Localization and mobility edges in a one-dimensional lattice with a self-similar Feigenbaum structure

1991 J. Phys.: Condens. Matter 3 1153

(http://iopscience.iop.org/0953-8984/3/9/010)

J. Phys.: Condens. Matter 3 (1991) 1153–1164. Printed in the UK

Localization and mobility edges in a one-dimensional lattice with a self-similar Feigenbaum structure

Tarun Kanti Roy† and Avijit Lahiri‡

† Saha Institute of Nuclear Physics, Calcutta 700 009, India

‡ Vidyasagar Evening College, Calcutta 700 006, India

Received 29 March 1990, in final form 15 October 1990

Abstract. We consider a one-dimensional tight-binding model with on-site potentials $V_n = \lambda g^{(n)}(0)$ where λ is a strength parameter and $g^{(n)}(x)$ is the nth iterate of $g(x)$, the universal function describing the structure of 2^∞ superstable cycles in infinitely bifurcated maps undergoing period doubling sequences. Interesting features of the model revealed in numerical computations are, firstly, the presence of a large number of mobility edges forming a clustered pattern for a certain range of values of λ and, secondly, non-smooth self-similar variation of inverse localization length γ as a function of energy E.

1. Introduction

The observation of various 'unusual' features of energy spectra and eigenfunctions of the Schrödinger equation for one-dimensional aperiodic chains has led to a widespread interest in such systems in recent years. More generally, one-dimensional systems in various contexts may be described in terms of the products of transfer matrices, which constitute an interesting study from the point of view of understanding wave propagation in inhomogeneous media (see, e.g., Ishii 1973, Sokoloff 1985, Kohmoto *et al* 1983, 1987, Ostlund *et al* 1983, Drummond 1989). The behaviour of Lyapunov exponents of such products as a function of some characterizing parameter, e.g. the frequency of lattice vibration or energy of one-electron states, sheds light, on the one hand, on fundamental theoretical question such as the existence and properties of singular continuous spectra of Schrödinger operators and, on the other hand, on a wide range of phenomena of practical interest (e.g. transport properties in solids, confinement of electromagnetic waves in stratified media).

The most widely studied types of aperiodicity are the random and the quasiperiodic chains in the tight-binding model (TBM), for which a range of exact results including scaling properties of spectra and eigenfunctions have been obtained (see, e.g., Aubry and Andre 1979, Kohmoto *et al* 1983, Ostlund *et al* 1983, Souillard 1984). The study of quasiperiodic chains, in particular, opens the door to considering various other types of aperiodicity (see, e.g., Würtz *et al* 1989, Fishman and Griniasty 1988; for some recent results on quasiperiodic chains with more than one incommensurate frequency, see Casati *et al* 1988 and Chulavesky and Sinai 1989). In contrast with random chains, a one-dimensional quasiperiodic chain with on-site potentials given by

$$V_n = \lambda \cos(2\pi Q n - \sigma) \tag{1}$$

0953-8984/91/091153 + 12 $03.50

(where Q is irrational, λ is a strength parameter and σ is a phase parameter) exhibits the phenomenon of 'metal–insulator' transition at $\lambda = 2$ and, for $\lambda > 2$, all states except one at the exact centre of the spectrum become exponentially localized. An interesting question in this connection is the existence of mobility edges in the spectrum. Thus, a TBM studied originally by Soukoulis and Economou (1982) corresponding to on-site potentials

$$V_n = \lambda[\cos(2\pi Qn) + \tfrac{1}{3}\cos(4\pi Qn)] \tag{2}$$

has recently been shown to involve a complicated mobility edge pattern (Sun 1989) in the spectrum. Another important class of aperiodic chains corresponds to on-site potentials of the form

$$V_n = \lambda \cos(2\pi Q|n|^{\nu} - \sigma). \tag{3}$$

Models of this type were considered in the weak-potential limit by Fishman and Griniasty (1988) and later by Thouless (1988). For $0 < \nu < 1$ these models come under the general classification of slowly varying potentials, and Das Sarma *et al* (1988) show that for $\lambda < 2$ the spectrum involves a pair of mobility edges located symmetrically. This means that the transition at $\lambda = 2$ is not a sharp metal–insulator type, since for $\lambda < 2$ the spectrum includes extended states covering an energy interval that gradually diminishes in width as λ is increased. Following a suggestion of Das Sarma *et al* (1988), Crisianty (1989) rigorously established the existence of mobility edges in square-well potential models of the slowly varying type.

2. Presentation of the model and numerical results

The existence of mobility edges and their location in the energy spectrum are expected to have important bearing on the transport properties of one-dimensional chains (see, e.g., Sokoloff 1985, Sun 1989). In this context, we present here some preliminary results of numerical investigations on a class of one-dimensional chains possessing a self-similar Cantor-set-like structure that is likely to prove interesting on the following counts.

(i) Studies on wave propagation in aperiodic systems with self-similar fractal structures are not common in the literature despite the fact that fractal structures arise in many diverse contexts, and experimental techniques such as molecular beam epitaxy can be resorted to for the artificial growth of such structures (see, e.g., Piertonero and Tosatti 1986, Vicsek 1989, Parker 1985).

(ii) For certain ranges of the strength parameter λ, there appear to exist a large number of mobility edges in the spectrum, and these mobility edges appear to be organized in a clustered fractal structure. In contrast with the work of Das Sarma *et al* (1988) and Crisianty (1989), the mobility edges are not a consequence of the slowly varying nature of the potential.

