The effect of non-linearity on one-dimensional periodic and disordered lattices

1999 J. Phys.: Condens. Matter 11 1823

(http://iopscience.iop.org/0953-8984/11/7/012)

J. Phys.: Condens. Matter **11** (1999) 1823–1832. Printed in the UK PII: S0953-8984(99)96999-0

The effect of non-linearity on one-dimensional periodic and disordered lattices

K Senouci†‡, N Zekri†‡, H Bahlouli†§ and A K Sen†‖

† AS-ICTP, 34100 Trieste, Italy

‡ Laboratoire d'Etude Physique des Materiaux, Departement de Physique, UST Oran, BP 1505, Oran El-M'naouer, Algeria

§ Physics Department, KFUPM, Dhahran 31261, Saudi Arabia

‖ LTP Division, Saha Institute for Nuclear Physics, 1/AF Bidhannagar, Calcutta 700 064, India

Received 24 August 1998, in final form 20 November 1998

Abstract. The Kronig–Penney model is used to study the effect of non-linear interaction on the transmissive properties of both ordered and disordered chains. In the ordered case, the non-linearity 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 γ is independent of the strength of the non-linearity in the case of disordered barrier potentials, while it varies with this strength for mixed potentials.

1. Introduction

Wave propagation in non-linear media is a subject that has recently been intensively researched [1]. The study of this phenomenon is of great practical importance in the understanding of transport properties of superlattices [2], electronic behaviour in mesoscopic devices and optical phenomena in general. The non-linear Schrödinger equation has been studied extensively in recent years and served as a prototype for studying non-linear phenomena. The origin of the non-linearity in the Schrödinger equation corresponds 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 has 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 for linear systems, to deduce the transmission and related properties of interest. However, there are differences from 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) and 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 non-linearity, 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 multi-stability and noise, and might give rise to a chaotic behaviour 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 non-linear interaction in an appropriate regime. Anderson's theory predicts the wavefunction

0953-8984/99/071823+10$19.50

of a non-interacting electron moving in a one-dimensional lattice with on-site energetic disorder to be localized even for an infinitesimal amount of disorder [7]. 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 non-linear systems. In fact, a power-law decay of the transmission had already been obtained for non-linear systems with on-site disorder [4, 8]. However, Kivshar [9], while studying the propagation of an envelope soliton in a 1D disordered system, has found that the decay is actually not of power-law type and that strong non-linearity washes out localization effects. This means that above a certain critical value of the non-linearity strength we can have wave propagation in non-linear disordered media, which is a situation of great practical interest. Molina and Tsironis [10], on the other hand, studied the transport properties of a non-linear disordered binary alloy using a tight-binding Hamiltonian. They confirmed the power-law behaviour of the transmission but concluded that the decay exponent does not depend on the degree of non-linearity and that delocalization disappears for large non-linearities.

The problem of wave propagation in non-linear, dynamical classical and quantum systems was examined mathematically by Frohlich *et al* [11]. These authors found, for some models of classical, disordered anharmonic crystal lattices, quasiperiodic lattice vibrations which remain localized for all times, and there is no transport of energy through the lattice.

The purpose of this work is to study how the decay of the transmission is affected by non-linear interactions in general for disordered systems and its effect in periodic systems. In particular, in a recent work on the effect of non-linearity on periodic systems [12], we found that the bandwidth decreases when the lattice potential has the same sign as the non-linear 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 establish how the nature of the eigenstates is affected by non-linearity.

2. Model description

In view of 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 non-linearity on the transmission of an ordered and disordered Kronig–Penney lattice model. We use the following standard model to describe this system [13]:

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\sum_n(\beta_n+\alpha|\Psi(x)|^2)\delta(x-n)\right\}\Psi(x)=E\Psi(x). \tag{1}$$

Here $\Psi(x)$ is the single-particle wavefunction at x, β_n the potential strength of the nth site, α the non-linearity 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 throughout this work. The potential strength β_n is a variable picked up from a random distribution with $-W/2 < \beta_n < W/2$ for the mixed-potential case and $0 < \beta_n < W$ for the potential barrier case (W being the degree of disorder). The local nature of the non-linear interaction in (1) stems not only from its simplicity as regards numerical computation, but also from the physical view that many of the interactions leading to non-linearity 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 [14]

