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Two-point statistics on multifractal analysis of resonant states

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Abstract. In order to characterize the resonant states described earlier by Basu *et al* (1991), we carry out the analysis of the two-point statistics on the multifractal measure associated with the transmittance of these states. We clearly demarcate the two regions to which the localized and the resonant states belong.

1. Introduction

It is well known that electronic states in tight-binding one-dimensional chains with nearest-neighbour overlap are exponentially localized. However, there is evidence of the existence of transmitting stochastic resonances (Azbel 1983a, b, 1984, Azbel and Rubinstein 1983, Pendry 1982a, b, 1984, 1986, 1987, Pendry and Kirkman, 1984, 1986, Godin and Haydock, 1988, Basu *et al* 1991). Pendry (1987) suggested that these transmitting states could be necklace states; that is, a superposition of localized states centred at different points and spanning the chain. Basu *et al* (1991) have looked at the transmittance as a function of the chain length [$T(L, E)$ versus L] and have noticed the necklace-like behaviour suggested by Pendry. The transmittance at the stochastic resonances shows a rich internal structure. In this communication we propose to examine this behaviour in some detail.

We note first that the $T(L, E)$ or $|\psi(L, E)|^2$ as functions of L differ in detail for different resonances for the same chain configuration or different chain configurations. Compare, for example, figures 2(*a*) and (*b*). One may, of course, inspect them directly one by one. The whole object of this communication is to suggest a method which will allow us to examine, not these individual differences, but the common characteristics resonant states. In particular, we wish to examine the question: are resonances due to special localized states peaked at the chain centre (as originally suggested by Azbel) or are resonant states necklace states (as suggested by Pendry)? To examine the clumped, multipeaked behaviour of $T(L, E)$ versus L curves, it is necessary to study the two point correlation functions on the probability measure defined on the chain. Knowledge of such correlations is useful in understanding the internal structure of multifractal measures. Lee and Halsey (1990) and Meneveau and Chhabra (1990) have suggested a generalization of the usual multifractal analysis. They define a function $f(\alpha, \alpha', \omega)$. This allows us to examine the probability of finding pairs of sites with singularity strength α and α' at a distance $r = a^{\omega}$ (a is the bin size $= 1/N$, assumed).

2. Formalism

In a narrow wire of length N described by the Anderson TB Hamiltonian, we have

$$H_{\text{sample}} = \sum_{n=1}^{N} \varepsilon_n \varphi_n^\dagger \varphi_n + V \sum_{n=1}^{N} (\varphi_n^\dagger \varphi_{n+1} + \varphi_n^\dagger \varphi_{n-1}). \tag{1}$$

At the two ends of the chain at $n = 1$ and $n = N$ we attach elementary perfectly conducting semi-infinite leads. We used the recursion technique with single site transfer matrices (Liu and Chao 1986) to find the transmittance $T(E)$ and reflectance $R(E)$ at different energies. At the stochastic resonances $T(E) = 1$ and $R(E) = 0$. At these energies the transmittance is observed along the length for a sample of size 3×10^4.

We define the correlation of transmittances between any two points on the chain at a distance r:

$$C(r) = \frac{1}{V} \sum_{i=1}^{N-r} T(i)\, T(i+r) \tag{2}$$

where V is the volume of the sample and equals N for a one-dimensional chain. $C(r)$ gives the correlation between pairs of points at a distance r from each other. This should reflect clumped or necklace-like behaviour, if there is any, and clearly distinguish between localized decaying states and necklace resonant states peaked at different points on the chain. This is a property which will clearly distinguish between extended and localized states also.

We define a generalized normalized measure, obtained from transmittances at different points, as

$$\bar{\mu}(i) = \left[T^p(i) T^q(i+r) \right] \Big/ \left[\sum_i T^p(i) T^q(i+r) \right]. \tag{3}$$

Then, following Lee and Halsey (1990), we define

$$\alpha = -\sum_{i=1}^{m} \bar{\mu}(i) \log T(i) / \log(N)$$

and

$$\alpha' = -\sum_{i=1}^{m} \bar{\mu}(i) \log T(i+r) / \log(N). \tag{4}$$

The probability of finding the two scaling exponents α' and α'' at a distance r is

$$P(\alpha, \alpha', r) \simeq N^{f(\alpha, \alpha', \omega) - D_0} \tag{5}$$

where $\omega = -\log(r)/\log(N)$ and D_0 is the fractal dimension at $q = 0$

$$\log P(\alpha, \alpha', r) = [f(\alpha, \alpha', \omega) - D_0] \log(N). \tag{6}$$

