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Nonlinear interaction effect on the phase distribution in one-dimensional disordered lattices

N Zekri† and H Bahlouli‡

† USTIO, Departement de Physique, LEPM, BP 1505 El M'Naouar, Oran, Algeria
‡ Physics Department, KFUPM, Dhahran 31261, Saudi Arabia

E-mail: nzekri@meloo.com

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Abstract. We studied in this paper the effect of nonlinear interaction on the PD of a one-dimensional Kronig–Penney chain. In the quasi-ballistic regime ($L \ll (2k_F)^{-1} \ll \lambda$ (localization length)), an attractive nonlinear potential leads to a smooth peak with an oscillatory shift in its position, while for repulsive potentials the peak becomes sharper and moves towards π. In the quasi-metallic regime ($(2k_F)^{-1} \ll L \ll \lambda$), the uniform PD becomes peaked as we increase the nonlinear potential. Depending on the sign of the nonlinear potential, this peak moves either away from or closer to π. In the strong disorder regime, the nonlinearity plays an identical role to disorder. It was found that the overall effect of nonlinear interaction in the mixed disorder case can be interpreted as a superposition of those for potential barriers and wells treated separately. Further results and discussion are also provided.

1. Introduction

The phase distribution (PD) of complex reflection amplitudes has been shown to be strongly related to the transport properties of disordered systems [1–4]. Two decades ago, several studies on one-dimensional (1D) disordered systems suggested that the random phase model supported the scaling theory of localization [5–8]. However, Lambert *et al* [4] examined in detail the PD in randomly distributed δ-potentials both in the Kronig–Penney and the tight-binding model and found it to become strongly peaked at the limit of a large disorder. This distribution was also found both numerically [4] and analytically, using the invariant embedding approach [9], to be doubly peaked at $\pi/2$ and $3\pi/2$ in the quasi-ballistic regime. These results have been confirmed recently by Sen [10] for the tight-binding model, in which the connection between these distributions and the scaling behaviour of the resistance was shown. However, these investigations have considered only mixed disorder (i.e. the energy site is randomly generated from a uniform distribution centred at the zero energy). A strong discrepancy has been found recently [11] in the behaviour of the transmission between mixed disorder and disordered potential barriers (wells). The behaviour of the transmission in disordered potential barriers and wells has been shown to give rise to a compensation effect in the transmission in mixed disorder [12]. This compensation will certainly affect the behaviour of the PD.

Therefore, some unexpected transport properties in some 1D systems can find their explanation in the behaviour of the PD. Indeed, nonlinear (NL) 1D models have been shown to exhibit delocalization [11, 13–15], instabilities and chaotic behaviour [16]. Although most of these properties have been extensively studied, they remain open for further investigations and have not been analysed by the PD approach. In particular, the non-uniqueness of the output wavefunction amplitude for a given input in the NL Schrödinger equation has certainly great consequences on the shape of the PD which is expected to play an important role in all phenomena based on phase coherence.

It is the purpose of this work to study the effect of NL interaction on the PD of the reflection amplitude of 1D Kronig–Penney disordered systems. We have examined the PD for mixed disorder as well as disordered barriers and wells, in different regimes of disorder. To avoid the multistability in the NL systems we restrict ourselves to a uniquely defined situation where the output is fixed and one is interested in finding the necessary input. We found in particular a new characteristic length scale (discussed in section 3.1), in addition to that separating the exponential decay of the transmission for smaller lengths from its power-law decay above this length scale [11].

The paper is organized in the following way. In section 2, we set up the general model used in studying the PD and provide the main expressions for determining the phase. In section 3, we present our numerical results and discuss their physical interpretation in different regimes and conclude in section 4 by summarizing our results and suggesting some future investigations.

2. Model

The model used in this paper is the Kronig–Penney model where the site potentials are δ-potentials. This model is a continuous multiband model and describes better short-range interactions than other models, such as the tight-binding model [17]. Furthermore, it is easier to include external fields in this model than in the tight-binding model. We consider a non-interacting electron of energy E moving through a linear chain of δ-potentials of strength β_n, where n is the site position. In each site a NL interaction is included to represent either a repulsive interaction (electron–electron interaction) or an attractive interaction (electron–phonon interaction). The Schrödinger equation then reads

