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LETTER TO THE EDITOR

Critical eigenfunctions in a quantum hierarchical system

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Abstract. The eigenstates of an electron in a hierarchical potential are investigated in the tight-binding approximation. The energy spectrum, which is known to be a Cantor set of measure zero, is found to possess wavefunctions which are self-similar and critical (i.e. the envelope has power law decay from the maximum). The wavefunctions are investigated in detail, with analytical and numerical results presented for their scaling properties.

There exist in one-dimensional quantum systems three qualitatively different types of energy spectra. For a periodic potential, one has a band structure with a continuum of possible energy values, giving rise to extended eigenfunctions. In a random potential, the spectrum is point-like, leading to exponentially localised wavefunctions. Third, there is the intermediate case of a singular continuous spectrum as has been seen in quasiperiodic systems (Sokoloff 1985). In this case, it has been proposed that the wavefunction is critical—i.e. the envelope of the wavefunction falls off from the maximum as some power of distance (Thouless and Niu 1983, Ostlund and Pandit 1984, Kohmoto *et al* 1987). In a previous paper (Ceccatto *et al* 1987), we proposed a model tight-binding equation for an electron in a hierarchical potential, a natural quantum extension of the classical problem of diffusion in hierarchical systems (Huberman and Kerszberg 1985). We found there that the energy spectrum is a Cantor set† of measure zero. In this letter we investigate in detail the nature of the wavefunctions corresponding to this set. We find that the eigenfunctions are self-similar and critical and we account analytically and numerically for their scaling properties.

We begin by considering the following tight-binding Hamiltonian for an electron in a hierarchical potential:

$$E\psi_n = t_{n+1,n}\psi_{n+1} + t_{n-1,n}\psi_{n-1} \tag{1}$$

where the transition matrix elements $t_{n-1,n} = t_{n,n-1}$ are given by

$$t_{n-1,n} = \begin{cases} 1 & n = 2j+1 \\ VR^{k-1} & n = 2^k(2j+1). \end{cases} \tag{2}$$

We take the hierarchy to be in the transition matrix elements, in natural correspondence to the master equation in the classical ultradiffusion problem. Also, we assume R to be in the interval $[0, 1]$ so that $t_{n-1,n}$ is an almost periodic function of n. Figure 1 gives a graphical representation of the transition matrix elements as a hierarchical array of barriers.

† By Cantor set, we mean a closed set containing no isolated or interior points (see, for example, Guckenheimer and Holmes 1983).

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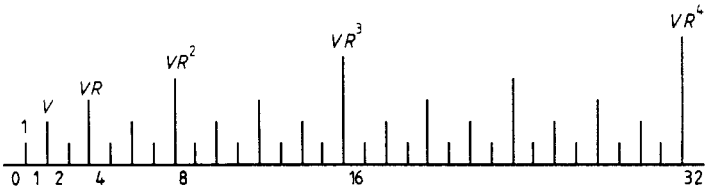


Figure 1. The off-diagonal transfer matrix elements, represented as barriers of heights inversely proportional to the hopping rates. The element $t_{n-1,n}$ corresponds to the barrier between cells $n-1$ and n.

To study the system of (1), it is convenient to consider it as the limit of increasingly larger periodic systems. The systems of period $p_n = 2^n$ is obtained by setting all transition matrix elements of the form VR^{k-1}, $k > n-1$, equal to VR^{n-1}. Thus (1) corresponds to $n \to \infty$. If we decimate cells $4j+1$ and $4j+2$, j integer, we obtain the p_{n-1} system, provided that we have renormalised values for E and V given by

$$V' = R(E^2 - V^2) \qquad E' = E(E^2 - V^2 - 1)/V. \tag{3}$$

The wavefunction is not renormalised. Let E_n and V_n be the nth iterates of E and V. If we define $T_{n+1} = (E_n^2 - V_n^2 - 1)/V_n$, then E is in the eigenspectrum of the period p_n system provided that $|T_n| \leq 2$. With this defintion, we may rewrite (3) in terms of T and V alone:

$$V_{n+1} = R(1 + V_n T_{n+1}) \qquad RT_{n+2} = T_{n+1}^2 + (1 - R^2) V_n T_{n+1} - (1 + R^2). \tag{4}$$

