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Abstract. A Kronig–Penney model with a constant electric field F for a non-interacting electron is used to study the transmission properties of the Anderson transition in one-dimensional systems with disordered δ-function potentials. We examine the cases where the potential varies uniformly from 0 to W (barriers) or from $-W$ to 0 (wells) for a given disorder W. We observe jumps in the transmission coefficient at the points $E + Fx = n^2\pi^2$ (where E is the electron energy and n an integer). These jumps are related to the small oscillations observed by Soukoulis *et al* in the mixed case (potentials from $-W/2$ to $W/2$). However, an interesting feature is found in the wells in the range between two jumps. It is observed that in the presence of a small field the states become more localized and the localization length decreases up to a minimum for a critical value F_m instead of increasing. Finally, we have studied the effect of the disorder on the Anderson transition by means of the participation ratio and the localization length.

1. Introduction

It is well established that almost all the eigenstates are exponentially localized in one-dimensional (1D) disordered systems in the absence of external fields irrespective of the amount of disorder [1–3]. Such localization properties have been extensively studied both analytically and numerically [4–14]. Two main models have been shown to be powerful in examining the transport properties of 1D systems: the Kronig–Penney model [8–12] and the tight-binding model [10, 13, 14]. The Kronig–Penney model is greatly appreciated for its simplified structure in introducing external fields. Two types of 1D disordered system have been proposed: substitutionally disordered systems with a constant lattice parameter [8–11] and spatially disordered systems with a constant potential [12].

The transmission coefficient is the relevant quantity for determining the localization properties [8, 11] and its logarithm has been shown to be statistically well behaved [15, 16] and to obey the central limit theorem [17].

Landauer [18] was the first to relate the transmission coefficients to the resistance:

$$R = T^{-1} - 1 \tag{1}$$

supported by experimental evidence at low temperatures on thin 'dirty' wires [19, 20]. The interest in the zero-temperature properties of these systems is that the resistance should increase exponentially with increasing length of the system:

$$R = \exp(\alpha L) - 1 \tag{2}$$

where α is the inverse localization length. At higher temperatures the localization of electron states will not be apparent because the phonon will cause the electron to hop from one state to another.

The electronic properties of disordered systems in the presence of electric fields are still less known and continue to be an attractive goal. For these systems, it has been proved that for a critical field F_c giving a total electrostatic energy across the sample equal to the electron energy, i.e. $F_c L = E$, the delocalization transition occurs. The relevant parameter in this problem is $X = FL/E$. In particular, at $X = 1$, a transition is observed from exponentially to power-law decaying states as confirmed by various calculations [9, 11, 21], while for large fields the transition from power law to extended states has been rigorously derived [10]. Most models considered uniformly distributed disordered potentials between $-W/2$ and $W/2$ (mixed case) for a given disorder W, and very few have been reported for the barriers case where the disordered potential varies from 0 to W or the wells case between $-W$ and 0.

Another relevant physical quantity for describing the nature of the eigenstates in the Anderson localization problem is the inverse participation ratio [22–24]. Furthermore a scaling law equation has been recently analytically derived for this quantity [25].

In this paper we are firstly concerned with the behaviour of the transmission coefficient in the presence of an electric field for two new systems: barriers and wells. Then we compare our data in the light of the mixed-case results [8, 10]. These systems may exhibit a new behaviour rather than the mixed case but we expect a compensation of the first two systems.

In a second step the inverse participation ratio and the localization length are used to examine the effect of the disorder on the delocalization transition in the mixed systems. It is important to confirm that the disorder does not change the Anderson transition qualitatively.

2. Formalism

We consider a linear chain of a finite L atoms with δ-peak potentials of random strengths V_n uniformly distributed. The Kronig–Penney model is used to calculate the wavefunctions of this system:

$$\left(-\frac{d^2}{dx^2} + \sum_{n=1}^{L} V_n \delta(x - na) - eFx \right) \psi(x) = E\psi(x) \qquad (3)$$

where E is the electron energy measured in $\hbar^2/2m$ units and the lattice parameter a is constant and taken here as the unit length. The disordered sample extends from $x = 0$ to $x = L = Na$, the two ends being connected ohmically to perfect leads maintained at a constant potential difference $|e|FL$, where e is a charge of the electron taken for convenience as unity.