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

where $\Psi(x)$ is the single particle wavefunction at x, β_n the potential strength at the nth site, α is the nonlinearity strength and E the single particle energy in units of $\hbar^2/2m$ where m is the free electron effective mass. For simplicity, the lattice spacing is taken to be unity in all this work. The potential strength β_n is a variable acquired from a random distribution where $-W/2 < \beta_n < W/2$ for the mixed potentials case, $0 < \beta_n < W$ for the potential barriers case and $-W < \beta_n < 0$ for the potential wells case (W is the degree of disorder). The local nature of the NL 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 the 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 (1). It reads [18]

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

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 these points, and it is very suitable for numerical computations. An iterative approach is taken to solve (2). For our initial conditions we used 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 that an electron has a wavevector k_F (at Fermi energy) incident at site $N + 3$ from the right (by taking the chain length $L = N$, i.e. $N + 1$ scatterers). The transmission and reflection amplitudes (t and r) can then be expressed as

$$t = \frac{-2\mathrm{i}\exp(-\mathrm{i}k(N+3))\sin k}{\Psi_{N+3}\exp(-\mathrm{i}k) - \Psi_{N+2}} \tag{3}$$

and

$$r = \frac{\exp(-2\mathrm{i}k(N+3))\,(\Psi_{N+2} - \exp(\mathrm{i}k)\Psi_{N+3})}{\Psi_{N+3}\exp(-\mathrm{i}k) - \Psi_{N+2}} \tag{4}$$

where the terms $\exp(-\mathrm{i}k(N + 3))$ and $\exp(-2\mathrm{i}k(N + 3))$, appearing respectively in the transmission and reflection amplitudes, originate from the fact that the electron is incident at site $N + 3$ with an incident phase $-k(N + 3)$. Therefore, these fictitious phases are to be disregarded. From (3) and (4) the phases of the transmission and reflection amplitudes depend 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). Without any loss of generality, we restrict ourselves in this work to the study of the PD of the reflection amplitude.

3. Results and discussion

In this section, we use three kinds of disorder: mixed disorder, potential barriers and potential wells and we investigate the NL potential effect on the PD for each of these disorder types separately. We study the NL potential effect on the PD in three different regimes: the quasi-ballistic regime ($L \ll (2k_F)^{-1} \ll \lambda$, where λ is the localization length), the quasi-metallic regime, also called weakly localized regime, ($(2k_F)^{-1} \ll L \ll \lambda$) and the strong disorder regime ($W \to \infty$). In the later regime we choose the sample length so large that the PD becomes stationary. All the distributions and averages are obtained for 10^4 realizations. We note here that to the best of our knowledge no work has been undertaken for the PD in the case of disordered barriers or wells (although some behaviours in mixed disorder can be understood on the basis of these two types of disorder). Neither has the NL influence on the PD in these three kinds of disorder been investigated. However, with our model we confirm the tight-binding and invariant embedding results obtained previously in the linear mixed disorder case [4, 9, 10], that is a doubly peaked distribution at $\pi/2$ and $3\pi/2$ in the quasi-ballistic regime and nearly uniform distribution in the quasi-metallic regime. For strong disorder the distribution has two peaks which tend to merge into a single peak and become sharper as we increase the disorder, and whose asymptotic position (ϕ_∞) depends only on the incoming electron energy. In this later case, it has been found previously [2, 4, 10] that the phase of the reflection behaves as $\phi_\infty = 2\cos^{-1}(E/2)$ (the energy E is $2\cos\ k$ for a lattice parameter taken to be unity). In the case of a Kronig–Penney model with δ-potentials, the incoming energy E behaves like k^2 and we easily obtain the energy dependence of the PD peak given by $\phi_\infty = 2\sqrt{E}$. We confirmed numerically this energy dependence and also the non-dependence of ϕ_∞ on other parameters. We point out here that the PD is peaked at $\pi/2$ for an energy at the band centre of the corresponding periodic system while it is peaked at π for an energy near the band edge.

3.1. Quasi-ballistic regime

In this regime we choose the parameters $E = 10^{-3}, W = 0.03$ and $L = 5$ which satisfy the condition $L \ll (2k_F)^{-1} \ll \lambda$, where the mean free path $(2k_F)^{-1}$ is about 17 and the localization