As D_0 and N are constants, $f(\alpha, \alpha', \omega)$ gives information about the probability.

$$f(\alpha, \alpha', \omega) = -\sum_{i=1}^{m} \bar{\mu}(i) \log \bar{\mu}(i) / \log(N) \tag{7}$$

r is always less than N, so ω is always less than 1. Hence $0 < 1 - \omega < 1$. Plotting

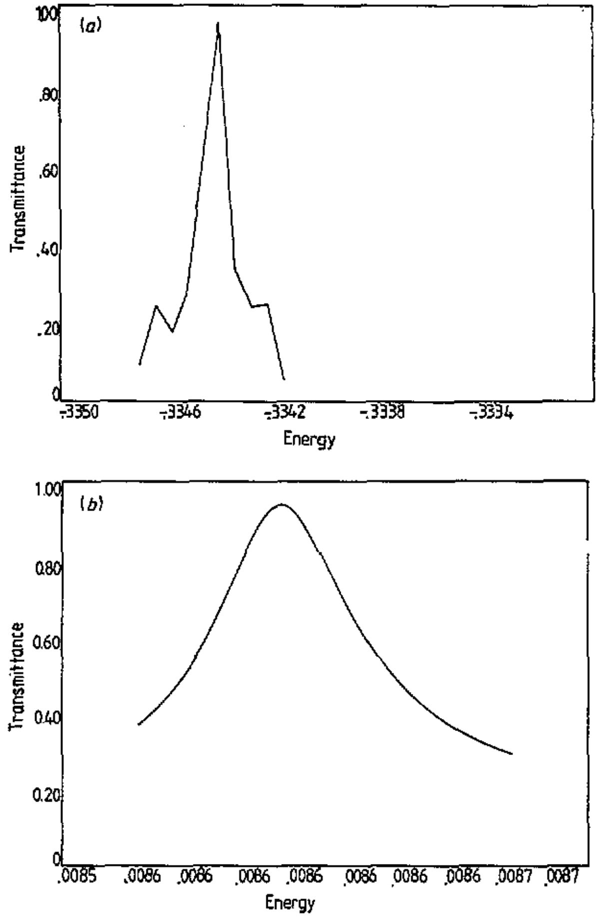

Figure 1. Transmittance versus energy for a chain of size 30000. (*a*) $E = -0.3344$; (*b*) $E = 0.0086$.

$f(\alpha, \alpha', \omega)$ versus $(1 - \omega)$, we expect to get an idea of how the probability of the α and α' sets (occurring at distances r) behave. We shall try to understand the resonant states from this viewpoint.

3. Results and discussions

Figures 1(*a*) and (*b*) give the transmittance versus energy curve for two different resonant states for a system of length 30000. These resonances occur at (*a*) $E = -0.3344$ and (*b*) $E = 0.0086$. The resonance is sharp with the width decreasing with size (Basu *et al* 1991).

Figures 2(*a*) and (*b*) show transmittance versus length for the two different resonances shown in figure 1. It has been suggested by Pendry (1987) that the resonant states have a necklace-like structure resembling localized clumps centred at different sites but overlapping. The transmittance (reflecting this behaviour) has clumped structures in it. As is seen, the clumped structures are not periodic.