The numerical resolution of equation (3) can be performed by taking advantage of the Poincaré map representation of the Schrödinger equation. This transformation consists in relating the wavefunction at different lattice sites. Specifically, by defining $\psi_n = \psi(x = na)$, Bellissard et al [26] showed in the absence of external field that equation (3) can be exactly mapped into a finite-difference equation of the form

$$\psi_{n+1} + \psi_{n-1} - V_n \frac{\sin \sqrt{E}}{\sqrt{E}} \psi_n = (2 \cos \sqrt{E}) \psi_n. \qquad (4)$$

In order to map equation (3) to a finite second-order differential equation it is convenient to approximate the potential Fx by a step function [9–11, 27], i.e. the so-called ladder approximation. This approximation is expected to be valid in the limit of weak fields $(Fa \ll E)$. By extrapolating the results obtained by Cota *et al* [11] of a comparison between the exact results and the approximate results to the parameters used in the present paper we expect that this approximation is valid for fields up to a few per cent of the electron energy. Once this is done, the solutions to equation (3) in between δ potentials are plane waves instead of Airy functions. The corresponding Poincaré map then reads

$$\psi_{n+1} = \left(\cos(k_{n+1}) + \frac{k_n \sin(k_{n+1})}{k_{n+1} \sin(k_n)} \cos(k_n) + V_n \frac{\sin(k_{n+1})}{k_{n+1}}\right) \psi_n - \frac{k_n \sin(k_{n+1})}{k_{n+1} \sin(k_n)} \psi_{n-1} \qquad (5)$$

with $k_n = \sqrt{E + naF}$. Equation (5) reduces to equation (4) for $F = 0$. This equation is a recursion formula and enables one to treat very large systems, being limited only by the computer time available. To carry out the iterations we introduce as initial values for ψ_1 and ψ_2 the plane waves $\psi_1 = \exp(-i\sqrt{E})$ and $\psi_2 = \exp(-2i\sqrt{E})$. We consider here an electron of wavenumber k_L incident at $x = L$ from the right. It is partially reflected with complex reflection amplitude and partially transmitted with a wavenumber $\sqrt{E}$. Iterating equation (5) we can calculate the wavefunctions ψ_{N+2} and ψ_{N+3} in order to obtain the transmission coefficient from the relation

$$T = \frac{k_0}{k_L} \frac{|\exp(2ik_L) - 1|^2}{|\psi_{N+2} - \psi_{N+3} \exp(-ik_L)|^2} \qquad (6)$$

where $k_L = \sqrt{E + FL}$ and $L = N + 2$. We examine here the quantity $\ln(T)$ because it is statistically well behaved [16].

The delocalization and the nature of the wavefunction can also be studied by means of the inverse participation ratio [23] and the localization length [4]. The inverse participation ratio is defined by

$$\mathcal{P} = \sum_{n=1}^{L} |\psi_n|^4 \Big/ \left(\sum_{n=1}^{L} |\psi_n|^2\right)^2 \leqslant 1. \qquad (7)$$

It behaves in the following way:

$$\mathcal{P} \propto O(N^{-1}) \qquad \text{for extended states} \qquad (8)$$

and

$$\mathcal{P} \propto O(N^0) \qquad \text{for localized states.} \qquad (9)$$

In a recent numerical work Mato and Caro [24] have confirmed the delocalization transition by means of this quantity at $X = 1$, providing some explanation for the results on the transmission coefficient.

The localization length λ is defined by [4, 26]

$$\lambda^{-1} = \lim_{N\to\infty} \left(\frac{1}{N} \langle \ln(|\psi_{N+1}|^2 + |\psi_N|^2)^{1/2}\rangle\right) \qquad (10)$$

where $\langle\,\rangle$ means the average. For $F = 0$ and using the Kronig–Penney model for mixed systems, the localization length can be expressed in terms of the electron energy and the disorder W [9] as follows:

$$\lambda(F = 0) = 96\frac{E}{W^2}. \qquad (11)$$

This expression is valid only in the mixed case ($\langle V_n \rangle = 0$).