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

where Ψ_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 carried out iteratively by taking for our initial conditions the following values at sites 1 and 2: $\Psi_1 = \exp(-\mathrm{i}k)$ and $\Psi_2 = \exp(-2\mathrm{i}k)$. 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

$$T = \frac{4\sin^2 k}{|\Psi_{N+2} - \Psi_{N+3}\exp(-\mathrm{i}k)|^2}. \tag{3}$$

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

3. Results

First let us examine how the allowed bands and bandgaps in the periodic systems (i.e., when the variable β has a constant value B for the whole system) are affected by the non-linear interaction. The non-linearity is expected under certain conditions to delocalize the electronic

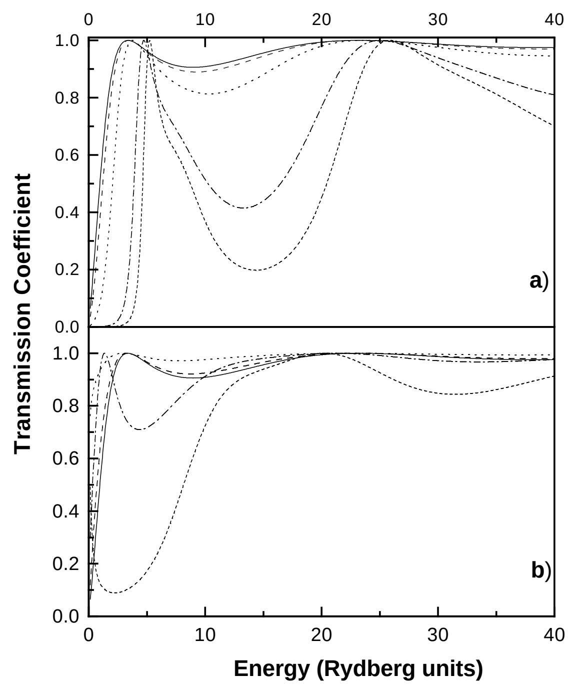

Figure 1. The transmission coefficient versus the energy for a double barrier with $\beta = 1$, $|\alpha| = 0$ (solid curve), 0.1 (dashed curve), 0.5 (dotted curve), 2 (dash–dotted curve) and 3 (short-dashed curve). (a) $\alpha > 0$, (b) $\alpha < 0$.

wavefunction [4, 13]. 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 a localization effect. To explain qualitatively the behaviour of the transmission for different signs of the non-linear interaction, we first start with a simple double-barrier structure. In recent work we examined the transmission spectrum for this structure but we restricted ourselves to small non-linearity strengths. In figure 1, we show the effect of non-linearity on the first two resonances of both double-barrier and double-potential-well systems. For the case of barriers, figure 1(a) shows that for positive α the resonances get displaced to higher energies and become sharper. As we increase α, the valleys deepen, which is a signature of confinement within the well between the two barriers. For negative α, figure 1(b) shows that for small values of $|\alpha| < B$, the resonances get displaced to lower energies while the valleys increase and get more and more suppressed as we increase α in magnitude. Thus one can conclude that for small values of α, the gap gets suppressed with increasing values of α provided that $|\alpha| < |B|$. On the other hand, for larger values of the non-linearity, $|\alpha| > |B|$, the effect is reversed; that is, the gap gets larger and larger.

If we consider a double potential well instead (figure 2), this behaviour is reversed. Thus for negative non-linearity (figure 2(b)) the valleys become deeper, while they become more and more suppressed for positive non-linearity as shown in figure 2(a) and, similarly to the case for the barriers, the valleys start becoming deeper for $|\alpha| > |B|$. In summary, the non-linear interaction seems to delocalize the electronic states when it is repulsive (attractive) for potential barriers (potential wells) and the non-linearity strength satisfies $|\alpha| < |B|$. For all of 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