(iii) The mobility edges disappear gradually as λ is increased, and, for λ larger than a certain value, all the states become localized.

(iv) In contrast with other potentials studied in the literature, the variation in the inverse localization length γ with energy E is highly non-smooth.

(v) The energy spectrum in general possesses a self-similar structure as revealed in the location of the mobility edges, variation in γ with E for localized states, and density of states.

The TBM that we study is given by

$$u_{n+1} + u_{n-1} + V_n u_n = E u_n \tag{4}$$

where u_n is the amplitude of the wavefunction at the nth site and V_n are the on-site potentials given by

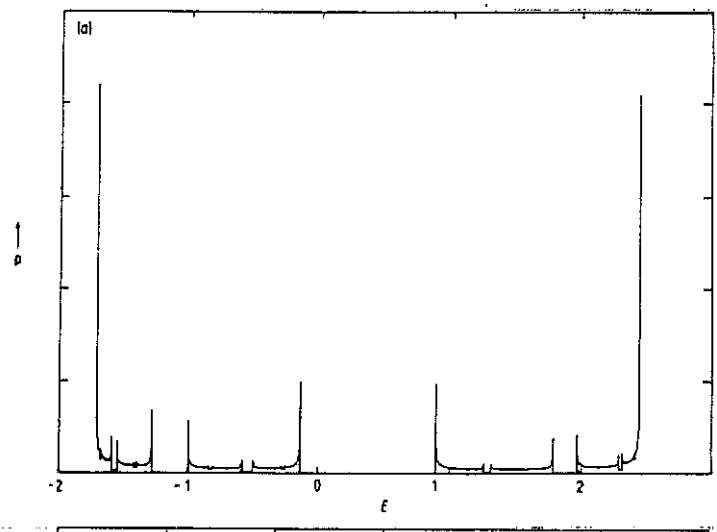
$$V_n = \lambda g^{(n)}(0). \tag{5}$$

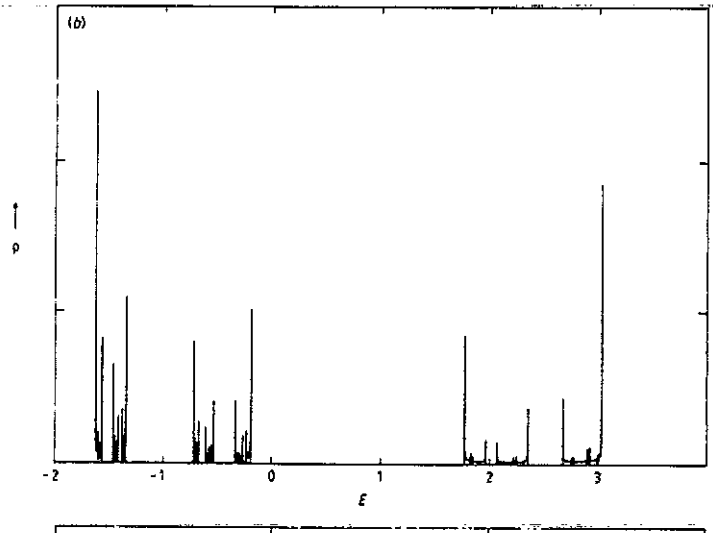
Here λ is the strength parameter already referred to, $g(x)$ is the well known universal function encountered in the scaling theory of period-doubling bifurcations (see, e.g., Feigenbaum 1978, 1979, 1980, Collet and Eckman 1980, Mira 1987), and $g^{(n)}(x)$ represents the n-times iterate of $g(x)$. Before presenting our results, a few comments may help to place the model in perspective.

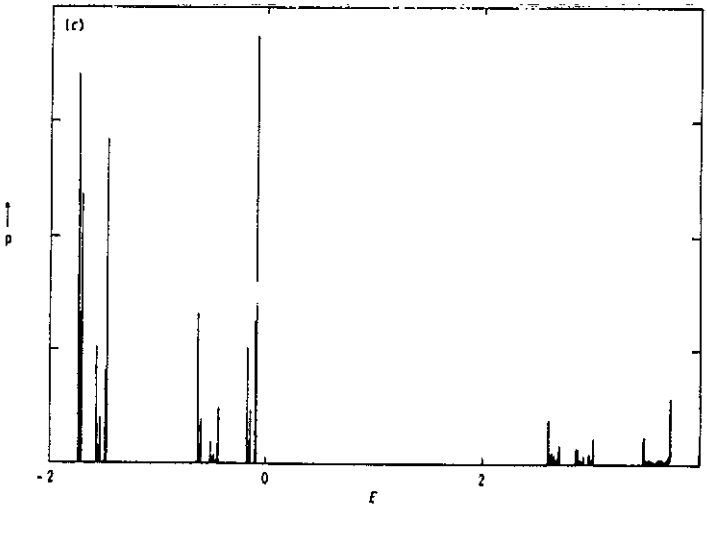
Recent years have witnessed interest in understanding how aperiodic functions and sequences of various types of complexity arise as trajectories of simple deterministic dynamical systems, such as low-dimensional dissipative and conservative maps. As a simple example, one may consider the case of quasiperiodic sequences that may be associated with phase-locked to quasiperiodic bifurcations of trajectories in circle maps (see, e.g., Kaneko 1986). In this context it is a useful exercise to consider wave propagation in one-dimensional chains characterized by aperiodicities of various types corresponding to different bifurcation regimes of maps. Indeed, important scaling properties of energy spectra and eigenfunctions in certain quasiperiodic one-dimensional chains appear to be natural extensions of a universal scaling theory of circle maps (Ostlund *et al* 1983). By analogy, we could consider periodic chains with arbitrarily large unit cells of length 2^N, and, in the limit $N \to \infty$, go over to an aperiodic chain as in Feigenbaum period-doubling sequence. For example, the on-site potentials may be taken to be proportional to the location of superstable cycle elements of cycle lengths 2^N of the logistic map