3. Results and discussion

In this section we discuss our numerical data on the transmission coefficient, the participation ratio and the localization length for different cases of 1D systems. The length of the system is $L = 4000$ and is sufficient to reproduce the global transport properties of the chain of finite length because the largest localization length ($\lambda_{max} = 55$ for the barriers) is much smaller than 4000. The quantities of interest are averaged over a number of 100 realizations (which is sufficient to obtain an accuracy of few per cent for $\langle \ln(T)/L \rangle$) for the transmission coefficient and 1000 realizations for the participation ratio and the localization length calculations (in order to obtain the same accuracy). The transmission coefficient is determined for two types of system, namely barriers and wells, while the participation ratio and the localization length are calculated in the mixed case.

3.1. Transmission coefficient

For comparison, we consider here the same parameters used by Soukoulis *et al* [9] for mixed systems, i.e. $E = 5$ and $W = \sqrt{12}$.

The transmission coefficient at $F = 0$ has been predicted to decrease exponentially with respect to the length of the system. In the barrier and well systems the same behaviour is seen in figure 1. It is also observed that the wells exhibit a smaller localization length ($\lambda \simeq 12$) while the barriers have a larger localization length ($\lambda \simeq 55$) and for the mixed case $\lambda \simeq 38$, satisfying equation (10). This result suggests, as expected, that the well systems strongly attract electrons, because of the typical nature of the short-range potential, while the barrier systems make transmission easier because of the tunnel effect. Obviously in mixed systems, the strong attraction of the wells competes with the tunnel effect in the barriers.
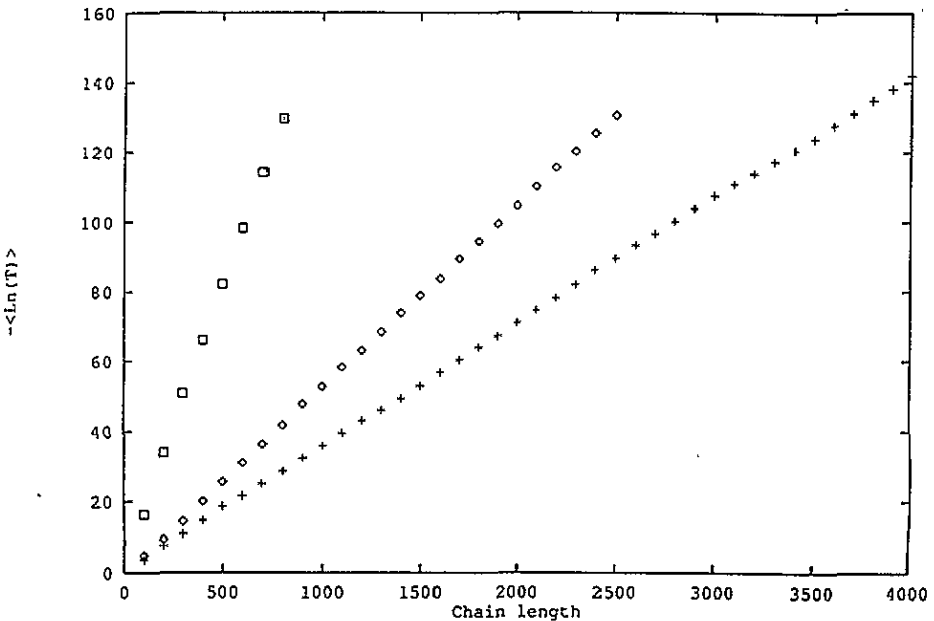

Figure 1. Comparison of the transmission coefficient between barriers (+), wells ($\square$) and the mixed case ($\lozenge$) for $F = 0$.

