The Spectrum of a One-Dimensional Hierarchical Model

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The spectrum of a discrete Schrödinger operator with a hierarchically distributed potential is studied both by a renormalization group technique and by numerical analysis. A suitable choice of the potential makes it possible to reduce the original problem to a two-dimensional map. Scaling laws for the band-edge energy E_{be} and for the integrated density of states η are predicted together with the global properties of the spectrum. Different scaling regimes are obtained depending on a hierarchy positive parameter R: for $R < 1/2$ the usual scaling laws for the periodic case are obtained, while for $R > 1/2$ the scaling behavior depends explicitly on R.

1. INTRODUCTION

Discrete Schrödinger operators with quasiperiodic potentials have attracted much attention in the last decade.[1] This interest has increased in connection with the experimental finding of quasicrystals[2] and also because these structures should exhibit spectral properties between the ones of ordered and disordered systems (e.g., ref. 3).

Recently, considerable attention also has been devoted to anomalous diffusion on hierarchical structures.[4,5] Renormalization group methods yield in this case exact results for the asymptotic behaviors of the mean

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square displacement of the autocorrelation function. Practical realizations of hierarchical models range from macromolecular systems to computing structures (for references see ref. 4); quasiperiodic heterostructures have also been achieved experimentally.[6]

In this paper we study the spectrum of a one-dimensional Schrödinger equation in a hierarchical potential, which exhibits novel features with respect to periodic, quasiperiodic, and disordered cases. A similar model was first proposed for the continuous case by other authors[7] and it is known as the limit periodic potential problem; at variance with this model, our discrete problem takes explicitly into account also the case corresponding to diverging coefficients of the Fourier series defining the limit periodic potential. Other types of hierarchical potentials were studied both rigorously[8] and numerically.[9]

The model we study in this paper is the following discretized Schrödinger equation on a chain of $2^n + 1 \equiv N + 1$ sites:

$$-(\psi_{x+1} - 2\psi_x + \psi_{x-1}) + V(x)\,\psi_x = E\psi_x; \qquad x = 1,..., N-1 \qquad (1)$$

where

$$V(x) = V_m; \qquad x = 2^m(2l + 1) \tag{2}$$

with l, $m = 0$, 1, 2,..., and with boundary conditions $|\psi_0| = |\psi_N| = 0$. A suitable definition of E always allows one to choose $V_0 = 0$. In this paper we address two main questions: the solution of the eigenvalue problem and some scaling properties of the spectrum. We also discuss some features of the eigenfunctions in different scaling regimes. It is not an aim of this paper to derive rigorous results for the mathematical properties of the spectral measure nor to draw any conclusion on the possible existence of localized states (this problem is under investigation by Kunz et al.[10]).

2. RENORMALIZATION GROUP

The renormalization group method based on the decimation procedure is a powerful tool to analyze the properties of model (1). To this purpose, let us write Eq. (1) as follows:

$$\psi_{x+1} = \alpha(x)\,\psi_x - \psi_{x-1} \tag{3}$$

where

$$\alpha(x) = \alpha_m = V_m - E + 2; \qquad x = 2^m(2l + 1) \tag{4}$$

The decimation procedure begins by eliminating the dependence on ψ_x with odd $x > 1$ in the set of equations (3), as far as $\alpha_0 \neq 0$. After that the new set of equations becomes

$$\psi_2 = \alpha_0 \psi_1$$
$$\psi'_{x+1} = \alpha'_m \psi'_x - \psi'_{x-1}; \qquad x = 2^m(2l+1) \tag{5}$$

with

$$\psi'_x = \psi_{2x} \tag{6a}$$

and

$$\alpha'_m = \alpha_{m+1}\alpha_0 - 2; \qquad m = 0, 1,..., n-1 \tag{6b}$$

Outside the spectrum one can iterate the above procedure $n-1$ times, reducing the original set of $2^n - 1$ equations (3) to n equations

$$\psi_{2^p+1} = \alpha_0^{(p)}\alpha_0^{(p-1)}\cdots\alpha_0^{(1)}\alpha_0\psi_1; \qquad p = 0, 1,..., n-1 \tag{7}$$

where $\alpha_0^{(p)}$ is the pth iterate defined by the recursion relation (6b). In particular, one has

$$\frac{\psi_N}{\psi_1} = \prod_{p=0}^{n-1} \alpha_0^{(p)} \tag{8}$$

Let us stress that if one chooses the values of E leading to $\alpha_0^{(p)} = 0$, which is an algebraic equation in E of degree 2^p, the $(p+1)$th step of decimation is not allowed. However, if this occurs, Eq. (5) at the pth step can be easily solved for ψ_x, giving an eigenstate for which $\psi_{2^p+m} = 0$, with $m = 0$, $1,..., n-p$. Therefore, the eigenvalues of the problem are obtained by solving the equations

$$\alpha_0^{(p)} = 0; \qquad p = 0, 1,..., n-1 \tag{9}$$

which, in this form, is still too hard a task. Let us stress that the recursions (6) and (9), which determine the eigenvalues of our model, do not depend on the choice of the boundary conditions $\psi_0 = \psi_N = 0$ (Dirichlet problem for the semi-infinite chain). For instance, it is easy to prove that one can obtain the same results choosing periodic boundary conditions $|\psi_0| = |\psi_N|$ and $V(0) = V(N)$.