$$x' = \Lambda(1 - 2x^2) \tag{6}$$

with the corresponding value of Λ denoted by Λ_N. Comparing this with the next value of Λ, namely $\Lambda = \Lambda_{N+1}$, we see that a unit cell of size 2^N is replaced by one of size 2^{N+1}, and hence each of the energy bands of the former splits into two in the latter. Thus, as N becomes large, we gradually encounter a highly fractured band structure until in the limit $N \to \infty$, we may end up with some exotic spectrum. The process is similar to the way in which a quasiperiodic chain may be thought of as a limiting case of a sequence of periodic chains of larger and larger unit-cell size. A notable difference between the two schemes, however, is the *self-similarity* in the first (each band splitting in exactly two at each stage), there being no corresponding self-similarity in the approximation of an irrational by successive truncations of its continued-fraction representation (Azbel 1979) that is involved in the second one (see, however, the work by Höfstadter 1976 and Xu 1986, 1987). Now, although 2^N superstable cycles of the map (6) differ somewhat from 2^N cycles of other similar maps, there is known to exist a *universal* structure of 2^N clusters in all infinitely bifurcated maps of a given type irrespective of their specific forms, given by the universal function $g_N(x)$ (Feigenbaum 1979, 1980), and the limit $N \to \infty$ of the sequence of these functions is another universal function $g(x)$. The sequence $g^{(n)}(0)$ of iterates of this function is known to be aperiodic with a self-similar Cantor-set-like structure having a fractal dimension of nearly 0.5388 (Grassberger 1981). An indication of the nature of its aperiodicity is given by its power spectrum which has a universal structure with peaks at periodicities 2^N for all N (Nauenberg and Rudnick 1981). It is


(a)
ρ
-2
-1
0
1
2
E


(b)
ρ
-2
-1
0
1
2
3
E


(c)
ρ
-2
0
2
E

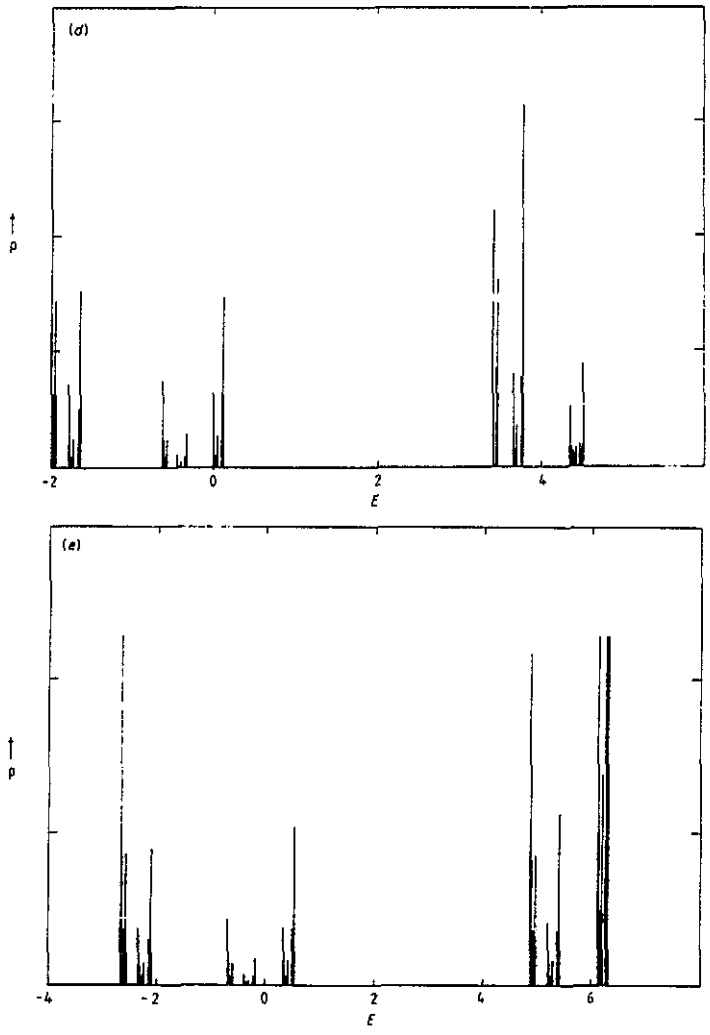
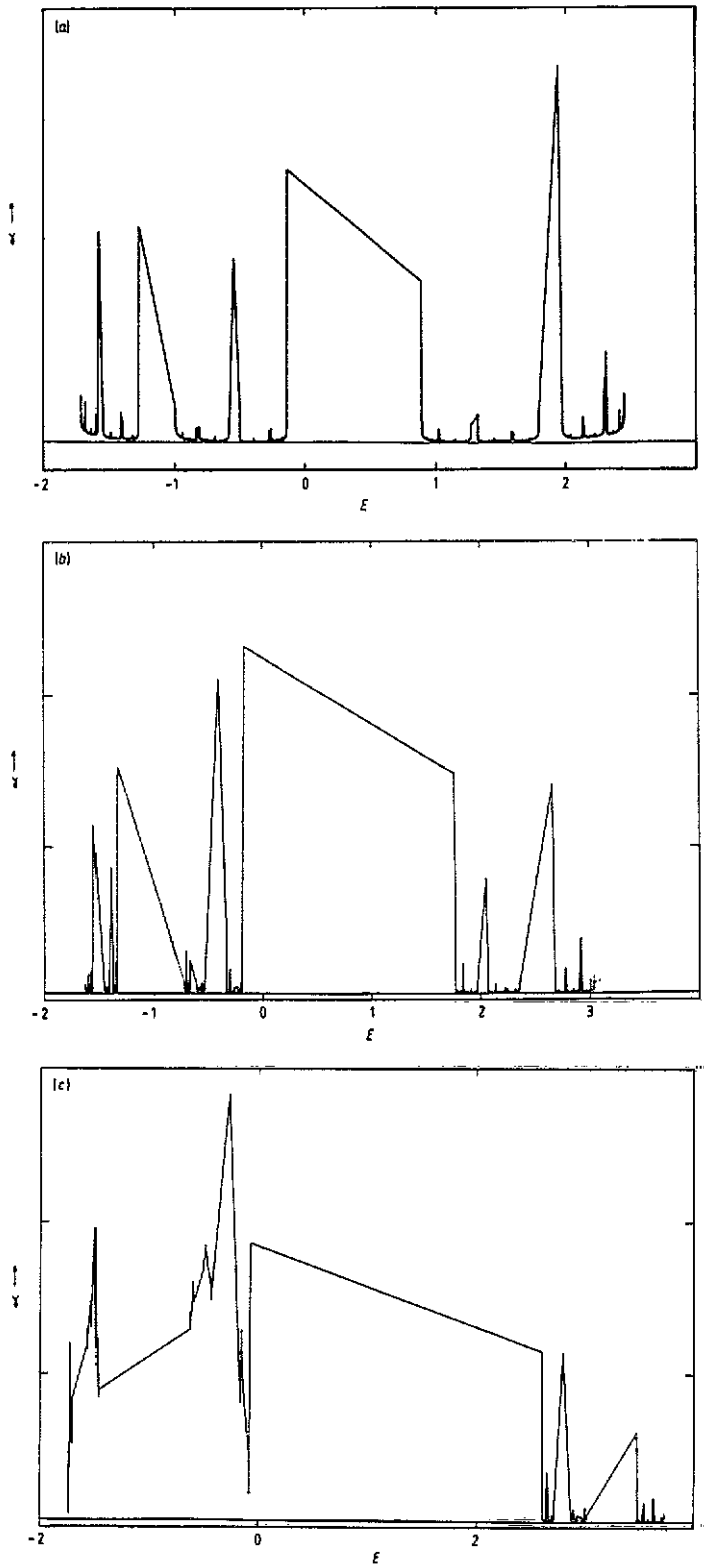