In applying an electric field to the barriers or the wells an abrupt jump appears in the transmission coefficient curves as seen in figure 2 for both the barriers and the wells at the particular values corresponding to $E + Fx = n^2\pi^2$, where n is an integer, in agreement with the predictions of Delyon *et al* [10] in the mixed case for $F = 0$. The strength of these jumps decreases for increasing F. Probably these jumps are related to the Zener-type transitions suggested by Soukoulis *et al* [9] and Cota *et al* [11]. This implies that power-law decays are not expected in such cases for length chains including these jumps.
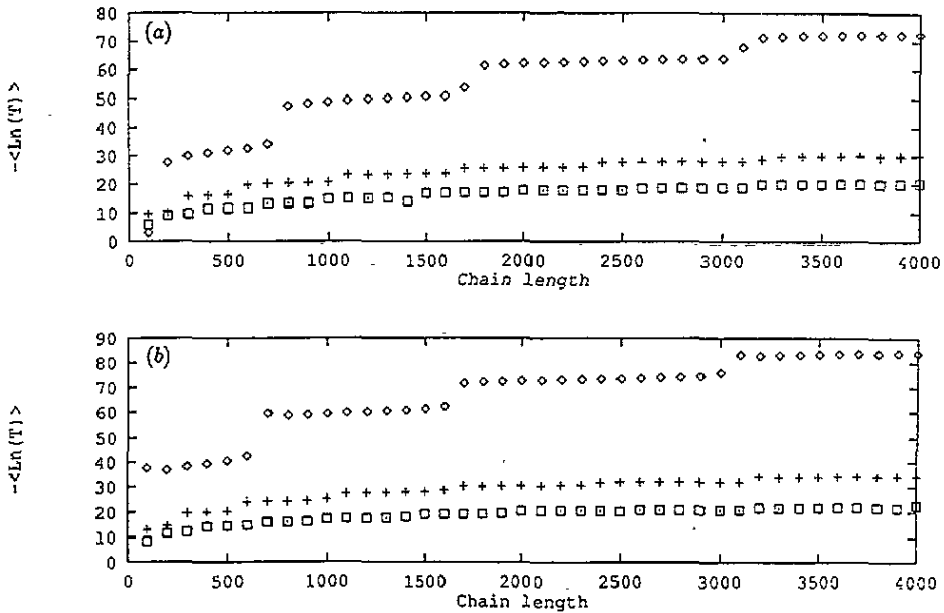

Figure 2. Transmission coefficient for different fields $F = 0.05$ ($\Diamond$), 0.15 (+) and 0.25 ($\Box$); (*a*) barriers; (*b*) wells.

For lengths before the first jump for the barriers the states undergo a transition from exponential to power-law decaying states (at $FL/E = 1$) as predicted by other works [9, 11] for mixed systems. In particular, figures 1 and 3(*a*) show the qualitatively similar behaviour (the curve of $-\langle \ln T \rangle$ as a function of the length chain fits a straight line at $F = 0$ and, for $F \neq 0$, $-\langle \ln T \rangle$ is a straight line as a function of the length chain on a logarithmic scale). However, surprisingly, the states associated with the wells do not behave similarly in figure 3(*b*). In this figure, $\langle -\ln T \rangle$ exhibits an exponentially divergent curve. Such unexpected features are reported here, indicating the existence of another type of localized *state observed in other situations* [28]:

