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Fractal wavefunctions in one-dimensional disordered systems with an electric field

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Abstract. We evaluate one of the generalised dimensions of the multi-fractal wavefunctions, the correlation dimension $D(2)$, and the participation ratio. We find that, when the system undergoes the delocalisation transition, the wavefunction loses its multi-fractal character. It is also observed that $D(2)$ is more sensitive to the electric field than are other core properties such as the participation ratio.

1. Introduction

The question of localisation of eigenstates in one-dimensional disordered systems in the presence of an electric field has been extensively studied. Both analytic (Prigodin 1980, Castello *et al* 1987) and numerical (Soukoulis *et al* 1983, Cota *et al* 1985) approaches in one dimension have clearly shown the existence of a transition from exponentially localised to power-law decaying states as a function of increasing electric field. Exponential or power-law decay are characteristics of the asymptotic region of the wavefunction, i.e. far from the centre of the mass of the charge distribution.

It is well established that the critical electric field F_c which produces the delocalisation transition is that giving a total electrostatic energy across the sample equal to the electron energy: $F_cL = E$, with L the sample length. The only relevant parameter in this problem is $X = FL/E$ and the transition is a smooth transition around $X = 1$. It is interesting to note that the disorder itself does not play a role in the determination of the critical field but only appears to affect the total change in the magnitude being considered, e.g. the transmission coefficient (Castello *et al* 1987).

An alternative characterisation of the wavefunctions of disordered systems is given by the fractal dimension (Mandelbrot 1977). The fractal dimension is evaluated over a length scale smaller than the localisation length around the centre of mass. Therefore it is a core property (Soukoulis and Economou 1984). However, this characterisation raised some controversies. In fact the results obtained by Soukoulis *et al* were hardly reproduced, in particular, in the work by Román (1986), Siebesma and Pietronero (1985) and Pietronero *et al* (1987).

Román suggests that the correct discrete version of equation (1) Soukoulis *et al* (1983) should not contain the contribution from the origin in order to scale correctly for small L. In doing so, he always obtained a fractal dimension equal to one. He concluded that the self-similar behaviour is a spurious effect of the contribution of $|\psi_0|^4$.

This result is curious because we have studied the multi-fractality of the wavefunction in the same model, eliminating the contribution from the origin, and our results show a non-trivial fractal behaviour (Mato and Caro 1987).

Similarly, Siebesma and Pietronero found not only a slope of unity at short distances but also a curvature in a length scale always smaller than the localisation length which presents a proper definition of the slope. Again this result is curious because we found a slope much lower than unity with a curvature starting at about half the localisation length.

Finally, Pietronero *et al* evaluated the moments of the wavefunction and found no evidence of multi-fractality or even fractality. However, this result is not convincing because they evaluated moments of a function which is not an eigenfunction of the Anderson Hamiltonian. For instance their function is not localised and the moments are not restricted to the core.

It is probable that the differences which we have just mentioned arise from the method of evaluation of the wavefunction. Our method of inverse iteration always gives the convergent solution and the boundary conditions corresponding to a scattering problem allow us to use an arbitrary eigenvalue (Román and Wiecko 1986).

This method which we used in a recent paper (Mato and Caro 1987) showed that the localised wavefunction is a multi-fractal object with an infinite number of generalised dimensions (Hentschel and Procaccia 1983, Munroe 1953) and a Hausdorff fractal dimension equal to one.

A multi-fractal object is a set that can be split into subsets each having its own fractal dimension (Halsey *et al* 1986). The characterisation of such an object is made by the scaling exponents of the correlation functions $\tau(q)$ of q points. The generalised dimensions $D(q)$ are given by $D(q) = \tau(q)/(q-1)$. The definition of the fractal dimension proposed by Soukoulis *et al* coincides with $D(2)$ and not with the Hausdorff dimension.

This magnitude $D(2)$, called the correlation dimension, has been extensively studied to characterise wavefunctions in several models (Román and Wiecko 1986, Zdetis *et al* 1986).

We shall use this correlation dimension to study the delocalisation transition. We shall also use the participation ratio (Bell and Dean 1970) as a measure of the size of the wavefunction.

2. Model

We shall use a Kronig–Penney model with the Poincaré map representation of the Schrödinger equation (Soukoulis *et al* 1983). We approximate the electrostatic potential by a step function, which has proved to be a good approximation (Nagai and Kondo 1980):

$$(K_{n+1}/\sin K_{n+1})\psi_{n+1} + (K_n/\sin K_n)\psi_{n-1}$$
$$= (K_{n+1}\cos K_{n+1})/\sin K_{n+1} + (K_n \cos K_n)/\sin K_n + b_n\psi_n \qquad (1)$$

where $K_n = (E + Fn)^{1/2}$ and b_n is a random variable which measures the strength of the nth δ-function. b_n is taken from a rectangular distribution of width W and centred at 1 (in units of $\hbar^2/2m$).