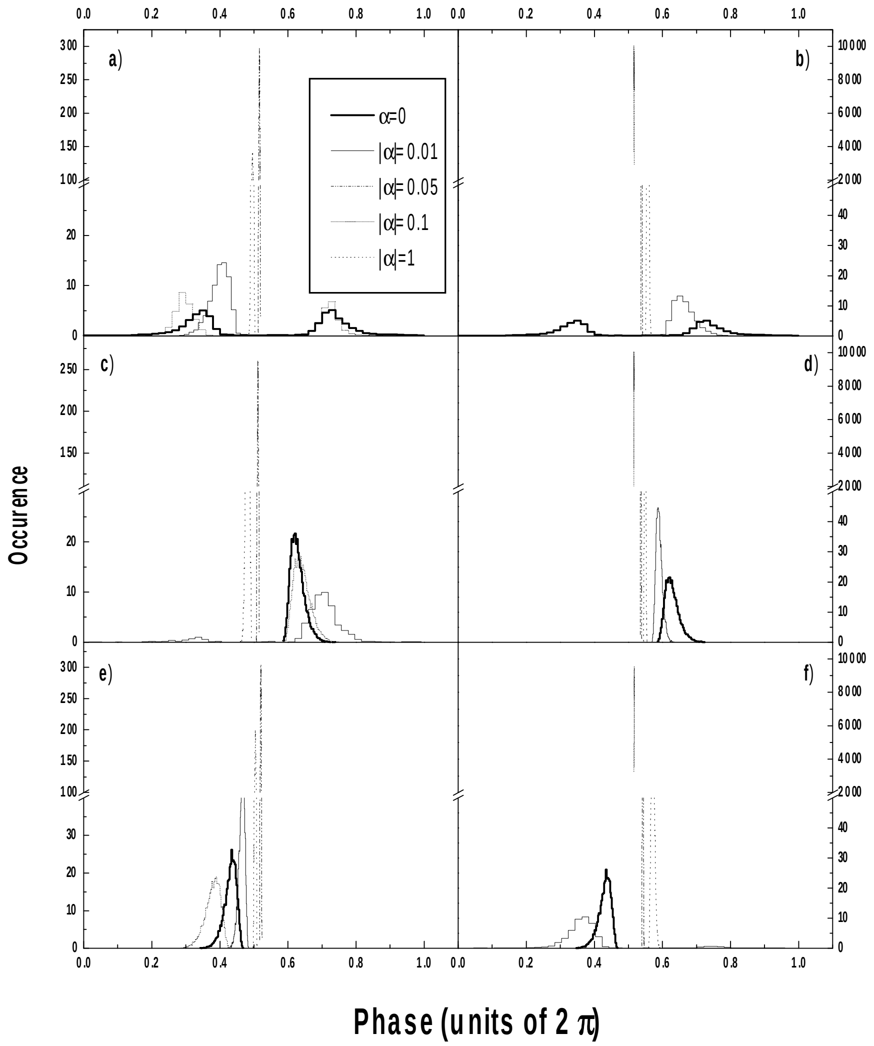

Figure 1. Phase distribution (in units of 2π) for $E = 0.001$, $W = 0.03$, $L = 5$ and different nonlinearity strengths ($|\alpha| = 0$, 0.01, 0.05, 0.1 and 1). For: mixed disorder (a) $\alpha < 0$, (b) $\alpha > 0$; potential barriers (c) $\alpha < 0$, (b) $\alpha > 0$; potential wells (e) $\alpha < 0$, (f) $\alpha > 0$.

length λ is close to 100 for mixed disorder, 70 for disordered barriers and 140 for disordered wells (these lengths are measured in units of the lattice parameter taken here to be unity).

In figure 1 we show the PD for different attractive (figures 1(a), (c) and (e)) and repulsive (figures 1(b), (d) and (f)) NL potentials and for the three kinds of disorder. In the case of mixed disorder (figures 1(a) and (b)) we notice that the PD is doubly peaked near $\pi/2$ and $3\pi/2$ in the absence of nonlinearity, while in disordered barriers and wells, only a single peak appears near $3\pi/2$ and $\pi/2$, respectively. Therefore the results obtained previously in this regime [4, 9, 10] cannot be extended to an arbitrary type of disorder and the superposition effect of these two types of disorder observed in the case of mixed disorder for the transmission properties [12] is also observed in the PD behaviour. In the presence of attractive (repulsive) NL potential, the peak at $3\pi/2$ ($\pi/2$) disappears in the mixed disorder case, while the other