$$\psi \simeq \exp(-x\beta) \qquad \text{with } \beta > 1. \tag{12}$$

In such systems the small electric field increases the attraction of the electron and then decreases the overlap of the wavefunctions. The localization length defined by equation (10) decreases to a minimum ($\lambda \simeq 5$) for a critical field ($F_c \simeq 0.01$). Owing to the jump in the transmission coefficient, this localization length varies with the length of the system. The transport properties of the wells will compete with the barriers in mixed systems.
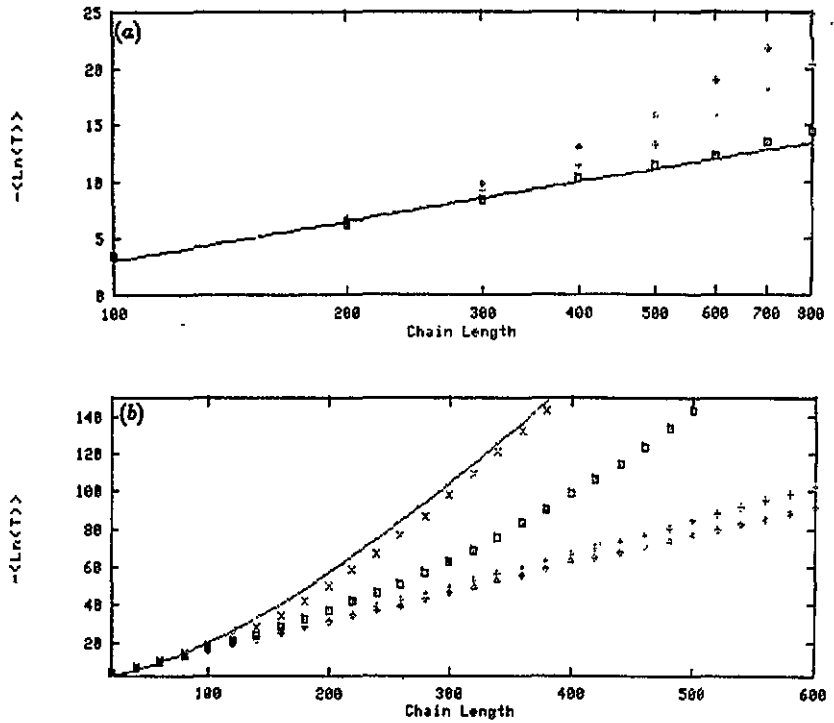
Figure 3. Transmission coefficient for different fields: (*a*) barriers for $F = 0.001$ ($\Diamond$), 0.002 (+) and 0.005 ($\square$) (log–log scale) (——, guide); (*b*) wells for $F = 0$ ($\bullet$), 0.001 (+), 0.005 ($\square$) and 0.005 ($\times$) (——($-\ln T = 0.02L^{1.5}$), guide).

In opposition to the global lengths (including the jumps) the transmission coefficient in the presence of an electric field for the systems studied here are both smaller than in the mixed case (figure 4). This is a curious result because we expect compensation between the effects of the wells and the barriers. Probably the mixture of the two cases will make the transmission of electrons easier.

3.2. Effect of the disorder on the Anderson transition

In this section, we study the effect of the disorder W on the delocalization transition, i.e. the inverse participation ratio $\mathcal{P}$ and the localization length λ. These quantities are essential in describing the nature of the eigenstates. In particular they are sensitive to the relevant parameter $X = FL/E$ [11]. In the following calculations we have considered for convenience $E = 1$.

It is well established from transmission coefficient calculations [9, 11] or from participation ratio calculations [24] that the delocalization transition occurs at $X \simeq 1$ and the states are exponentially localized for $X < 1$ while for $X > 1$ the wavefunctions become extended. Furthermore in the transition region ($X \simeq 1$) the wavefunctions are power law localized [9, 11, 21]. In figure 5 the inverse participation ratio $\mathcal{P}$ is reported as a function of $\ln X$ for different disorders W. These results clearly confirm the expected transition at $X = 1$. The results of Mato and Caro [24] on the participation ratio show a transition slightly shifted to the right of $X = 1$. This is presumably because they have averaged over a small number of iterations (15) and then their results are less accurate rather than ours
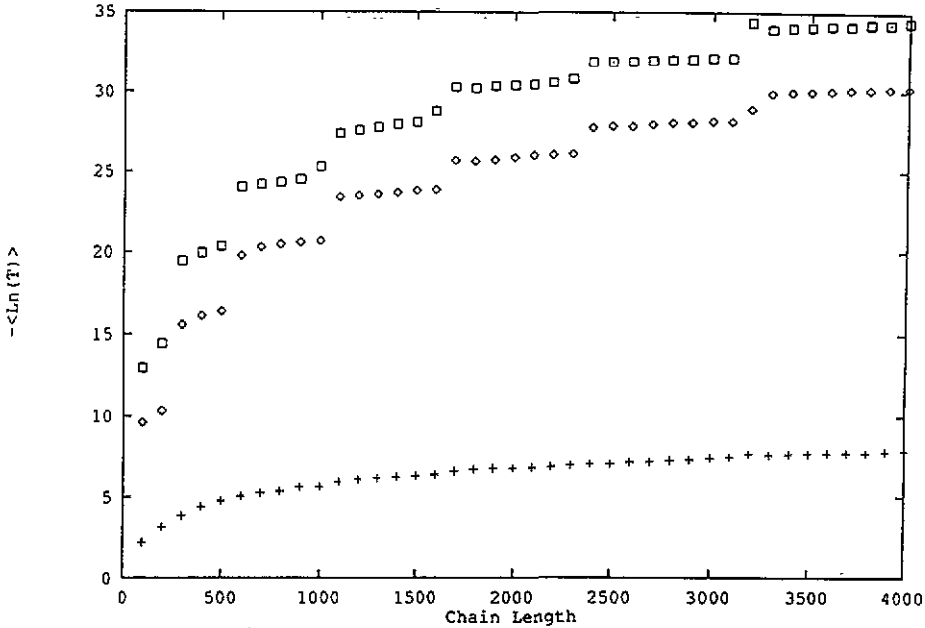
Figure 4. Comparison of the transmission coefficient between the barriers ($\Diamond$), the wells ($\square$) and the mixed case ($+$) for $F = 0.15$.