Figure 1. Density-of-states ρ plots (versus energy E) computed numerically for our model (equations (4) and (5)) with a lattice size $N = 2048$: (*a*) $\lambda = 1.0$; (*b*) $\lambda = 2.0$; (*c*) $\lambda = 3.0$; (*d*) $\lambda = 4.0$; (*e*) $\lambda = 6.0$. Numerical values of ρ have not been indicated since different plots have been rescaled differently along the ρ axis for convenience of presentation and are not essential for our purpose.

with reference to this particular sequence that we construct the TBM given by equation (4).

Figure 1 gives the density-of-states plots and figure 2 the corresponding inverse localization length versus energy plots for this model for five arbitrarily chosen values of λ that may be considered to be more or less representative (see below). For any given λ, the spectrum consists of two major clusters of eigenvalues separated by a gap, and there are smaller gaps within the clusters, the pattern being repeated on progressively finer scales. For low λ the gaps decrease in width very rapidly as we look at smaller intervals on the energy scale, so that the energy spectrum has a predominantly continuum character and most of the states are extended in nature (figures 1(*a*) and 2(*a*)). As λ is


(a)
N
-2
-1
0
1
2
E
(b)
N
-2
-1
0
1
2
3
E
(c)
N
-2
0
2
E

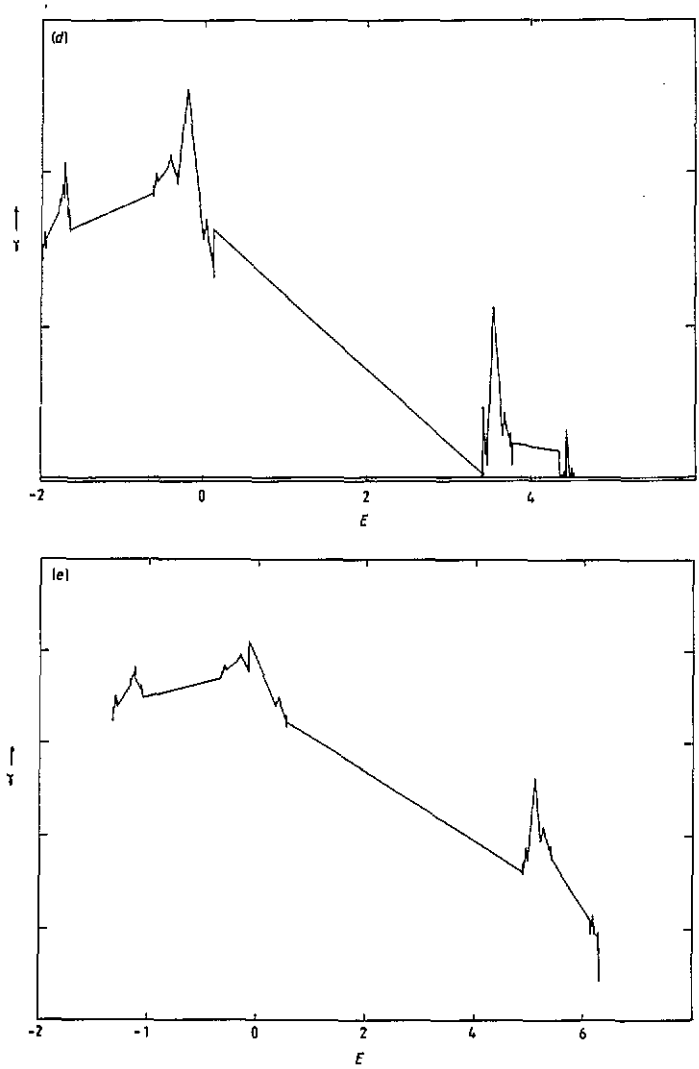


Figure 2. Inverse localization length γ versus energy E plots: (a)–(e) correspond, respectively, to the density-of-states plots in figures 1(a)–1(e). Points corresponding to allowed states have been joined with straight lines (corresponding to energy gaps for the finite-size lattice) so as to obtain a piecewise continuous plot. As in figure 1, numerical values of γ have not been indicated.

increased, small groups of localized states appear in the lower-energy cluster of the spectrum, attended by mobility edges (figures 1(b) and 2(b)). Initially the localized states appear to have a 'thin' fractal structure, covering a vanishingly small measure of the entire energy spectrum, but, with increasing λ, entire intervals of the spectrum acquire Cantor-set-like structures until at λ near about 2.7 we find very few mobility edges in the lower-energy half, while the upper-energy half continues to have a predominantly continuum structure. It is important to note the non-smooth self-similar nature of the γ versus E plot in the lower-energy portion as most of the states become localized. (We do not include in this paper quantitative discussion on self-similarity in various features

of the spectra since our numerical investigations are based on rather small lattice size. Detailed statements will be made in a future publication.) This is to be contrasted with chains given by equations (1) and (3). For example, figures 3(*a*) and 1(*a*) of Das Sarma *et al* (1988) show a typical density-of-states plot and the corresponding γ versus E plot, respectively, in a model of type (3), of which the former shows that the spectrum has a fragmented and clustered structure, but the clustering does not have a scale