Equation (4) has two relevant fixed points, namely

$$T^* = a = \pm 1 \qquad V^* = \frac{R}{1 - aR} \qquad E^{*2} = \frac{1 - aR + R^2}{(1 - aR)^2}. \tag{5}$$

Note that these fixed points have $|T^*| < 2$, and hence initial points which iterate to them correspond to energies in the spectrum of the infinite system. Let us investigate in greater detail how points iterate to either of the fixed points. The $a = 1$ fixed point has eigenvalues satisfying $0 < \lambda_1 < 1 < \lambda_2$, and is thus hyperbolic. The $a = -1$ fixed point has eigenvalues $\lambda_2 < -1 < \lambda_1 < 0$, and thus is hyperbolic with reflection. From examination of the (T, V) phase space diagram, it is apparent that there exist two heteroclinic points where the stable invariant manifold of one fixed point intersects the unstable invariant manifold of the other. As is well known (see, for example, Berry 1978), the existence of one heteroclinic point implies the existence of an infinity of them. Thus, the stable invariant manifolds near the two fixed points must be extraordinarily complicated twisted objects. The intersections of these curves with the line $V = V_0$, $T \in [-2, 2]$, gives rise to the set of initial T values which iterate to the fixed points. From our first paper, we know that these two sets of points each have fractal measure zero and thus correspond to only a small part of the total spectrum. We anticipate that the rest of the spectrum, an uncountable set with non-zero fractal dimension, corresponds to bounded chaotic solutions to (4).

To provide a picture of the wavefunctions at the fixed points, introduce the transfer matrix M_n defined by

$$\begin{pmatrix} \psi_{p_n+1} \\ \psi_{p_n} \end{pmatrix} = M_n \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \begin{pmatrix} \alpha_n & \beta_n \\ \gamma_n & \delta_n \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \tag{6}$$

where $p_n = 2^n$. The quantity T_n defined above is related to the transfer matrix by $T = \mathrm{Tr}\, M_n$. One may easily show that there exists a recursion relation among the transfer matrices, namely that $M_{n+1} = AM_n^2$, where the matrix A is given by

$$A = \begin{pmatrix} R & E(1-R^2)/R \\ 0 & 1/R \end{pmatrix}. \tag{7}$$

The starting value is

$$M_1 = \begin{pmatrix} (E^2 - V^2)/V & -E/V \\ E/V & -1/V \end{pmatrix}. \tag{8}$$

At the fixed point, we may rewrite the recursion relation as a linear one: $M_{n+1} = A(aM_n - I)$, $n \geq 1$, where I is the identity matrix. This expression may be explicitly evaluated, with the result that $M_{n+1} = (aA)^n(M_1 + B) - B$, where the matrix B is given by

$$B = \frac{1}{1-aR}\begin{pmatrix} R & -aE(1+aR) \\ 0 & -a \end{pmatrix}. \tag{9}$$

Next, let us take into account the boundary conditions for the wavefunctions at the fixed points. For the periodic system of period p_n, Bloch's theorem implies that $\psi_{j+p_n} = \exp(\mathrm{i}kp_n)\psi_j$, for some wavenumber k. Thus, if we fix our overall normalisation and phase by taking $\psi_0 = 1$, we have $\psi_1 = [\exp(\mathrm{i}kp_n) - \delta_n]/\gamma_n \to E^*$, as $n \to \infty$. We have used these initial values with (1) to plot the wavefunction at the two fixed points, $a = \pm 1$. In figure 2(a), we have plotted the first 1024 cells of the absolute value of the wavefunction for the $a = 1$ fixed point; in figure 2(b), we show the first 128 cells. Note in particular the identical shape of the two wavefunctions, exhibiting the self-similarity of the wavefunction. In figures 2(a) and (b), we have plotted the wavefunction at the $a = -1$ fixed point in the same manner. Again, note the self-similarity.