(1000 realizations). It is mainly observed in figure 5 that the transition is smooth for small disorder W and the curve becomes a horizontal line when $W \to 0$, leading as expected to extended states. On increase in the disorder, the transition becomes abrupt. As predicted by Mato and Caro [24], these effects do not affect the critical point of the transition. It has been shown for infinite chains that this transition occurs at $X = 0$ when the potential is arbitrarily smooth [29].

In the localized states the values of the inverse participation ratio correspond approximately to the core of the wavefunction ($\mathcal{P}^{-1} \simeq \lambda/2$). From figure 5 the inverse participation ratio takes the following values in the localized states:

$$W = 1.5 \qquad \mathcal{P}^{-1} \simeq 20$$
$$W = 1 \qquad \mathcal{P}^{-1} \simeq 50$$
$$W = 0.5 \qquad \mathcal{P}^{-1} \simeq 200$$

and then the extended states are expected for $W \to 0$ ($\mathcal{P}^{-1} \to \infty$). It is then possible to parametrize the inverse participation ratio as

$$2\mathcal{P}^{-1} \simeq L \simeq \frac{1}{|X - X_c|^\nu}(\nu > 0 \qquad \text{and} \qquad X_c = W = 0). \tag{13}$$

This transition is also observed in figure 6 where the localization length λ is shown as a function of X. This behaviour is seen in quasi-periodic systems at a critical point [4]. However, in this way, it seems that the disorder affects the transition weakly (the transition is shifted slightly to the right of $X = 1$ for large values of W).
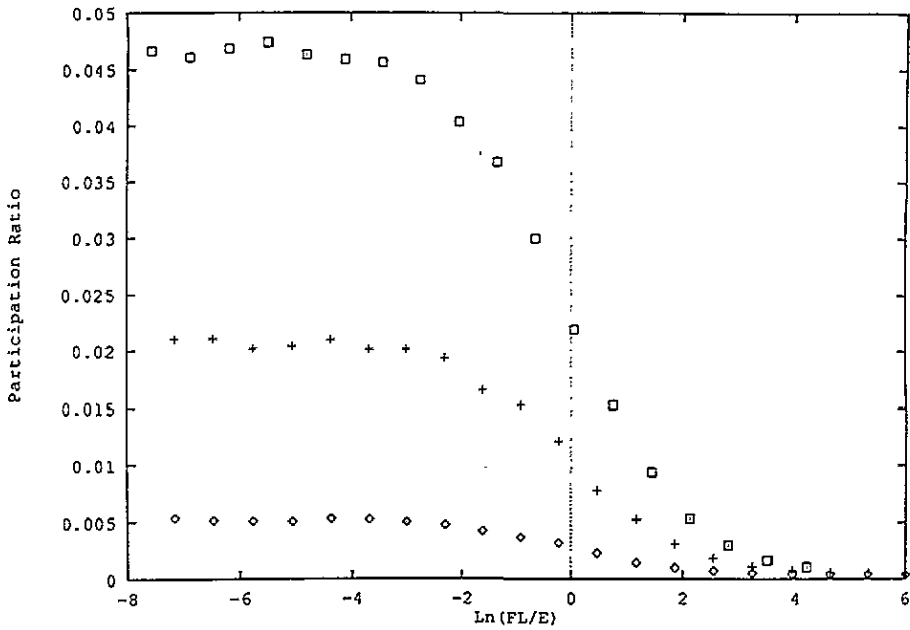
Figure 5. Participation ratio as a function of $\log(FL/E)$ for $E = 1$ and different disorders: $\Diamond$, $W = 0.5$; $+$, $W = 1$; $\Box$, $W = 1.5$.
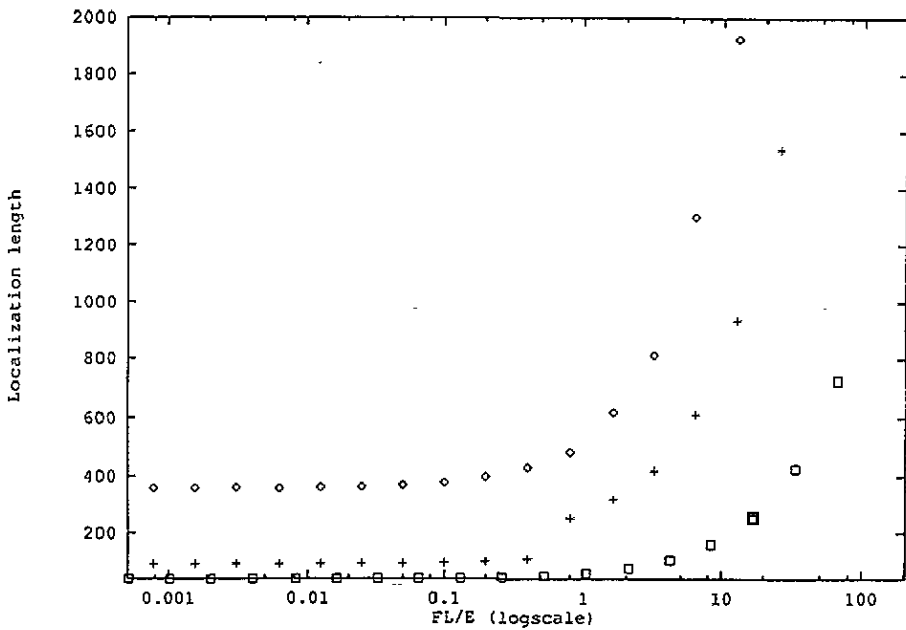

Figure 6. Localization length λ as a function of FL/E for $E = 1$ and different disorders: $\Diamond$, $W = 0.5$; $+$, $W = 1$; $\Box$, $W = 1.5$.

4. Conclusion