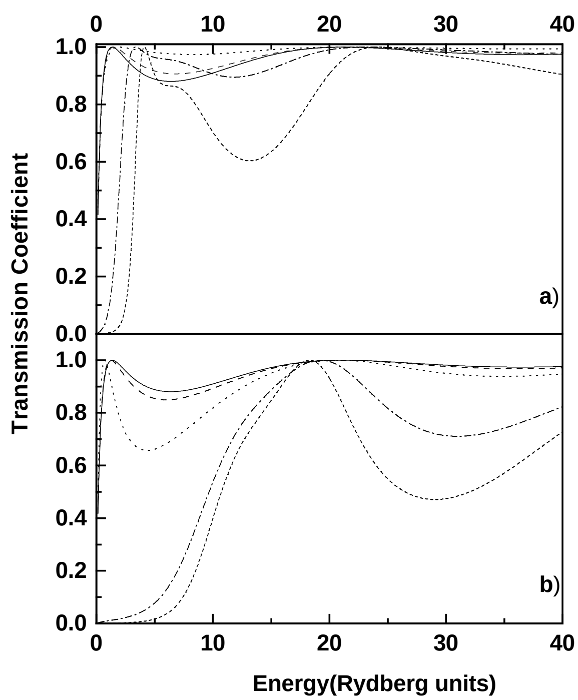

Figure 2. As figure 1, but for a double well ($\beta = -1$).

and the interaction potential (represented by non-linearity) have opposite signs, the effective potential decreases in equation (1) and vanishes for $|\alpha| = |B|$. Therefore, the electron tends to become free in this case. When the non-linear strength increases, the effective potential starts increasing and the electron will 'see' the effective potential.

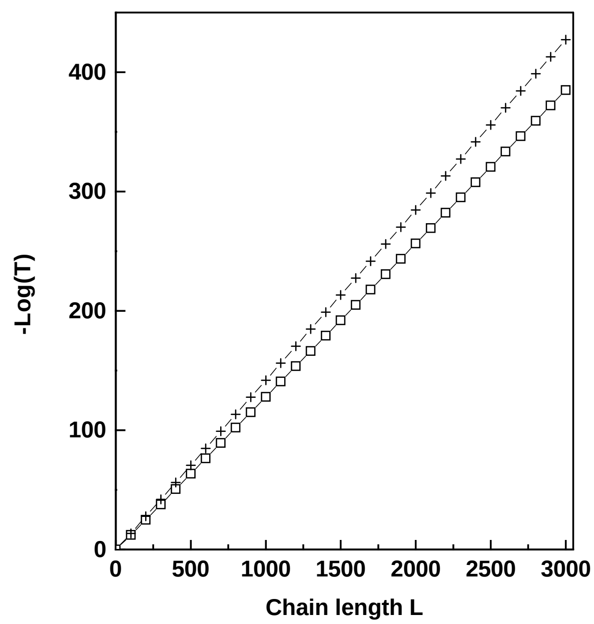

Figure 3. $-\log T$ versus L for a linear periodic system ($\alpha = 0$) for both potential barriers, $\beta = 1$, $E = 11$ (open squares), and potential wells, $\beta = -1$, $E = 9$ (crosses, +).

However, we found in previous work [12] that the delocalization (the 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 non-linearity. 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 non-linearity 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 non-linear 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 4(a)) and for potential wells (figure 4(b)). It is shown in these figures that when the non-linear strength increases (in absolute value) but remains smaller than the absolute value of the potential strength ($|\alpha| < |B|$), the amplitude of the transmission oscillations becomes larger (while its period increases), reaching a constant unity transmission at the critical non-linearity strength ($|\alpha_c| = |B|$), while for larger non-linearity strengths ($|\alpha| > |B|$) the amplitude of these oscillations keeps increasing and its period decreases. This behaviour means that the eigenstates in the gap region of the corresponding linear systems become extended even for a small amount of non-linearity but the transmission is maximum at the critical non-linearity strength α_c (or in other words the resistance vanishes at this critical strength).