invariance associated with it, which results in a smooth variation in γ with E along the spectrum (except at the two mobility edges). Indeed, we expect that the nature of fragmentation in models of form (3) will not be much different from that in an incommensurate quasiperiodic chain, which has been thoroughly investigated by Azbel (1979), Höfstadter (1976) and Xu (1986, 1987); as already noted, there is no strict self-similarity in the continued-fraction representation of any given irrational. By contrast, the self-similarity of the sequence $\{g^{(n)}(0)\}$ (this self-similarity is based primarily on two scale factors, α and α^2, $\alpha = 2.502\,9\ldots$; in a more accurate description, however, an infinite number of scale factors are to be taken into account) leads to a self-similar Cantor-set-like spectrum which in turn causes the non-smooth γ versus E graph to possess a self-similar appearance. For comparison we plot in figures 3(*a*) and 3(*b*) the density-of-states plot and the γ versus E graph, respectively, for hypothetical one-dimensional chain whose energy spectrum has an exact middle-thirds Cantor set structure (one does not know what sequence of on-site potentials in a TBM would give rise to this spectrum, but a plausible guess is that this sequence itself will have to have a Cantor-set-like structure (see figure 4 caption); this 'inverse problem' of constructing chains which give rise to different types of spectrum has not been discussed in the literature but appears to be interesting from the point of view of potential applications). One can see the pronounced non-smooth scale-invariant structure of the graphs, very much similar to that arising in the TBM that we are considering.

Returning to figures 1 and 2, we observe that the lower half of the spectrum becomes entirely dominated by localized states at some λ near 3.0 (figures 1(*c*) and 2(*c*)), although the upper half remains dominated by extended states. As λ is increased further, the upper half in turn becomes 'infected' (figures 1(*d*) and 2(*d*)) and the mobility edges are pushed more and more to the right-hand end of the spectrum until, at λ somewhere near 6.0, almost *all* states become localized and both halves acquire similar structures (figures 1(*e*) and 2(*e*)).

A comparable system which is somewhat easier to investigate would be a TBM with on-site potentials given by the sequence (the point set corresponding to which is an exact middle-thirds Cantor set) $0, \frac{2}{3}, (\frac{2}{3})^2, \frac{2}{3}+(\frac{2}{3})^2, (\frac{2}{3})^3, \frac{2}{3}+(\frac{2}{3})^3, (\frac{2}{3})^2+(\frac{2}{3})^3, \frac{2}{3}+(\frac{2}{3})^2+(\frac{2}{3})^3, \ldots$, each term multiplied by a strength parameter λ. A typical density-of-states plot and γ versus E plot for this model are shown in figures 4(*a*) and 4(*b*), respectively. Similarity with the corresponding plots for the model studied above is quite apparent, particularly in respect of the non-smooth variation in γ with E. Results of more detailed investigations will be reported separately.