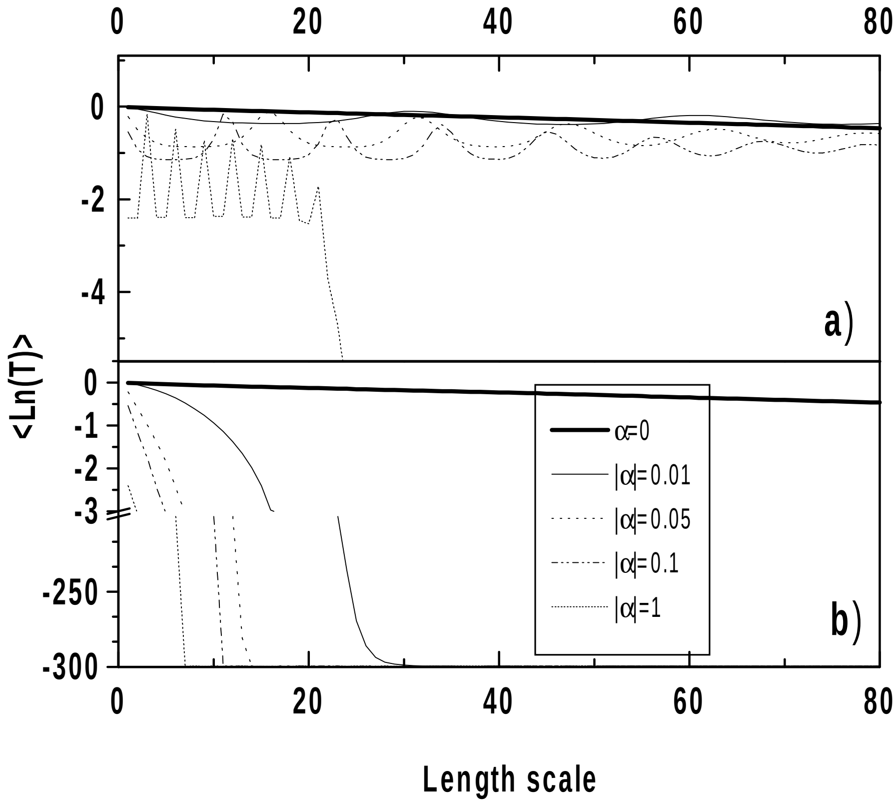

Figure 2. Transmission coefficient against length for the same parameters as in figure 1 in the mixed disorder case and for different nonlinearity strengths ($|\alpha| = 0$, 0.01, 0.05, 0.1 and 1). (a) $\alpha < 0$, (b) $\alpha > 0$.

peak is shifted towards π. As we increase the NL strength for repulsive potentials the peak at $3\pi/2$ converges towards π. For attractive NL potentials, the peak position at first gets closer to π and then moves away from it as we increase the strength of the NL potential. Thus repulsive and attractive NL potentials play different roles regarding their effects on the PD. This non-monotonic behaviour in the case of attractive NL potentials is also observed in disordered potential barriers (see figure 1(c)) and wells (figure 1(e)), while the monotonic behaviour observed in the mixed disorder case for repulsive NL potentials is also seen in the case of disordered barriers (figure 1(d)) and wells (figure 1(f)).

The oscillating behaviour of the PD peak position for attractive NL potentials gives rise, in this regime, to a Bloch-like behaviour of the transmission against length (see figure 2(a)), while the monotonic shift of the PD peak towards π for repulsive NL potentials enhances the decay of the transmission as a function of the length (figure 2(b)). This can be explained with the help of the strong correlation between the position of the PD peak and the transmission coefficient. Indeed a convergence of the peak in the PD towards π seems to lead to a strong decay of the transmission while peaks near zero or 2π seem to be related to a weaker decay or even an enhancement of the transmission.

Figure 2(b) shows that by increasing the NL repulsive potential strength we have already moved away from the quasi-ballistic regime (the localization length estimated from the slope of the transmission against length for $L \to 0$ becomes smaller than the lattice parameter and the condition $L \ll (2k_F)^{-1} \ll \lambda$ will not be satisfied). Thus, in addition to the disorder effect which decreases the transmission, the repulsive NL potentials lead to a chain composed mostly of barriers, which strengthens the transmission decay corresponding to the stronger growth of $|\Psi|^2$, again enhancing this decay. As we increase the NL strength the number of effective potential barriers increases while the potential wells tend to disappear. In this case, the disorder combined with repulsive nonlinearity makes the transmission decay stronger than the exponential decay.