In order to explain this delocalization qualitatively, we note that the non-linear term in equation (1) contains $|\Psi^2|$ which behaves as the inverse of the transmission coefficient

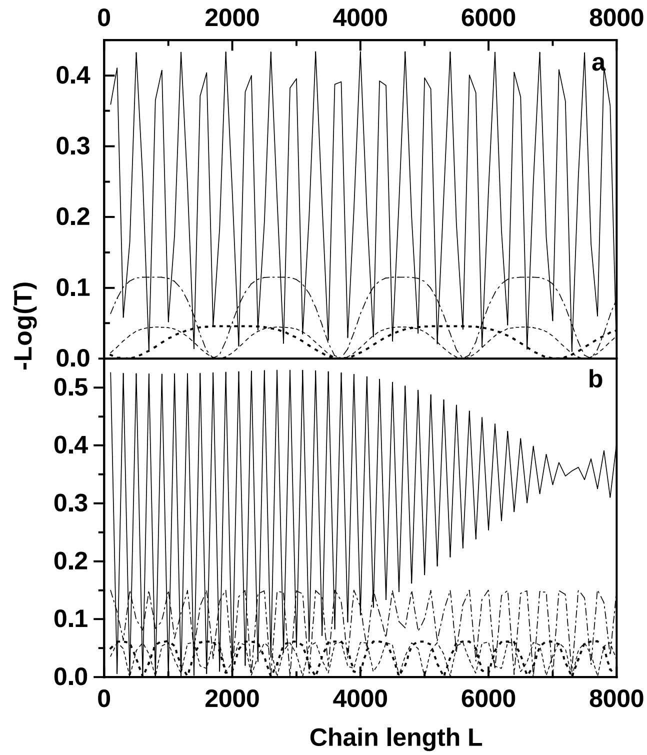

Figure 4. $-\log T$ versus L for $|\alpha| = 0.1$ (solid curve), 0.5 (dashed curve), 2 (thick dotted curve) and 3 (dash–dotted curve) for (a) potential barriers ($\beta = 1$, $E = 11$ and $\alpha < 0$) and (b) potential wells ($\beta = -1$, $E = 9$ and $\alpha < 0$).

from equation (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 strength of the non-linearity. 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 non-linearity strength.

Let us now examine the effect of disorder on the non-linear Schrödinger equation. We consider here two kinds of disorder as discussed above (mixed disorder and potential barrier disorder) in order to check the kind of disorder dependence shown by the power-law behaviour observed in recent work [10, 13]. 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, and the lattice parameter a 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

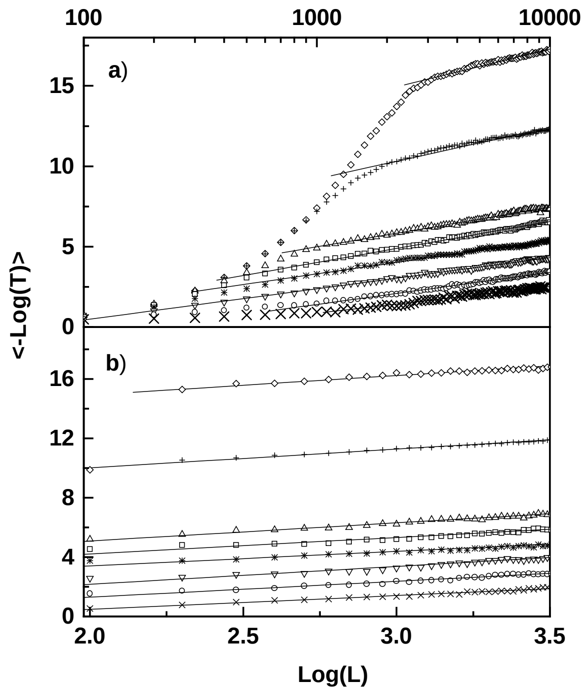

Figure 5. $\langle -\log T \rangle$ versus $\log L$ for $|\alpha| = 10^{-15}$ (open diamonds), 10^{-10} (crosses, +), 10^{-5} (open upright triangles), 10^{-4} (open squares), 10^{-3} (stars), 10^{-2} (open inverted triangles), 10^{-1} (open circles) and 1 (crosses, $\times$) for $\alpha < 0$, $W = 4$, $E = 10$ and for 100 disorder realizations. (a) The mixed case. (b) Potential barriers. Solid lines correspond to the power-law fittings.

the energy taken by Cota *et al* [13] (their model is exactly the same as our mixed-potential model) is $E = 5$ instead of $E \simeq 10$ (probably due to a misprint in their paper). As found by Cota *et al* [13], for $E = 5$ the mixed case shows a power-law decay above a critical non-linearity strength (in fact, they did not fit a power-law behaviour 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 α, but faster than exponentially for larger disorder and/or non-linearity. 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 the non-linearity strength as clearly shown in figure 5(a) (below this length L_c, the transmission is exponentially decaying). Furthermore, even for very small non-linearity 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 behaviour is also shown in the case of disordered barrier potentials (figure 5(b)) 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 non-linearity.