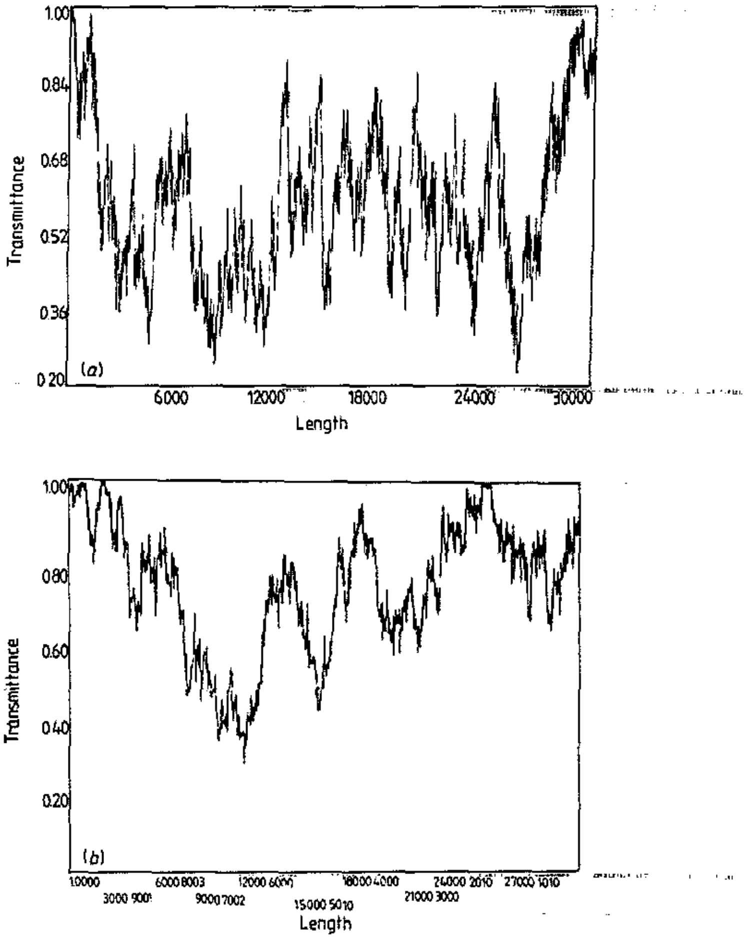

Figure 2. Transmittance versus length for resonances (a) at $E = -0.3344$; (b) $E = 0.0086$.

In order to analyse the nature of these resonant states we study the two-point correlation function $C(r)$. Figure 3(a) shows the two point correlation function $C(r)$ versus r, the distance between any two points in the measure, for a localized state (broken curve) and the resonant state at $E = -0.3344$ (full curve).

For the localized state the transmittance falls off exponentially with length. So with increasing r, the correlation between $T(i)$ $(=|t_i|^2)$ and $T(i + r)$ decreases. As no two points are significantly correlated to each other, the curve falls off sharply with an increase in r.

For the resonant state, $C(r)$ falls off slowly with r, exhibiting prominent oscillations. This behaviour is a common feature of resonant states. Figure 3(b) shows $C(r)$ versus r for the two different resonant states described in figures 1(a) and (b). Although the curves differ in detail, the general oscillatory decay is a common feature.

For small r, $T(i)$ and $T(i + r)$ represent transmittances for two nearby points in the same clump and are strongly correlated for a significant fraction of sites i. As r is increased, this correlation, as well as the number of sites for which this correlation is

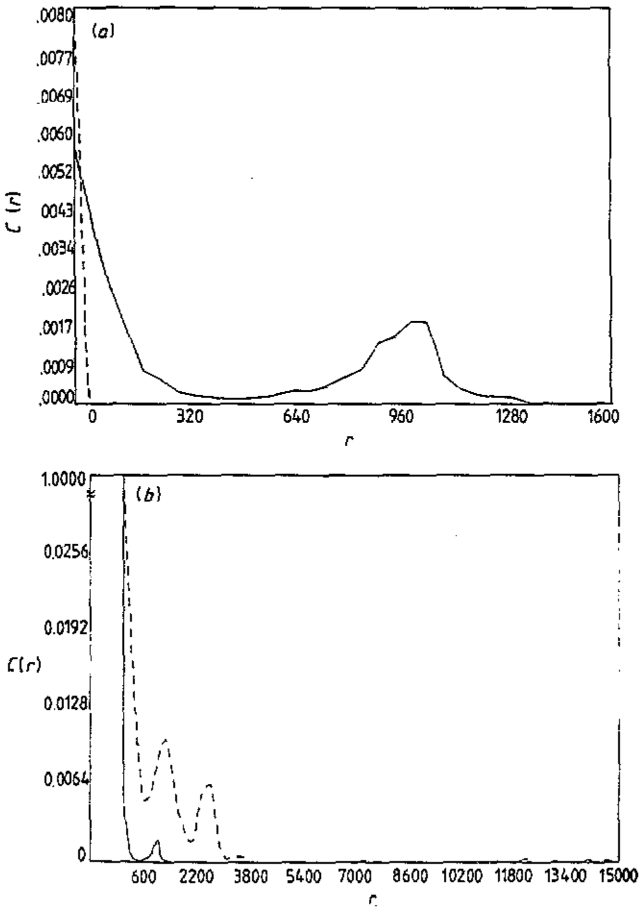

Figure 3. Correlation function $C(r)$ versus r for (a) a localized state (broken curve) and a resonant state at $E = -0.3344$ (full curve); (b) the two resonant states at $E = -0.3344$ (full curve) and at $E = 0.0086$ (broken curve).