Let us now show how one can construct recursively, at least in principle, the eigenstates as a function of the $\alpha_0^{(p)}$. The simplest case occurs for $\alpha_0 = 0$, i.e., $E = 2$; the set of equations (3) is solved immediately to give

$$\psi_{2x+1} = (-1)^x \psi_1, \qquad \psi_{2x} = 0; \qquad x = 0, 1,... \tag{10}$$

When $\alpha_0^{(1)} = 0$ one has $E = [(4 + V_1) \pm (8 + V_1^2)^{1/2}]/2$ and the eigenstates are

$$\psi_{2x-1} = (-1)^{[x/2]} \psi_1, \quad \psi_{2(2x+1)} = \alpha_0 (-1)^x \psi_1, \quad \psi_{4x} = 0; \quad x = 0, 1,...$$
(11)

where $[x]$ is the integer part of x. In principle, one can go further iteratively to any finite order p; it is straightforward to verify that all these eigenfunctions, which do not depend on the chain length, are periodic functions of period 2^{p+1}, so that they are not localized states. One can write explicitly the form of the family of eigenstates corresponding to the solutions of Eq. (9). Choosing $\psi_1 = 1$, one obtains

$$\psi_2 = \alpha_0, \quad \psi_3 = 1 + \alpha_0', \quad \psi_4 = \alpha_0 \alpha_0', \quad \psi_5 = 1 + \alpha_0' + \alpha_0'',...$$

and in general

$$\psi_{2x+1} = \hat{P}(\psi_x + \psi_{x+1}), \quad x < 2^{n-2} - 1$$

$$\psi_{2^p(2x+1)} = \psi_{2^p} \hat{P}^p \psi_{2x+1}, \quad x < 2^{n-2-p} - 1 \qquad (12)$$

$$\psi_{2^{n-1}+x} = \psi_{2^{n-1}-x}, \quad x = 0,..., 2^{n-1}$$

where, considering that all the ψ_x are expressed in terms of the $\alpha_0^{(p)}$, the linear operator $\hat{P}$ acts as follows:

$$\hat{P}1 = 1; \quad \hat{P}^i \alpha_0^{(p_1)} \alpha_0^{(p_2)} \cdots = \alpha_0^{(p_1+i)} \alpha_0^{(p_2+i)} \cdots \qquad (13)$$

It is a much harder task to obtain some information about the nature of the 2^p eigenfunctions coming from the solution of Eq. (9) in the $p \to \infty$ limit. For instance, the fundamental energy is the lowest energy solution of Eq. (9) in this limit; as a consequence of what we have shown, it is also clear that if localized states exist, they must be looked for in this set of solutions.

3. REDUCTION TO A TWO-DIMENSIONAL MAP

A suitable choice of the potential (2) allows us to reduce the infinite set of recursion relations (6b) to a 2D map. To this purpose, we first perform the following transformation:

$$\beta_m = \alpha_m - \alpha_{m-1}; \quad m = 1, 2,... \qquad (14)$$

$$\gamma_m = \beta_{m+1}/\beta_m; \quad m = 1, 2,... \qquad (15)$$

In terms of these new variables, Eqs. (6b) can be rewritten in the set

$$X' = 2 + XY - X^2 \tag{16a}$$

$$Y' = -XY\gamma_1 \tag{16b}$$

$$\gamma'_m = \gamma_{m+1}; \qquad m = 1, 2,... \tag{16c}$$

where $X^{(p)} = -\alpha_0^{(p)}$ and $Y^{(p)} = \beta_1^{(p)}$. In this way the recursion (16c) is decoupled from the others and its fixed point is

$$\gamma_m^* = R; \qquad m = 1, 2,... \tag{17}$$

Using Eqs. (14) and (15), one obtains at the fixed point (17) the following form for the potential:

$$V_m = V_1(R^m - 1)/(R - 1) \tag{18}$$

while recursions (16a), (16b) simplify to the two-dimensional map

$$X' = 2 + XY - X^2 \tag{19a}$$

$$Y' = -XYR \tag{19b}$$

with initial conditions $X = E - 2$ and $Y = V_1$. For $R > 1$, choosing the potential such that $V_m/V_{m-1} \to R$ as $m \to \infty$, the form (18) is reached after a transient. For instance, this occurs if $V_m \sim R^m$ for large m. The general properties of the spectrum will not be affected by the initial choice of V_m and this justifies our studying directly the potential (18). In this case the map (19) contains all the information on the spectrum. For fixed p the determination of the eigenvalues coming from Eq. (9) amounts to looking for the intersections of the pth preimages of the axis $X = 0$ with $Y = V_1$. All these preimages are branches of nonintersecting hyperbolic curves with the common vertical asymptote $X = 0$ and the set of straight lines