As shown in figure 5, the exponent of the power-law decay, γ, seems to be slightly dependent on the non-linearity strength for the mixed case while it seems to be almost constant for disordered barrier potentials. This behaviour is confirmed in figure 6 where we fitted the power-law behaviour only above L_c. This figure shows a qualitative agreement with the results of Cota *et al* [13] (except for the fact that there is no critical α) for a mixed disorder, while

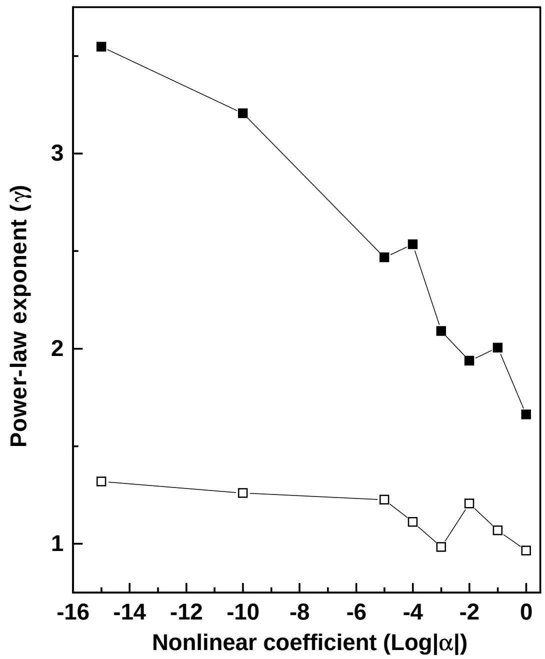

Figure 6. The exponent γ versus the non-linearity strength $\log(|\alpha|)$ for both the mixed case (filled squares) and potential barriers (open squares). The solid lines are simply guides to the eye.

for barrier-type disorders the exponent is smaller and seems to become independent of the non-linearity strength. This last result has been also found by Molina and Tsironis [10] for disordered binary alloys; they first of all used a tight-binding Hamiltonian and then included the disorder in the non-linear coefficient itself (this is entirely different from the model that we used). On the other hand, Cota *et al* [13] used the same model as we do, but the behaviour observed by them is not universal and depends on the kind of disorder. Indeed, for disordered potential barriers the negative non-linearity strength tends to delocalize the eigenstates, as shown for the double barriers (figure 1(a)) and for the periodic systems (figures 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 behaviour becomes very sensitive to some particular configurations for the large length scale, and tends to give very large values of the resistance, making the calculations of the average properties unstable. We used different random generating routines proposed in numerical recipes [15] (i.e. 'ran0.for', 'ran1.for', 'ran2.for' and 'ran3.for') and found this behaviour to be independent of which routine was used. We found also that the instability appears for all of the routines used and the large statistical fluctuations of the transmission remain at large length scales.