significant, decreases. For a particular r, say, the points of the first clump may not be altogether correlated to subsequent points at a distance r. However, two of the subsequent clumps may be such that points in them are strongly correlated at the same r. From (2), $C(r)$ has a summation in it, so all points separated by that r contribute to $C(r)$ which has a significant value. The signature of this extra correlation shows up in a much slower decay in $C(r)$. The inhomogeneous distribution of the clumped structure is responsible for the initial slow fall of $C(r)$. As r increases, the correlation between points far apart naturally decreases. If the transmittance has a clumped, necklace-like structure, for some specific large values of r we may again have significant correlation between points belonging to different clumps. This is reflected in the oscillatory behaviour of $C(r)$.

Our aim is to characterize the resonant states and distinguish them clearly from extended and localized states. For this, we shall look at a particular generalized measure μ^*, which is the $\tilde{\mu}$ defined before with $p = -q$.

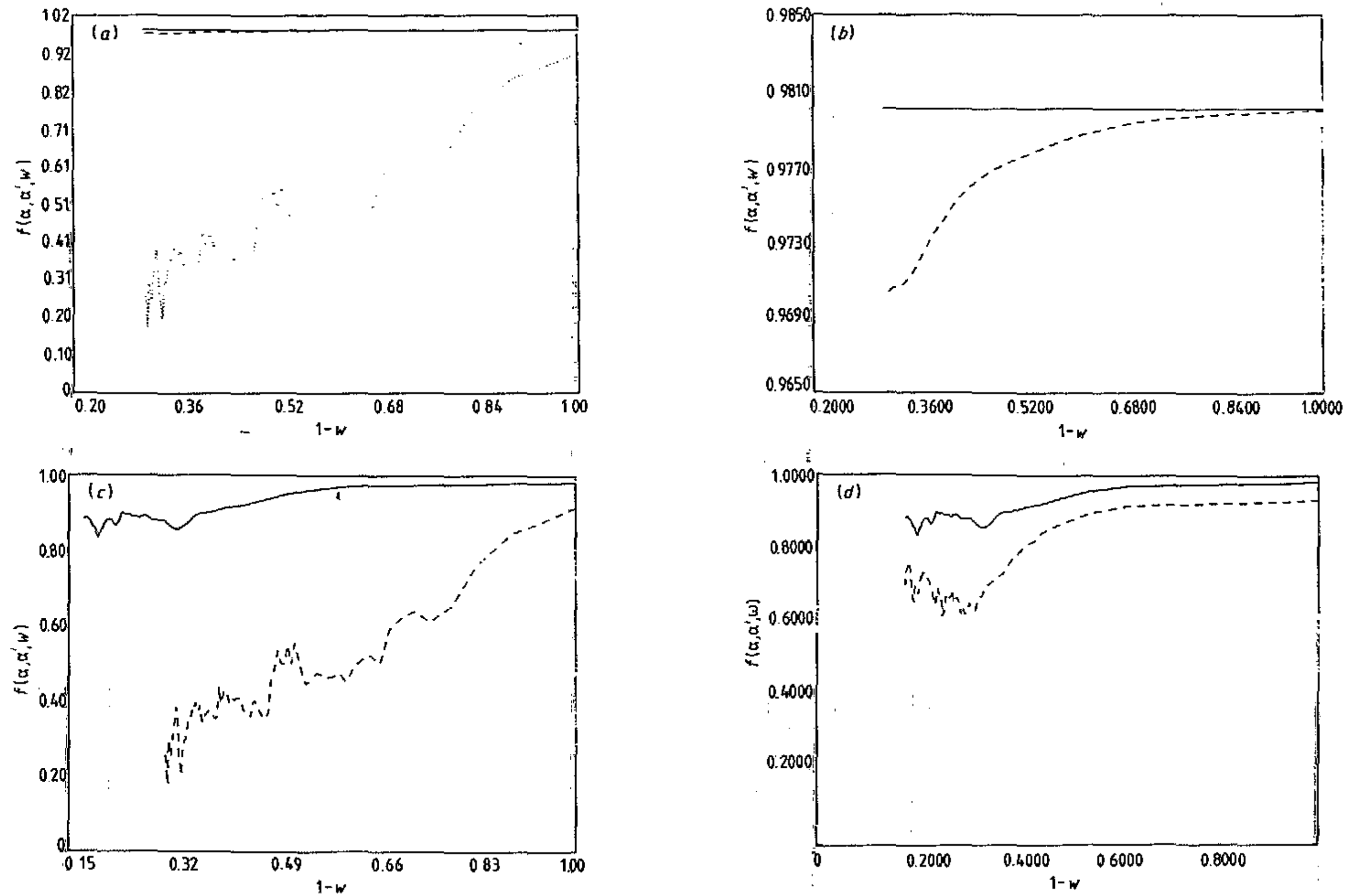

Figure 4. $f(\alpha', \alpha'', \omega)$ versus $(1 - \omega)$ for the measure μ^* (*a*) for an extended state (full curve); the resonant state at $E = -0.3344$ (broken curve); and a localized state (dotted curve); (*b*) (in an expanded scale along the *y*-axis) for extended state (full curve) and the resonant state (broken curve). High resolution near 0.98 is made to distinguish clearly between the two states: (*c*) for a localized state (broken curve) and the resonant state (full curve): (*d*) for the two resonant states at $E = -0.3344$ (full curve) and $E = 0.0086$ (broken curve).

With this definition,

$$\mu^* = [T^{-q}(i)T^q(i+r)] \Big/ \Big[\sum_i T^{-q}(i)T^q(i+r)\Big].$$

For an extended state $\mu^* \simeq [(1/N)^{-q}(1/N)^q]/[m(1/N)^{-q}(1/N)^q] = 1/m$. We have taken $m \simeq 15000$ when $N \simeq 30000$.

So

$$f(\alpha, \alpha', \omega) \simeq \Sigma\mu^*(i) \log \mu^*(i)/\log(1/N) \simeq 1.$$

Figure 4(a) shows $f(\alpha, \alpha', \omega)$ versus $(1-\omega)$ for extended (full curve), localized (dotted curve) and resonant (broken curve) states. $f(\alpha, \alpha', \omega)$ may be interpreted as $\simeq \log P(\alpha, \alpha', r)$ from (6) where $P(\alpha, \alpha', r)$ is the probability of finding α and α' at a distance r.