On first inspection, we appear to have two different types of wavefunctions. For the fixed point, corresponding to $a = 1$ (figure 2), we see that the envelope of the wavefunction monotonically increases with position. We will show in a moment that the dependence is in fact algebraic, i.e. $\psi_n^{\max} \sim n^{\beta}$. This corresponds to a wavefunction intermediate between extended (as in a periodic potential) and exponentially localised (as in a random potential). This intermediate behaviour has been found in quasiperiodic systems and has been postulated to be a signature of a singular continuous energy spectrum. In figure 3, where we have plotted the wavefunction corresponding to the $a = -1$ fixed point, we see something somewhat different. The wavefunction is extended in the sense that the envelope is at a constant height as a function of position. It is, however, rather an odd extended state because the maxima become more and more spread out with increasing position. In fact, we will argue that, in a suitably averaged sense, this wavefunction is qualitatively the same as that at the first fixed point.

We may account for the details of figures 2 and 3 from the above work. Consider first the properties of the wavefunction at the fixed point with $a = 1$. Examination of the numerical plots reveals that the maxima occur at sites $i_n = (4^n - 1)/3$ and $j_n = 2(4^n - 1)/3$, n integer. Plotting the values of $|\psi|$ at these points on a log-log plot shows the power law behaviour of the envelope, as shown in figure 4. For $R = \frac{1}{2}$, the numerically determined exponent is $\beta = 0.3358 \pm 0.0002$.

To calculate β analytically, consider the following. Let $P_n = \psi_{i_n}$, $Q_n = \psi_{i_{n-1}}$, and define $\Lambda_n = M_2 M_4 \ldots M_{2n}$. (Note that a similar scheme can be followed for the maxima