Equation (1) is solved by the inverse iteration method (Román and Wiecko 1986) with $0 \leqslant n \leqslant L$. The boundary conditions are those corresponding to plane waves connected to the ends of the finite system. In this way, we can evaluate the eigenfunctions for arbitrary energy. Once the normalised eigenfunction is known, the participation ratio P and the correlation dimension $D(2)$ are evaluated using

$$P^{-1} = \sum_{n=0}^{L} |\psi_n|^4 \tag{2}$$

$$l^{D(2)} \propto \sum_{n_0} \left(|\psi_{n_0}|^2 \sum_{n=n_0+1}^{n_0+l} |\psi_n|^2 \right) \tag{3}$$

with n_0 such that every term in the sum belongs to the core. Note that the term $\Sigma_{n_0} |\psi_{n_0}|^4$ has been omitted in equation (3) in order to obtain the correct scaling for small l (Román 1986).

3. Results and discussion

We have evaluated P and $D(2)$ for a system of length $L = 1024$, $E = 1$, $W = 1$, $10^{-4} \leqslant FL/E \leqslant 10^3$ and 15 realisations of the random potential. The wavefunction was evaluated for each realisation of the random potential and equations (2) and (3) were used to obtain P and $D(2)$ and then they were averaged. The results are shown in figures 1 and 2.

It is interesting to note that non-trivial fractal behaviour is obtained for a single realisation of the random potential although $D(2)$ and P are slightly different for each sample. According to the values adopted for W and E the localisation length for small fields is around 100. In these cases of small fields the participation ratio takes a constant value of approximately 30 which is a measure of the core size. As X increases, the participation ratio grows significantly and at $X \simeq 1$ shows the delocalisation transition. For large fields ($X \gg 1$), the wavefunction spreads over the whole sample. This result agrees with the huge decrease in the differential resistivity found by Castello *et al* (1987).

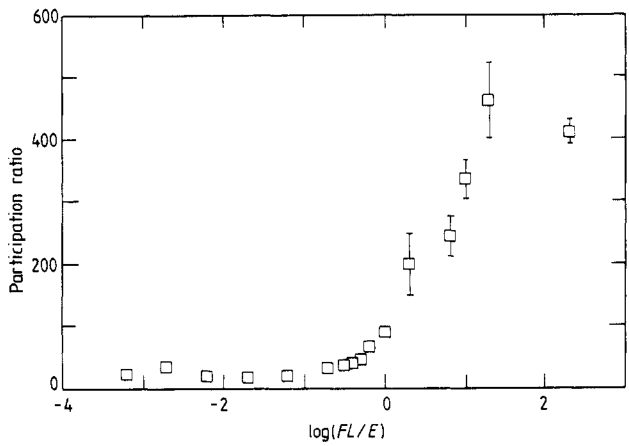

Figure 1. Participation ratio as a function of $\log(FL/E)$. The error bars are obtained after averaging over 15 samples.

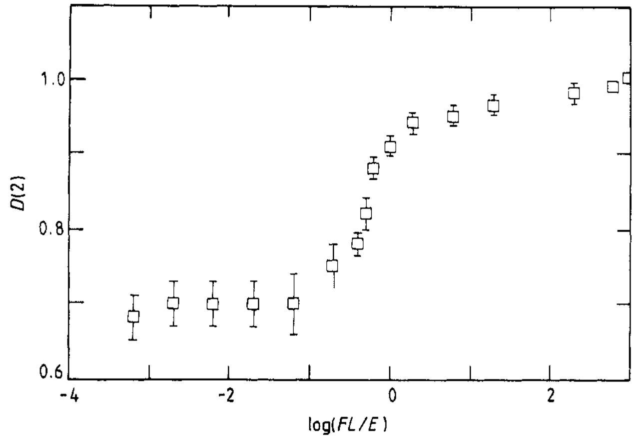

Figure 2. Correlation dimension $D(2)$ as a function of $\log(FL/E)$. The error bars are obtained after averaging over 15 samples.

The correlation dimension shows a similar behaviour. For small fields ($X \leqslant 0.1$), $D(2)$ is almost constant and its value is in agreement with the results of Soukoulis and Economou (1984) and Román and Wiecko (1986). For very large fields ($X \geqslant 10^3$), $D(2)$ approaches the value 1, the Euclidean dimension of the space; therefore the fractal character of the wavefunction disappears. For such a large field the disordered potential becomes irrelevant and the wavefunction is completely determined by the solution of the Schrödinger equation with an electric field, i.e. the Airy function.

In fact, the delocalisation transition is already shown in $D(2)$ for $X \simeq 0.1$. This is interesting because $D(2)$ is a short-range property. Such a value for X represents a potential drop from site to site of the order of 10^{-4}, which is four orders of magnitude smaller than the average change in site energy due to disorder. This shows that $D(2)$ is much more sensitive to the electric field than is the participation ratio, which is contrary to intuition. For $q \neq 2$, the $D(q)$-values behave in a similar fashion; for very large fields $D(q)$ approach the value 1. In conclusion, we have shown that the electric field, through the delocalisation transition destroys the multi-fractal character of the wavefunction in a disordered system. Moreover, the evaluation of one of the generalised dimensions, the correlation dimension $D(2)$, shows that it is as sensitive to the effects of the electric field as is an asymptotic property, such as the differential resistivity (Castello *et al* 1987), and more sensitive than is a core property such as the participation ratio.

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