When attractive NL potentials increase, their negative sign strengthens the effective potential wells ($\beta_n + \alpha|\Psi|^2$ from (1)) while the effective potential barriers tend to disappear from the chain. This is in contrast to the repulsive NL case. However, since the transmission decay is slower in the disordered potential wells in comparison to potential barriers [19], a competition between the easier transmission in the effective potential barriers of small strength (remaining in the chain) and the slow decay of the transmission in the effective potential wells makes the overall transmission coefficient (as well as the wavefunction amplitude $|\Psi|^2$) oscillate as shown in figure 2(a). This oscillatory-like behaviour disappears when the effective potential barriers disappear from the chain (the chain becomes composed only with effective potential wells) leading to the strong enhancement of the transmission decay, as in the case of repulsive NL potentials described above ($|\Psi|^2$ will grow strongly and the nonlinearity contributes to the transmission decay). As we increase the attractive NL strength, a more rapid increase of $|\Psi|^2$ takes place. Hence the period of the oscillating cycle decreases, as seen in figure 2(a). The amplitude of this oscillatory behaviour decreases as the length increases up to a characteristic length scale L_c. Above L_c the NL potential strengthens the disorder effect (this length corresponds also to the disappearance of the effective potential barriers from the chain). The characteristic length L_c decreases as the NL strength increases. Therefore, there are two characteristic length scales in the presence of nonlinearity: one (L_c) characterizing the oscillatory-like behaviour of the transmission in the quasi-ballistic regime and the other separating its exponential decay from its power-law decay for larger length scales, studied in detail in our previous work [11].

3.2. Quasi-metallic regime

In this regime, we choose $L = 10$, $W = 1$ and $E = 1$. These parameters satisfy the quasi-metallic condition $(2k_F)^{-1}(= 0.5) \ll L(= 10) \ll \lambda$ ($\approx$100 for mixed disorder, $\approx$70 for disordered potential barriers and $\approx$140 for disordered potential wells). In this case, the PD is nearly uniform in the mixed disorder case, as shown in figure 3 and in agreement with the tight-binding results [10]. In the case of disordered potential barriers and wells, this distribution is slightly peaked near the edges (0 or 2π). As we increase the attractive NL potential (figure 3(a)) a peak appears around π and moves towards higher phases while becoming sharper. For repulsive NL potentials (figure 3(b)) the peak shifts towards smaller phases (the peak for $\alpha = 2$ appears near 2π because we plotted the phase between 0 and 2π). A similar behaviour was found for potential barriers and wells (not presented here). We point out here that in these cases, when the NL potential has the opposite sign to the site potential, then the distribution flattens as the NL potential increases. This then leads to an enhancement of the transmission because the effective potential strength in (1) decreases [11]. When the NL potential becomes larger than the site potential, the effective potential starts increasing and gives rise to a sharper PD peak and a stronger exponential decay of the transmission.

We note here also, that for attractive NL potentials, the same finite size oscillatory-like behaviour described above in the quasi-metallic regime appears in the transmission.

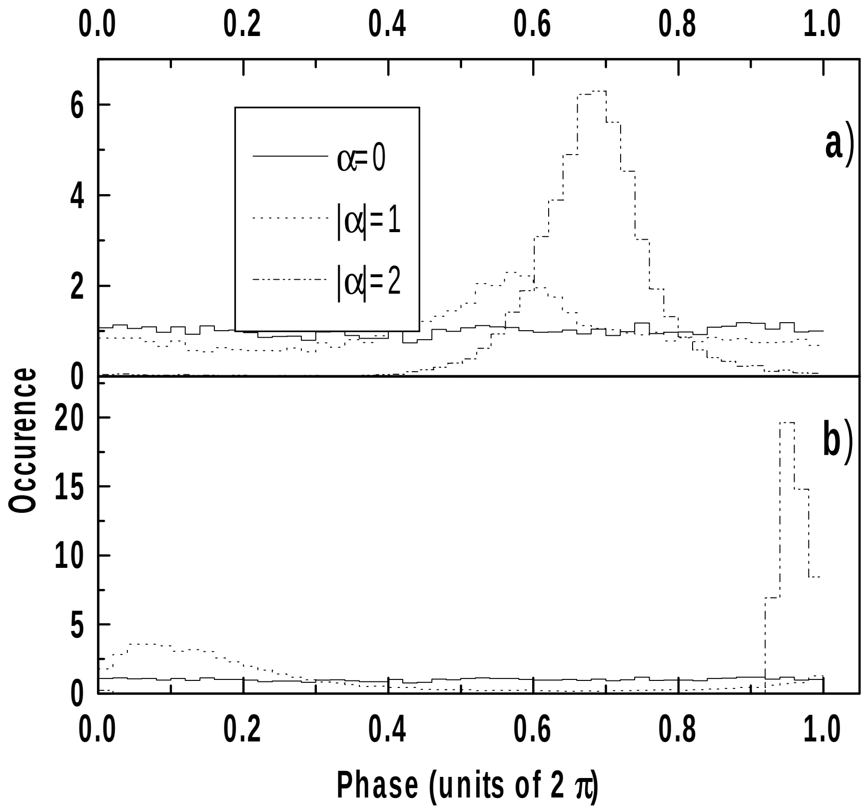

Figure 3. Phase distribution (in units of 2π) for $E = 1$, $W = 1$, $L = 10$ and different nonlinearity strengths ($|\alpha| = 0$, 1 and 2) in the mixed disorder case: (a) $\alpha < 0$, (b) $\alpha > 0$.