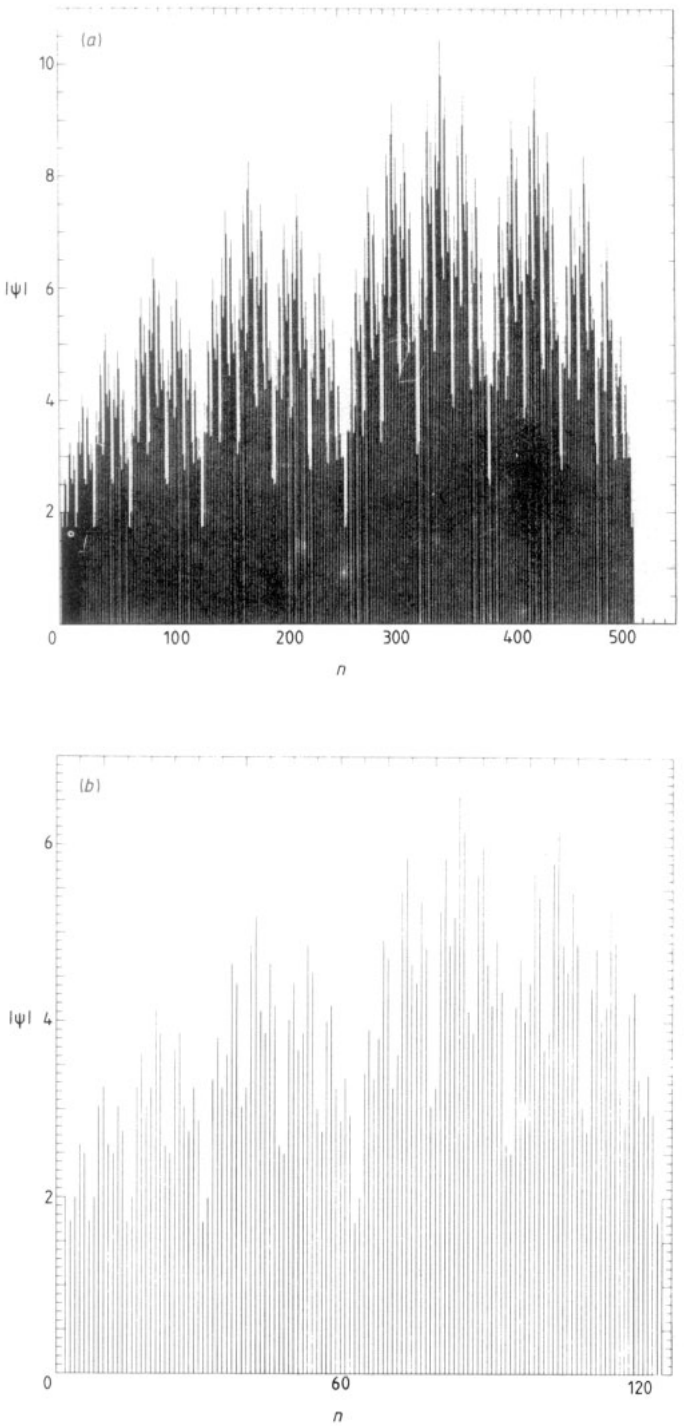
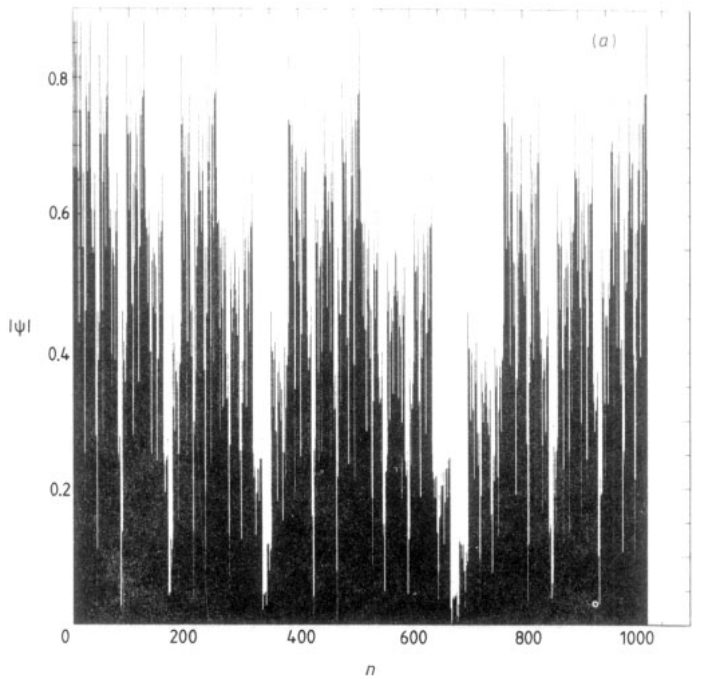


Figure 2. (*a*) The absolute value of the wavefunction corresponding to the fixed point $E=(1-R+R^2)^{1/2}/(1-R)$, $V=R/(1-R)$, for $R=0.5$, plotted against position for the first 512 cells. (*b*) The first 128 cells of the same wavefunction. Note the similarity to (*a*).