All spectra in our TBM have been computed by using the 'LR decomposition with shift' algorithm of diagonalization of tridiagonal matrices (Wilkinson 1965) with a lattice size of 2048. Inverse localization lengths have been calculated from the spectra by using the formula

$$\gamma(E) = (N-1)^{-1} \sum{}' \ln|E - E'| \tag{7}$$

where N is the lattice size. The universal function $g(x)$ has been approximated with a polynomial of degree 14 as done by Feigenbaum (1979).

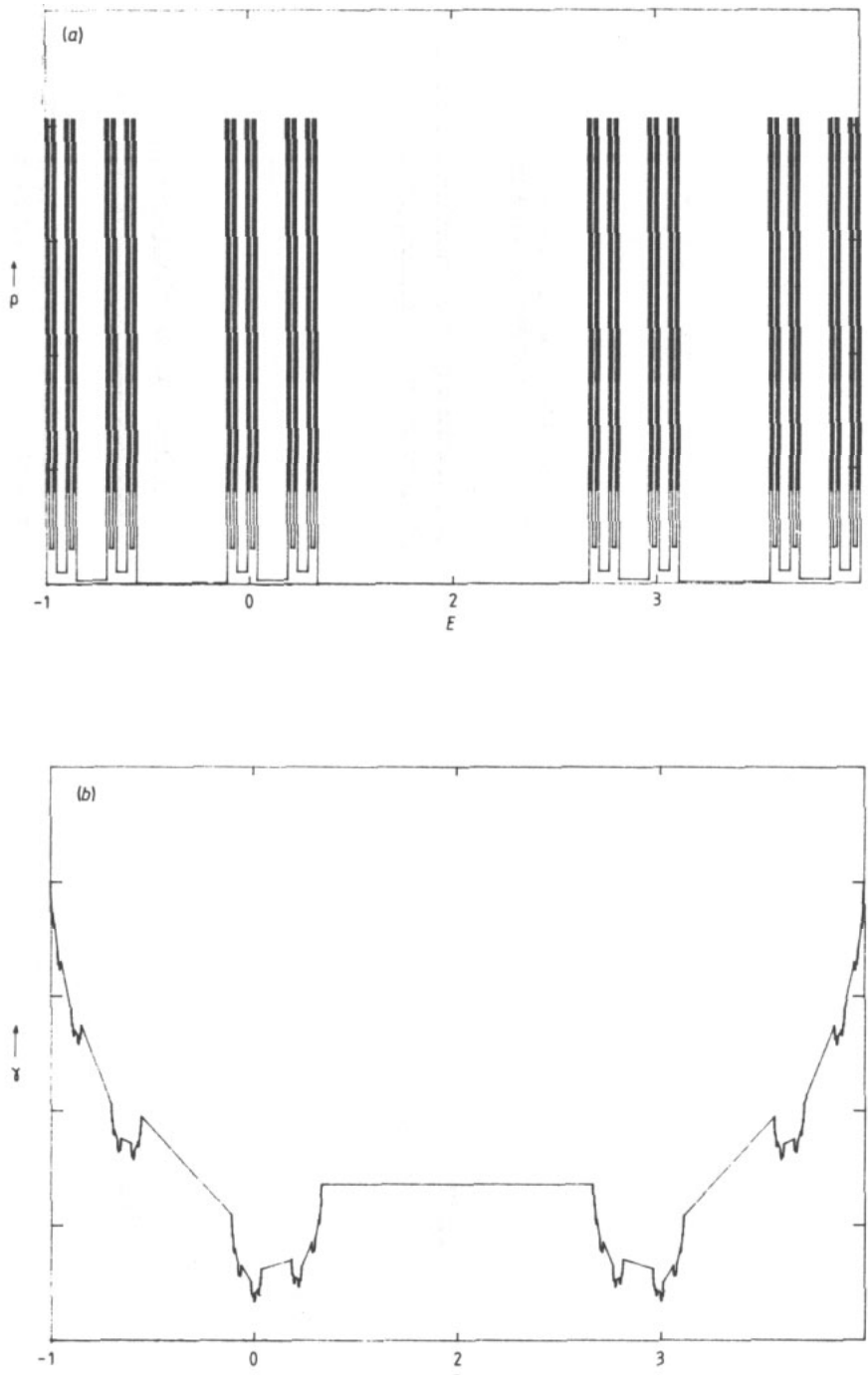


Figure 3. (*a*) Density-of-states and (*b*) γ versus E plots for a hypothetical lattice whose energy spectrum is an exact middle-thirds Cantor set. The numerical values indicated along the axes are arbitrary to the extent of a multiplicative constant in E and an additive constant in γ. Numerical values along ρ have not been indicated as they are not relevant. Points representing allowed energies are joined by straight lines.