As seen from the figure, for the extended state, the probability of α and α' existing at r is always ~ 1. For the resonant state, because of its clumped nature spread all over the system, there is no gap in the measure (transmittance) and so $f(\alpha, \alpha', \omega)$ cannot fall to zero as r increases, as discussed by Lee and Halsey (1990). For localized states, the transmittance exists up to points which fall within the localization length. After that the transmittance for the rest of the length scales is negligible. As r increases $T(i+r) \ll T(i)$ and so μ^* decreases. From (7) it is clearly visible that as μ^* decreases, $f(\alpha, \alpha', \omega)$ also decreases.

In order to distinguish better between the extended and resonant states in figure 4(b), we show $f(\alpha, \alpha', \omega)$ versus $(1-\omega)$ in an extended scale. Here, as is clearly visible, the resonant state is not exactly like an extended state. It has some localized property incorporated in it such that it also has a tendency to fall off after some sufficiently large r values.

Figure 4(c) shows the same for a resonant state (full curve) and a localized state (broken curve). Here, the r variation for the resonant state curve is made very large. Even then, $f(\alpha, \alpha', \omega)$ decreases but does not fall off to zero. As resonant states have a gapless transmittance spread throughout the system this is very much expected (Lee and Halsey 1990).

In order to make sure that the signature of the resonant states are not specific to a particular resonance, we have compared the same curves for the two different resonances described in figures 1(a) and (b). This is shown in figure 4(d). From this figure we see that although the exact specific values are slightly different for the two different states, the general nature of the curves is very similar.

We could clearly demarcate the two different scaling regions to which the Azbel and localized states belong. This is very similar to the works of Meneveau and Chhabra and Lee and Halsey on a different model Cantor set. The two-point statistics method of multifractal measures is, according to us, a very good method of distinguishing transmittances at different scaling regions.

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