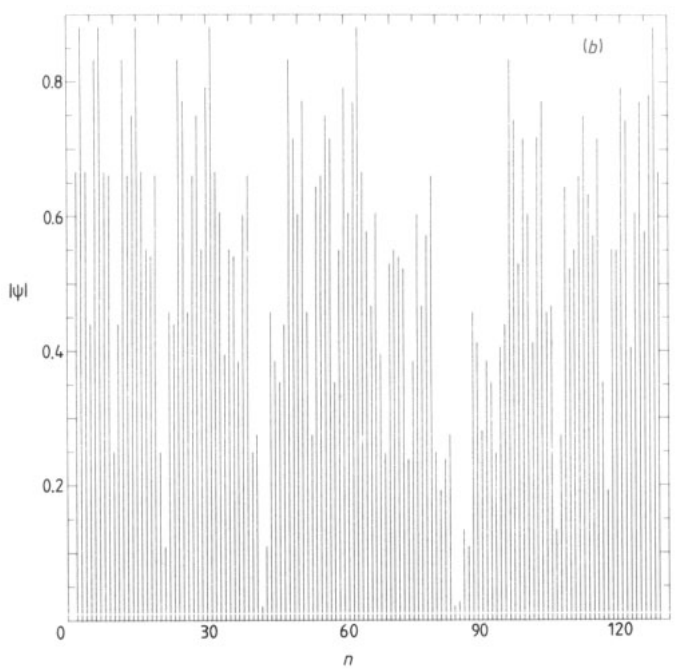


Figure 3. (*a*) The absolute value of the wavefunction corresponding to the fixed point $E=(1+R+R^2)^{1/2}/(1+R)$, $V=R/(1+R)$, for $R=0.5$, plotted against position for the first 1024 cells. (*b*) The first 128 cells of the same wavefunction. Note the similarity to (*a*).

at sites j_n using $\Lambda_n = M_1 M_3 \ldots M_{2n-1}$; the result is the same.) Then P_n and Q_n are related to ψ_1 and ψ_0 by

$$\begin{pmatrix} P_n \\ Q_n \end{pmatrix} = \Lambda_n \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \Lambda_{n-1} \begin{pmatrix} \psi_{2^{2n}+1} \\ \psi_{2^{2n}} \end{pmatrix}. \tag{10}$$

Using our expression for the matrix M_k and using the above boundary condition, we can write

$$\begin{pmatrix} \psi_{2^{2n}+1} \\ \psi_{2^{2n}} \end{pmatrix} = M_{2n} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \frac{a}{1-aR} \begin{pmatrix} E \\ 1 \end{pmatrix} - \frac{Ea(aR)^{2n}}{1-aR} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{11}$$

Now, assume a scaling, as suggested by figure 4, of the form $P_n \sim [(4^{n+1}-1)/3]^{\beta}$. Defining $\eta_n = P_n / P_{n-1}$, we have $\eta_n \sim [4+3/(4^n-1)]^{\beta}$. In the large-$n$ limit this gives us $\eta_n \to \eta \sim 4^{\beta}$. If one now explicitly evaluates η from (10) and (11), a short calculation will yield

$$\eta = \frac{(1+R+R^2) \pm [(1+R+R^2)^2 - 4R^2]^{1/2}}{2} \qquad (a=1). \tag{12}$$

Only the positive sign gives $\eta > 1$ (and hence an increasing envelope) and thus the positive root is the relevant one here. From the above, we have $\beta = \ln \eta / \ln 4$ which, when evalued at $R = \frac{1}{2}$, gives $\beta = 0.3359$. The agreement with the above numerically determined slope is excellent.

Consider now the wavefunction corresponding to the other fixed point ($a = -1$), as pictured in figure 3. We see from the figure that the maxima occur at sites $2^{m+1}-1$,