The characteristic length L_c defined above is about 5 for $\alpha = -1$ while it is about 20 for $\alpha = -0.1$. On the other hand, for attractive NL potentials the transmission decays rapidly for any arbitrary strength of the nonlinearity.

3.3. Strong disorder regime

From previous works [2, 4, 10] the strong disorder regime is reached when the two distribution peaks (appearing for the mixed disorder case when increasing the disorder strength) merge into a single, sharper peak. The PDs of concern to us in this regime are of a stationary nature, that is they are obtained for large sizes and are not affected by any further increase in the system length. As discussed previously, this peak is affected only by the energy in the mixed disorder case. However, this situation may not be the same for other types of disorder and in particular a compensation effect can occur for disordered potential barriers and wells. Indeed, as shown in figure 4, the peak is slightly shifted to higher phases in the case of disordered barriers. This peak becomes sharper as we increase the disorder strength and saturates at about 1.62π for infinite disorder strength. For disordered potential wells, the shift in the distribution peak is reversed (shifts to smaller phases) and saturates at approximately 1.64π. Hence there seems to be a compensation between the effects of potential wells and barriers, resulting in the mixed case, in the non-dependence of the peak position on disorder strength.

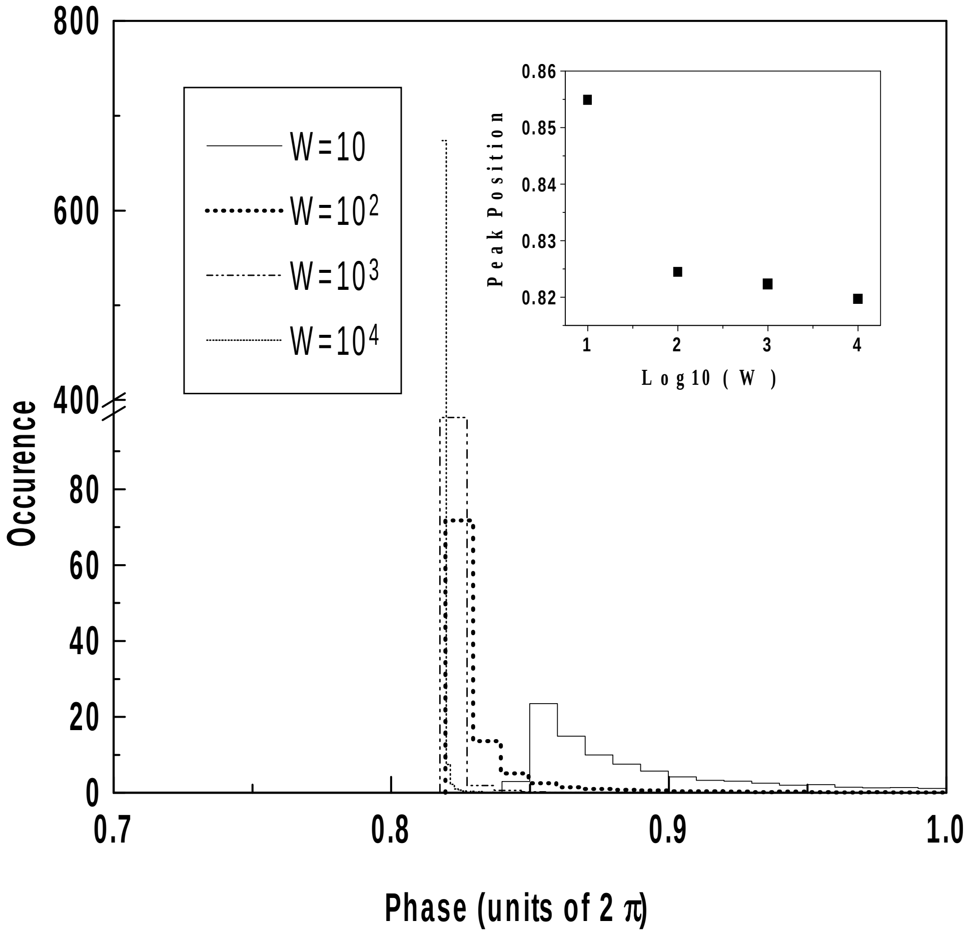

Figure 4. Phase distribution (in units of 2π) in the case of barriers for linear system with $E = 1$, $L = 1000$ and different disorder strengths ($W = 10$, 10^2, 10^3 and 10^4). The insert represents the peak position against disorder.