In this paper we examined the Anderson transition for different disordered 1D systems (barriers, wells and mixed systems) and also the effect of the disorder on this transition. For this, we calculated the transmission coefficient, the inverse participation ratio and the localization length. In the barriers and wells we found that the transmission coefficient also behaves like the mixed systems at $F = 0$ (i.e. exponentially localized states) but the well states are more strongly localized than the mixed states while, in the barriers, localization is weaker.

The wells and barriers are also found to exhibit jumps which are suggested by Soukoulis *et al* [9] in the mixed case to be of Zener type at particular points, i.e. for $Fx + E = n^2\pi^2$. The jumps in the $-\langle \ln T \rangle$ curves indicate that the localization length goes to infinity at these points as predicted by Delyon *et al* [10].

The other new effect is observed for the wells in the transmission curves before the first jump. The localization length decreases to a minimum for sufficiently small fields, leading to super localized states. This suggests the existence of a critical field (for which the localization length is a minimum). This effect disappears when the wells and the barriers are mixed.

Finally we examined the effect of disorder on the Anderson transition for mixed systems by calculating the inverse participation ratio and the localization length. This transition is strong for large disorders and becomes smooth when $W \to 0$ without affecting the critical point $X = 1$ as expected by Mato and Caro [24].

The systems examined here open up the following new questions.

(1) What is the origin of the super localization in the wells and the jumps in the barriers and the wells in the transmission coefficient?

(2) For which disorder W and energy E is super localization in the wells observed?

(3) What is the behaviour of the exponent α of the super localized states (equation (12)) as a function of the field?

(4) What are the multifractal character, and the inverse participation ratio of the eigenstates in the wells and the barriers?

These questions are the subject of a forthcoming paper.

Acknowledgment

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