed above (mixed disorder and potential barriers disorder) in order to check the kind of disorder dependence of the power law behavior observed in recent works [10, 12]. We note here that we observe a power-law decay of the transmission near the band edges of the corresponding periodic system (i.e., around $k = n\pi/a$, $n$ being a positive integer number and the lattice parameter $a$ is taken here to be unity). For all other energies, the decay of the transmission with the length becomes either exponential or even stronger (we did not show these results here). In this connection, we would like to remark that the energy taken by Cota et al. [12] (their model is exactly the same as our mixed potentials model) is $E = 5$ instead of $E \simeq 10$ (probably
due to a misprint in their paper). As found by Cota et al. [12], for $E = 5$ the mixed case shows a power-law decay above a critical nonlinearity strength (actually they did not fit a power-law behavior for the strengths of $\alpha = 10^{-15}$ and $10^{-10}$). In contrast, what we find is that for $E = 5$, the transmittance decays exponentially for small disorders and small $\alpha$, but faster than exponentially for larger disorder and/or nonlinearity. However, if we choose $E = 10$ (which is close to the band-edge for a periodic system but inside the gap), there is a finite size effect and the power-law decay of the transmission is observed only above a characteristic length $L_c$ which seems to decrease with nonlinearity strength as clearly shown in Fig.5a (below this $L_c$, the transmission is exponentially decaying). Further, even for very small nonlinearity strengths (e.g., $\alpha = 10^{-15}$ and $10^{-10}$) there is a crossover to a power-law decay of the transmittance for $L > L_c$. This power-law behavior is also shown in the case of disordered barrier potentials (Fig.5b) but the characteristic length $L_c$ seems to be smaller. We did not show here the case of disordered potential wells because it is similar to that of the potential barriers but for a positive sign of the nonlinearity.

As shown in Figs.5, the exponent of the power law decay $\gamma$ seems to be slightly dependent on the nonlinearity strength for the mixed case while it seems to be almost constant for disordered barrier potentials. This behavior is confirmed in Figure 6 where we fitted the power-law behavior only above $L_c$. This figure shows a qualitative agreement with the results of Cota et al. [12] (except for the fact that there is no critical $\alpha$) for a mixed disorder while for barrier type disorders, the exponent is smaller and seems to become independent of the nonlinearity strength. This last result has been also found by Molina et al. [10] for disordered binary alloys who first of all used a tight binding Hamiltonian and then lumped the disorder in the nonlinear coefficient itself (this is entirely different from the model we used). On the other hand, Cota et al. used the same model as we do, but the behavior observed by them is not universal and depends on the kind of disorder. Indeed, for disordered potential barriers the negative nonlinearity strength
tends to delocalize the eigenstates as shown for the double barriers (Fig.1a) and for the periodic systems (Figs.4) while in the mixed case, there is always a competition between the delocalization in potential barriers and the strong localization in the remaining potential wells which increases the characteristic length $L_c$. We would also like to point out that the power-law behavior becomes very sensitive on some particular configurations in the large length scale, and tends to give very large values of the resistance making the calculations on the average properties unstable.

4 Conclusion

We studied in this paper the effect of nonlinearity both on double barriers, periodic and disordered systems using a simple Kronig-Penney Hamiltonian. We found in the double barriers system a range of nonlinearity strengths for which the delocalization takes place and a critical nonlinearity strength above which the behavior is reversed (At this critical value the transparency becomes unity). It seems also that the nonlinearity suppresses the gap in periodic systems. Indeed, for finite size systems, the transmission for energies corresponding to the gap in infinite systems is exponentially decaying while, with any small amount of nonlinearity it becomes Bloch like. Finally in the presence of disorder and in the regime of nonlinearity strengths delocalizing the gap states of the periodic system, we found that the transmission becomes power-law decaying around the band edges of the corresponding periodic system while for other energies the transmission is at least exponentially decaying if not faster. The exponents of the power-law behavior (above the $\alpha$-dependent crossover length scale $L_c$) of the transmittance depends on the nonlinearity strength for mixed systems in qualitative agreement with the results of Cota et al. [12], while it seems to be constant for potential barriers in agreement with the results of Molina et al. [10] even though the system used by these last authors is different from ours (they used a tight binding model with a disorder in the nonlinearity strength.
itself). Therefore, the variation of this exponent with nonlinearity depends strongly on the type of disorder used and is not universal as claimed recently [12]. On the other hand, this exponent is much larger in mixed systems than in disordered potential barriers. It is then interesting to examine within this model the effect of disordered nonlinearity on the transport properties in order to compare them with the results of Molina et al. [10]. Also, this power-law behavior is observed only above a characteristic length $L_c$. It is then interesting to study the finite size effect of this behavior. Furthermore, since metallic and insulating behaviors are well characterized by the statistical properties of their transport coefficients [14], it seems to be adequate to examine the transition from exponentially localized states in linear disordered systems to power law decaying states in nonlinear ones using the above technique.

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Figure Captions

**Fig.1** Transmission coefficient versus energy for a double barrier with $\beta = 1$, $|\alpha| = 0$. (solid curve), 0.1 (dashed curve), 0.5 (dotted curve), 2 (dash-dotted curve) and 3 (short dashed curve). a) $\alpha > 0$, b) $\alpha < 0$.

**Fig.2** Same as Fig.1 for double well ($\beta = -1$).

**Fig.3** $-\log T$ versus $L$ for linear periodic system ($\alpha = 0$) for both potential barriers $\beta = 1, E = 11$ (open squares) and potential wells $\beta = -1, E = 9$ (cross symbols +).

**Fig.4** $-\log T$ versus $L$ for $|\alpha| = 0.1$ (solid curve), 0.5 (dashed curve), 2. (thick dotted curve) and 3. (dash-dotted curve) for a) potential barriers ($\beta = 1, E = 11$ and $\alpha < 0$) and b) potential wells ($\beta = -1, E = 9$ and $\alpha < 0$).

**Fig.5** $< -\log T >$ versus $\log L$ for $|\alpha| = 10^{-15}$ (open diamond), $10^{-10}$ (cross symbol +), $10^{-5}$ (open triangle up), $10^{-4}$ (open square), $10^{-3}$ (star symbol), $10^{-2}$ (open triangle down), $10^{-1}$ (open circle) and 1. (cross symbol x) for $\alpha < 0$, $W = 4$, $E = 10$ and for 100 disorder realizations a) Mixed case b) Potential barriers. Solid lines correspond to the power-law fittings.

**Fig.6** The exponent $\gamma$ versus nonlinearity strength $\log(|\alpha|)$ for both mixed case (filled square) and potential barriers (open square). The solid lines are simply guides to the eye.
FIGURE 1

Transmission Coefficient

Energy (Rydberg units)
FIGURE 2

Transmission Coefficient vs. Energy (Rydberg units)
FIGURE 3

-Log(T) vs. Chain length L
FIGURE 4
FIGURE 5

\[ \log(\langle T \rangle) \]

\[ \log(L) \]
FIGURE 6

Power-law exponent ($\gamma$) vs. Nonlinear coefficient ($\log|\alpha|$).