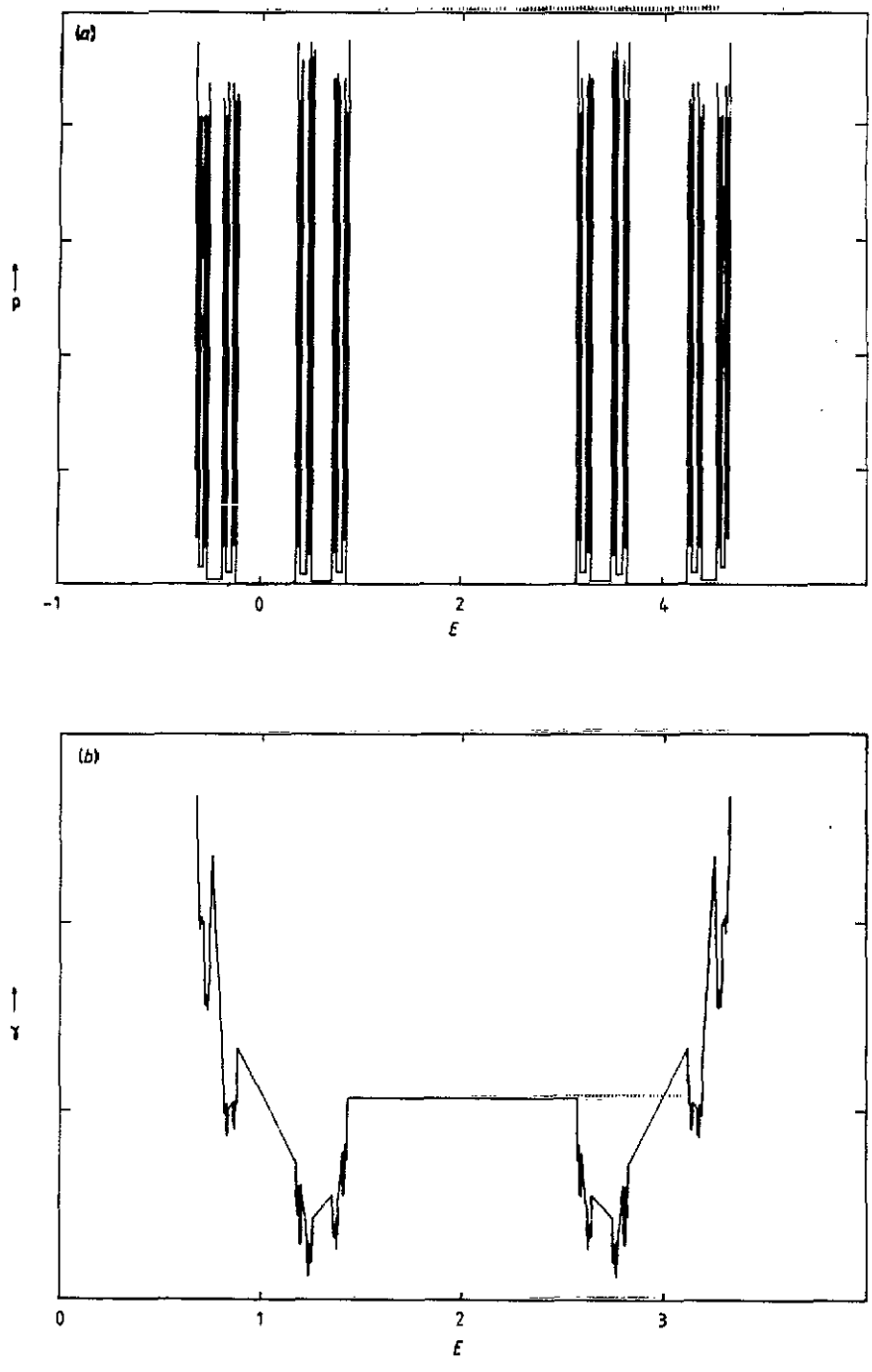


Figure 4. (*a*) Density-of-states and (*b*) γ versus E plots for a TBM with on-site potentials V_n given by the sequence $0, \frac{2}{3}, (\frac{2}{3})^2, (\frac{2}{3}) + (\frac{2}{3})^2, \ldots$ (see text), where each term is multiplied by the strength parameter $\lambda = 4.0$. Note the non-smooth self-similar nature of the γ versus E plot. The close resemblance of (*b*) with figure 3(*b*) is significant. As before, numerical values for ρ and γ have not been indicated. Points representing allowed energies are joined by straight lines.

3. Concluding remarks

The realization of systems with structures intermediate between spatially periodic and random has in recent times acquired substantial plausibility. The new techniques to produce semiconductor heterostructures (Merlin *et al* 1985, Todd *et al* 1986) with control of the growth of each layer allow experimental constructions of pre-assigned spatial arrangements of barriers. Properties of such heterostructures perpendicular to the layers can be modelled, e.g. in terms of appropriate chains of transfer matrices. Other important instances of irregular deterministic potential structures are to be found in the context of classical diffusion (Rammal and Toulouse 1986) and anomalous relaxation in spin glasses (Hoffmann *et al* 1985, Mezard *et al* 1984, Kutasov *et al* 1986).

Of particular significance in this context is the correspondence, discussed by Lahiri and Ghosal (1987, 1988), between stable spatially inhomogeneous states of certain model reaction–diffusion systems and hyperbolic trajectories of reversible mappings (Sevryuk 1986). Such correspondence could be invoked to produce desired spatial inhomogeneities in, say, appropriate chemical reaction tanks. It has been recently pointed out (Lahiri 1990) that four-dimensional reversible maps can undergo *inverted* period-doubling sequences of the Feigenbaum type, giving rise to chaotic hyperbolic orbits having a self-similar structure. Taken together, these two observations lead to the possibility of precisely the type of spatial structure that we have considered in this paper. The physical possibility of such structures has recently received a boost through the experimental observation of Turing-type patterns in reaction–diffusion systems (Castets *et al* 1990).