In figure 5 we show the PD for the mixed case for different NL potential strengths. Figure 5 shows that the NL potential plays the role of disorder. This is in the sense that it makes the peak sharper while its position is only slightly affected and for very strong NL repulsive (attractive) potentials it approaches the limiting positions observed in the strong disorder case for potential barriers (wells). In this regime and in the strong nonlinearity case, the transmission becomes vanishingly small and the effective potential will be either attractive or repulsive (dominated by the NL potential). This situation corresponds to that of figure 4 for potential barriers (and the equivalent one for potential wells). For disordered potential barriers the attractive NL flattens the distribution peak giving rise to a uniform distribution in agreement with the delocalization effects found for the transmission in our previous work [11]. For repulsive NL the distribution peak shifts towards smaller phases and seems to saturate around 1.64π. The peak becomes sharper as we increase the NL potential strength. For disordered potential wells the situation is reversed, that is for attractive nonlinearity the peak moves to higher phases and seems to saturate around 1.62π. Again it becomes sharper as we increase the NL potential.

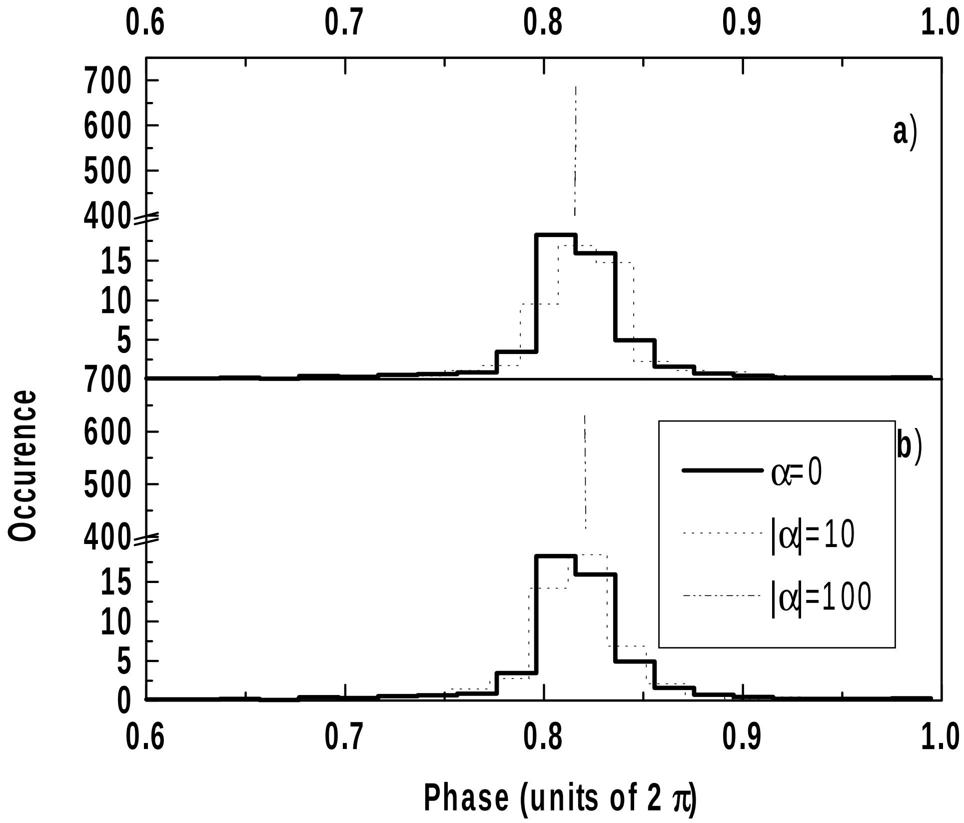

Figure 5. Phase distribution (in units of 2π) for $E = 1$, $W = 100$, $L = 10\,000$ and different nonlinearity strengths ($|\alpha| = 0$, 10 and 100) in the mixed disorder case: (a) $\alpha < 0$, (b) $\alpha > 0$.