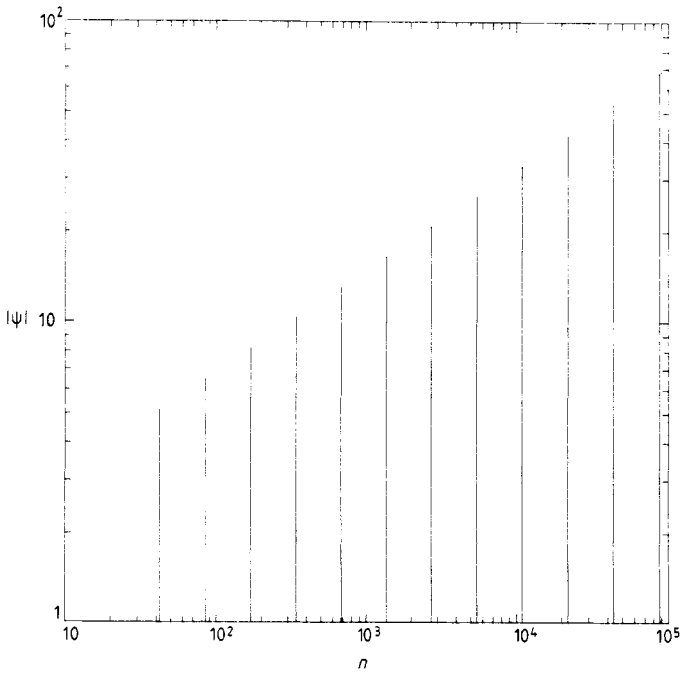


Figure 4. The absolute value of the wavefunction corresponding to the fixed point $E = (1-R+R^2)^{1/2}/(1-R)$, $V = R/(1-R)$, for $R = 0.5$, plotted only at sites $i_n = (4^n-1)/3$, to show the scaling of the envelope. The numerically determined slope is 0.3358.

$m = 0, 1, \ldots$, and have a constant magnitude. We may calculate this value exactly. During the renormalisation transformation (equation (3) above), cells 2^{m+1} and $2^{m+1}-1$ go to positions 2^m and $2^m - 1$, respectively. Because we are at a fixed point, the values of E and V are unchanged by the renormalisation and hence we are left with exactly the same system afterwards. If we repeat the process m times, then we see that cell $2^{m+1}-1$ iterates to cell 1. Thus the value of the wavefunction at cell $2^{m+1}-1$ must be identical to the value at cell 1, i.e.

$$\psi_{2^{m+1}-1} = \psi_1 = E^*. \tag{13}$$

For $R = 0.5$, this gives the envelope of the wavefunction at the constant height of $E^* = 0.8819$. The agreement with figure 3 is excellent.

One should note that, for $R \to 1$, the location of the maxima changes to cells 3×2^j, $j = 1, 2, \ldots$, and the value increases above E^*. However, the envelope is still at a constant height.

The flatness of the envelope of the wavefunction for the second fixed point suggests that the state might be extended. On the other hand, the fact that the maxima become more widely spaced at large positions suggests that the state might be in some sense localised. Let us investigate this question in more detail. To distinguish between localised and extended states, introduce an averaged function $\bar{\psi}$ defined by

$$\bar{\psi}_k = \frac{1}{2^{n-1}} \sum_{j=2^{n-1}}^{2^n-1} |\psi_j|^\lambda \qquad k \in [2^{n-1}, 2^n - 1]. \tag{14}$$

We see that $\bar{\psi}$ is equal to the value of $|\psi|^\lambda$ (assume $\lambda > 0$) averaged over the interval between successive maxima. For a strictly extended state, where the value of $|\psi|$ is periodic, we see for large n that $\bar{\psi}_n$ is constant. For an exponentially localised state, the value of $\bar{\psi}$ also falls off exponentially with position. For a critical state where the wavefunction decays algebraically from the maximum, such as the wavefunction corresponding to the $a = 1$ fixed point above, $\bar{\psi}$ also falls off like a power law. Thus $\bar{\psi}$ mimics the behaviour of the wavefunction. We have calculated $\bar{\psi}$ for the fixed point eigenfunctions, with $\lambda = 2$, and find for both cases that $\bar{\psi}$ decays algebraically from its maximum, i.e. $\bar{\psi}_n \sim x^{-\gamma}$ where x is the distance from the maximum. For $R = \frac{1}{2}$ and $a = 1$, $\gamma = 0.4987$ and for $R = \frac{1}{2}$ and $a = -1$, $\gamma = 0.2269$. So we see that, in this averaged sense, both wavefunctions are critical. As might be expected, the value of γ is closer to zero (and hence $\bar{\psi}$ close to constant) for the $a = -1$ fixed point, and hence that eigenfunction is closer to extended than the other.