Eigenvalue spectra and localization properties of one-dimensional aperiodic structures, when interpreted in the context of electronic properties, are directly responsible for the transmission characteristics such as the resistance of finite chains. While a discrete spectrum leads to a resistance increasing exponentially with the length of the chain, singular continuous spectra have been shown to lead to various power-law dependences (Sokoloff 1985, Würtz *et al* 1989, Sun 1989). As already mentioned, mobility edges are expected to play a significant role in determining these transmission characteristics. Of yet greater importance of the types of model considered here is their possible implication in respect of *AC transmission* properties of linear chains. In contrast with one-dimensional chains with completely bound states (e.g. insulators), linear chains with mobility edges included in a singular continuous spectrum present the novel possibility of *quantum diffusion* under time-periodic external perturbation (Roy and Lahiri 1990). Thus we are led to a situation where a one-dimensional chain can possibly possess sharply contrasting DC and AC transmission properties.

Investigations regarding the possibilities indicated are in progress.

Acknowledgments

We acknowledge with thanks the computational facilities provided by M Engineer and S Mukherjee.

References

Aubry S and Andre C 1979 *Proc. Israel Phys. Soc.* vol 3, ed O G Kuper (Bristol: Adam Hilger) p 133
Azbel M Y 1979 *Phys. Rev. Lett.* **43** 1954

Casati G, Guarneri I and Shepelyansky D L 1989 *Phys. Rev. Lett.* **62** 345
Castets V, Dulos E, Boissouade J and De Kepper P 1990 *Phys. Rev. Lett.* **64** 2953
Chulavesky V A and Sinai Ya G 1989 *Comments Math. Phys.* **125** 91
Collet P and Eckman J P 1980 *Iterated Maps on the Interval as Dynamical Systems. Progress on Physics* vol 1 (Boston, MA: Birkhausser-Boston)
Crisianty A 1989 *J. Phys. A: Math. Gen.* **22** L681
Das Sarma S, He S and Xie S C 1988 *Phys. Rev. Lett.* **61** 2144
Drummond I T 1989 *J. Phys. A: Math. Gen.* **22** 1275
Feigenbaum M J 1978 *J. Stat. Phys.* **19** 25
—— 1979 *J. Stat. Phys.* **21** 669
—— 1980 *Los Alamos Sci.* **1** 4
Fishman S and Griniasty M 1988 *Phys. Rev. Lett.* **60** 1334
Grassberger P 1981 *J. Stat. Phys.* **26** 173
Hoffmann K H, Grossmann S and Wegner F 1985 *Z. Phys.* **60** 401
Hofstadter D 1976 *Phys. Rev.* B **14** 2239
Ishii K 1973 *Prog. Theor. Phys. Suppl.* **53** 77
Kaneko K 1986 *Collapse of Tori and Genesis of Chaos in Dissipative Systems* (Singapore: World Scientific)
Kohmoto M, Kadanoff L P and Tang C 1983 *Phys. Rev. Lett.* **50** 1870
Kohmoto M, Sutherland B and Iguchi K 1987 *Phys. Rev. Lett.* **58** 2436
Kutasov A, Aharony A, Domany E and Kinzel W 1986 *Phys. Rev. Lett.* **56** 2229
Lahiri A 1990 *Preprint*
Lahiri A and Ghosal S S 1987 *Phys. Lett.* **124A** 47
—— 1988 *J. Chem. Phys.* 7459
Merlin R, Bajema K, Juang F Y, Clarke R and Bhattacharya P 1985 *Phys. Rev. Lett.* **55** 1768
Mezard G, Parisi G, Sourlas N, Toulouse G and Virasoro M 1984 *Phys. Rev. Lett.* **56** 1156
Mira C 1987 *Chaotic Dynamics* (Singapore: World Scientific)
Nauenberg M and Rudnick J 1981 *Phys. Rev.* B **24** 439
Ostlund S, Pandit R, Rand D, Schellnhuber H J and Siggia E D 1983 *Phys. Rev. Lett.* **50** 1873
Parker E H C (ed) 1985 *The Technology and Physics of Molecular Beam Epitaxy* (New York: Plenum)
Piertonero L and Tosatti E 1986 *Fractals in Physics* (Amsterdam: North-Holland)
Rammal R and Toulouse G 1986 *Rev. Mod. Phys.* **58** 765
Roy T K and Lahiri A 1990 preprint
Sevryuk M B 1986 *Reversible Systems (Springer Lecture Notes in Mathematics* 1211*)* (Berlin: Springer)
Sokoloff J B 1985 *Phys. Rep.* **126** 190
Souillard B 1984 *Phys. Rep.* **103** 41
Soukoulis C M and Economou E N 1982 *Phys. Rev. Lett.* **48** 1043
Sun J 1989 *Phys. Rev.* B **40** 8270
Thouless D J 1988 *Phys. Rev. Lett.* **61** 2141
Todd R, Merlin R, Clarke R, Mohanty M and Axe J D 1986 *Phys. Rev. Lett.* **57** 1157
Vicsek T 1989 *Fractal Growth Phenomena* (Singapore: World Scientific)
Wilkinson J H 1965 *The Algebraic Eigenvalue Problem* (London: Oxford University Press) p 506
Würtz D, Schneider T, Politi A and Zanetti M 1989 *Phys. Rev.* B **39** 7829
Xu H 1986 *J. Phys. C: Solid State Phys.* **19** L795
—— 1987 *J. Phys. C: Solid State Phys.* **20** 5999