For repulsive NL potentials the distribution peak flattens and corresponds to an enhancement of the transmission. Therefore, in agreement with our previous results on the transmission [11, 20], it seems that a flattening of the distribution gives rise to a delocalization effect when the linear and NL potentials are of opposite signs. However, if they are of the same sign it leads to an enhancement of the localization. The NL effects on potential barriers and wells are not shown here to avoid a lengthy paper. Therefore, we conclude from this work that a uniform PD cannot be taken as a signature of localization as claimed in previous works [5–8]. On the basis of our present results, strong localization occurs when the PD becomes sharply peaked and moves towards π, while in the case where this distribution become nearly uniform, it means a delocalization effect.

4. Conclusion

We have presented in this paper the effect of NL interaction on the PD and the transmission properties of a 1D Kronig–Penney system in three different regimes: quasi-ballistic regime, quasi-metallic regime and strong disorder regime. Our results in the mixed disorder case seem to be a superposition of disordered potential barriers and wells. We found that in the quasi-ballistic regime an attractive NL potential leads to an oscillatory shift of the PD peak position giving rise to a Bloch-like behaviour of the transmission. The transmissive properties, in the presence of attractive NL potentials have a second characteristic length scale L_c in addition to that separating the exponential from the power-law decay of the transmission, described in our previous work [11]. Repulsive NL potentials, on the other hand, seem to make the PD peak sharper and shift towards π. In the quasi-metallic regime, the uniform distribution in the mixed disorder becomes peaked and moves in a direction dependent on the sign of the NL potential. Finally in the strong disorder regime and for mixed disorder, the nonlinearity plays an identical role to disorder, in the sense that the distribution peak becomes sharper and seems to saturate to a limiting position for very strong nonlinearity. For disordered potential barriers or wells, the peak flattens out if the site potential and the NL potential have opposite signs. This gives rise to a delocalization effect, in agreement with our previous results on the effect of NL on the transmissive properties of these systems [11]. However, an extensive characterization of the transmissive properties of 1D systems by their PD should be completed in order to understand some unexpected behaviours in the transmission, such as the multistability, the chaotic behaviour for NL systems and the asymptotic exponential decay of transmission for amplifying systems [21]. Some of these interesting topics will be the subject of some forthcoming investigations.

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References

[1] Kappus M and Wegner F 1981 *Z. Phys.* B **45** 15
[2] Lambert C J and Thorpe M F 1982 *Phys. Rev.* B **26** 4742
[3] Azbel M and Soven P 1982 *Phys. Rev.* B **49** 751
[4] Stone A D, Allan C and Joannopoulos J D 1983 *Phys. Rev.* B **27** 836
[5] Anderson P W, Thouless D J, Abrahams E and Fisher D S 1980 *Phys. Rev.* B **22** 3519
[6] Economou E N and Soukoulis C M 1981 *Phys. Rev. Lett.* **46** 618
[7] Sak J and Kramer B 1981 *Phys. Rev.* B **24** 1761
[8] Melnikov V I 1980 *Pis'ma Zh. Eksp. Teor. Fiz.* **32** 244 (Engl. Transl. 1980 *JETP Lett.* **32** 225)
[9] Heinrichs J 1995 *J. Phys.: Condens. Matter* **7** 6291
[10] Sen A K 1997 *Mod. Phys. Lett.* B **11** 555
[11] Senouci K, Zekri N, Bahlouli H and Sen A K 1999 *J. Phys.: Condens. Matter* **11** 1823
[12] Zekri N, Schreiber M and Ouasti R 1995 *J. Phys.: Condens. Matter* **7** L275
[13] Cota E, Jose J V, Maytorena J and Montsivais G 1995 *Phys. Rev. Lett.* **74** 3302
[14] Molina M and Tsironis G P 1994 *Phys. Rev. Lett.* **73** 464
[15] Frohlich J, Spencer T and Wayne C E 1986 *J. Stat. Phys.* **42** 247
[16] For a review, see Hennig D and Tsironis G P 1999 *Phys. Rep.* **307** 333
Abdullaev F, Bishop A R and Pnevmaticos S (eds) 1992 *Disorder with Nonlinearity* (Berlin: Springer)
[17] Sanchez A, Macia E and Dominguez-Adame F 1994 *Phys. Rev.* B **49** 147
[18] Bellisard J, Formoso A, Lima R and Testard D 1982 *Phys. Rev.* B **26** 3024
[19] Ouasti R, Zekri N, Brezini A and Depollier C 1995 *J. Phys.: Condens. Matter* **7** 811
[20] Zekri N and Bahlouli H 1998 *Phys. Status Solidi* b **205** 511
[21] Zekri N, Bahlouli H and Sen A K 1998 *J. Phys.: Condens. Matter* **10** 2405 and references therein