Other details of the wavefunctions at the two fixed points may also be derived using the general formalism described above. For example, from (11) we see that, as $k \to \infty$, we have $\psi_{2^k+1} = aE^*/(1 - aR)$ and $\psi_{2^k} = a/(1 - aR)$ (note that this holds even when k is not even). Examination of figures 2 and 3 confirms this statement. Furthermore, if we define $\xi_n = Q_n/Q_{n-1}$ for the $a = 1$ fixed point, we find that, as $n \to \infty$, $\xi = \eta$. Thus the subsidiary maxima in figure 2 scale in the same way as the principal ones.

Finally, we must consider the wavefunction at the uncountable set of points in the spectrum which do not iterate to one of the fixed points. Presumably, these points correspond to bounded chaotic solutions to (4). To examine the shape of such a wavefuction, consider one of the periodic systems described above, for some large value of p_n. Figure 5 shows the eigenstate corresponding to an energy chosen at random in the 140th band of the period $p_8 = 256$ system for $V = R = 0.5$. This state corresponds to a Bloch wavenumber $kp_8 = 1.38$. Note that this value does not correspond to either one of the fixed points: one can easily show that, for $a = 1$, $kp_n = \pm\pi/3$,

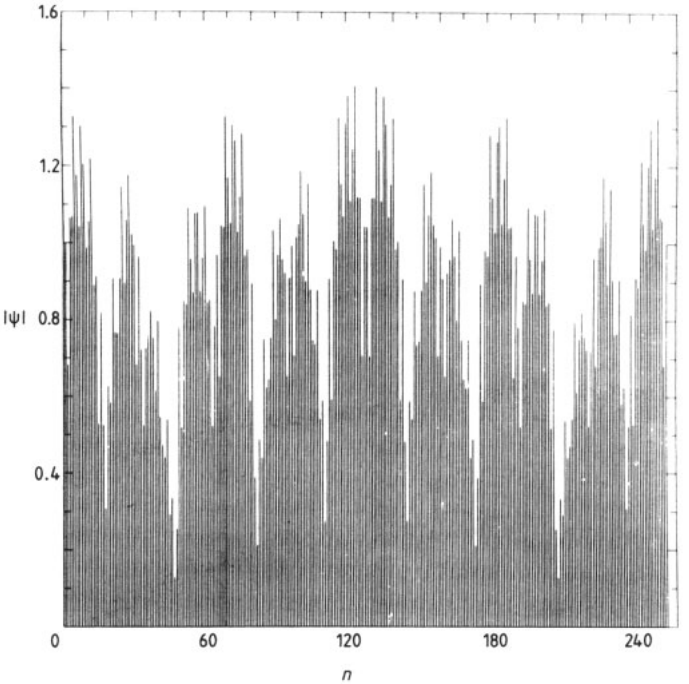


Figure 5. The absolute value of the wavefunction plotted against position for the point $E = 0.6849$, $V = R = 0.5$, for the period $p_8 = 256$ system. This point lies in the 140th band (counting from lowest to highest energy, with 256 total).

and for $a = -1$, $k = \pm 2\pi/3$. Examination of figure 5 shows that $|\psi|$ is symmetric about the centre, a reflection of the basic symmetry of the potential around the centre in the finite period system. For the infinite period case of (1), the centre itself is at infinity and hence the symmetry is not seen in pictures of the wavefunction. Other detailed properties of this wavefunction and similar such states are currently under investigation.

In summary, we have presented an analysis of the eigenstates of a tight-binding model of an electron in a hierarchical potential. We have found that the zero measure Cantor set energy spectrum contains wavefunctions which, in a suitably defined average way, decay algebraically from their maxima. We have discussed the boundary conditions for the problem and have determined analytically and numerically the precise shape of the envelope for the wavefunction at the fixed points. We have also presented an example of an eigenfunction at one of the energies in the spectrum which does not iterate to either of the fixed points. Details of the nature of these states, as well as the problem of the spreading of a wavepacket with time, will be presented in the future.

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