4. Conclusion

We studied in this paper the effect of non-linearity both on double barriers, and on periodic and disordered systems using a simple Kronig–Penney Hamiltonian. We found in the double-barrier system a range of non-linearity strengths for which the delocalization takes place and a critical non-linearity strength above which the behaviour is reversed (at this critical value the transparency becomes unity). It seems also that the non-linearity 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 non-linearity, it becomes Bloch-like. Finally, in the presence of disorder and for the signs of the non-linearity strength leading to delocalization in periodic systems, we found that the transmission exhibits power-law decay around the band edges of the corresponding periodic system, while for other energies the transmission decays at least exponentially if not faster. We note here that the delocalized states in the non-linear interaction are different in their nature from those in correlated disorder. Indeed, in correlated disorder this corresponds to resonant-tunnelling-extended states [16], while in non-linear disordered systems the delocalized states still exhibit power-law decay. It is found also that this delocalization is broken asymptotically and the transmission becomes more than exponentially localized, supporting the mathematical results given by Frohlich *et al* [11]. The exponent of the power-law behaviour (above the α-dependent crossover length scale L_c) of the transmittance depends on the non-linearity strength for mixed systems, in qualitative agreement with the results of Cota *et al* [13], while it seems to be constant for potential barriers, in agreement with the results of Molina and Tsironis [10] even though the system used by these latter authors is different from ours (they used a tight-binding model with a disorder in the non-linearity strength itself). Therefore, the variation of this exponent with non-linearity depends strongly on the type of disorder and is not universal as claimed recently [13]. On the other hand, this exponent is much larger for mixed systems than for disordered potential barriers. It is thus interesting to examine within this model the effect of disordered non-linearity on the transport properties in order to compare with the results of Molina and Tsironis [10]. Also, this power-law behaviour is observed only above a characteristic length L_c. It is thus interesting to study the finite-size effect of this behaviour. Furthermore, since metallic and insulating behaviours are well characterized by the statistical properties of their transport coefficients [17], it seems to be adequate to examine the transition from exponentially localized states in linear disordered systems to power-law-decaying states in non-linear ones using the above technique.

Acknowledgments

We would like to acknowledge the support of the ICTP during our stay at Trieste. HB would also like to acknowledge the support of the Physics Department at King Fahd University of Petroleum and Minerals (KFUPM) enjoyed during the progress of this work.

References

[1] Tsironis G P and Economou E N (ed) 1998 *Proc. Conf. on Fluctuations, Non-linearity and Disorder in Condensed Matter and Biological Systems (Heraklion, Crete, 1996); Physica* D **113** 115–412
Abdullaev F, Bishop A R and Pnevmatikos S (ed) 1992 *Disorder with Nonlinearity* (Berlin: Springer)
[2] Zhang Y, Kastrup J, Klann R, Ploog K H and Grahn H T 1996 *Phys. Rev. Lett.* **77** 3001
[3] Griffin A, Snoke D W and Stringari S 1995 *Bose–Einstein Condensation* (Cambridge: Cambridge University Press)
[4] Devillard P and Souillard B 1986 *J. Stat. Phys.* **43** 423
[5] Wan Y and Soukoulis C M 1990 *Phys. Rev.* A **41** 800
See also
Bishop A R (ed) 1989 *Disorder and Nonlinearity* vol 39 (Berlin: Springer) p 27
[6] Wan Y and Soukoulis C M 1989 *Phys. Rev.* B **40** 12 264
[7] Anderson P W 1958 *Phys. Rev.* **109** 1492
[8] Abdullaev F, Bishop A R and Pnevmatikos S (ed) 1992 *Disorder with Nonlinearity* (Berlin: Springer)

[9] Kivshar Y S 1993 *Phys. Lett.* **173** 172
[10] Molina M I and Tsironis G P 1994 *Phys. Rev. Lett.* **73** 464
[11] Frohlich J, Spencer T and Wayne C E 1986 *J. Stat. Phys.* **42** 247
[12] Zekri N and Bahlouli H 1998 *Phys. Status Solidi* b **205** 511
[13] Cota E, Jose J V, Maytorena J and Monsivais G 1995 *Phys. Rev. Lett.* **74** 3302
[14] Sanchez A, Macia E and Dominguez-Adame F 1994 *Phys. Rev.* B **49** 147
[15] Press W H, Teukolsky S A, Vetterling W T and Flannery B P (ed) 1997 *Numerical Recipes in Fortran 77. The Art of Scientific Computing* (Cambridge: Cambridge University Press)
[16] Sanchez A, Macia E, Dominguez-Adame F and Diez E 1995 *Phys. Rev.* B **51** 6769
[17] Casati G and Cerdeira H A (ed) 1993 *Chaos in Mesoscopic Systems* (Singapore: World Scientific)
Beenakker C W J 1997 *Rev. Mod. Phys.* **69** 731
Guhr T, Mueller-Groeling A and Weidenmueller H A 1998 *Phys. Rep.* **299** 189