$$Y = X/C \tag{20}$$

as oblique asymptotes. The angular coefficients C^{-1} are easily obtained using Eq. (19),

$$C_l = 1 + RC_{l-1}, \qquad C_1 = 1; \qquad l = 1, 2,... \tag{21}$$

whose solution is

$$C_l = \frac{R^l - 1}{R - 1} \tag{22}$$

It is also easy to show that all hyperbolic curves intersect the $Y = 0$ axis between $X = -2$ and $X = 2$. Half of these branches lie on the lhs of the axis $X = 0$. The branches which lie on the rhs group in classes such that a fraction $1/2^l$ have asymptote of type (20) with $C = C_l$. The hyperbolic curves corresponding to the first three preimages of the axis $X = 0$ are shown in Fig. 1. Let us derive the first consequences of these results. The $Y = V_1 = 0$ case corresponds to the uniform potential, whose spectrum is easily determined by the recursions (19) for $Y = 0$. In the infinite-chain limit the spectrum is dense on the energy interval $(0, 4)$ (see, e.g., ref. 11). For $V_1 > 0$ the very existence of the oblique asymptotes allows for the classification of the eigenenergies in zeroth-order bands (ZOBs) of serial index l, each containing a fraction $1/2^l$ of states. The separation of these ZOBs becomes neater as V_1 increases as long as $R > 1$. Inside these bands we find numerically smaller gaps, corresponding to the existence of hyperbolic-like asymptotes. The distance between two consecutive left borders of ZOBs scales as $V_1 R^{l-1}$ as V_1 and/or E increase. This implies that for $R > 1$ the gaps separating the ZOBs increase exponentially. For
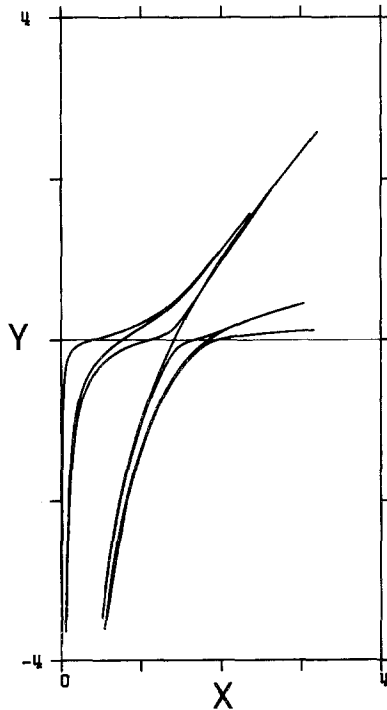

Fig. 1.   The right branches of the first three preimages of the axis $X = 0$ for $R = 4$ (the left branches are obtained by the symmetry $X \to -X$, $Y \to -Y$).

$R = 1$ one has asymptotically equal length gaps, which is a consequence of Eq. (22) in the $R \to 1$ limit. This case separates two distinct regimes. For $R < 1$ the limiting oblique asymptote has angular coefficient $1 - R$ and, at variance with the $R > 1$ case, the spectrum is bounded also from above and the ZOBs accumulate near the upper band edge. Figure 2 shows the numerical results for the number of states with energy lower than E, $\delta(E, V_1)$, as a function of the energy in the various cases. The above theoretical predictions on the edges of the ZOBs are well verified numerically.

4. SCALING LAWS

The combination of the renormalization group treatment with standard methods allows us to discuss the scaling behavior of the density of states and of the Liapunov exponent for particular values of the energies. An immediate theoretical prediction that one can obtain on the basis of the existence of the ZOBs is the scaling behavior of the integrated density of states $\eta(E, V_1) = \delta(E, V_1) 2^{-n}$ for large E and $R > 1$. In fact, the fraction of states $1 - \eta(E_l, V_1)$ with energy $E > E_l = 2 + V_1 C_l$ is

$$1 - \eta(E_l, V_1) = 1/2^{l-1} \tag{23}$$

Using Eq. (22), one can rewrite this in terms of E only, i.e.,

$$\eta(E, V_1) = 1 - \left(\frac{E(R-1)}{V_1}\right)^{-\log 2/\log R} \tag{24}$$

From Eqs. (19) one can derive the scaling of the band-edge energy E_{be} in the $V_1 \to 0$ limit. In order to obtain it, one has to compute the limit hyperbolic curve $f(X)$ passing through $(X = -2, Y = 0)$ (see Fig. 1) in the region of small Y. We note that $(-2, 0)$ is a fixed point of the map (19) and that the limit curve we are looking for is an invariant set of this two-dimensional mapping. This amounts to solving the functional equation $Y' = f(X')$ with X' and Y' given in Eqs. (19) and $Y = f(X)$. Linearizing the recursions (19) around $(-2, 0)$ and requiring that $Y = f(X) \sim A(X+2)^z$ is an invariant set, one finds

$$z = \begin{cases} \log(2R)/\log 4, & R > 2 \\ 1, & R < 2 \end{cases} \tag{25}$$

where $A = 2 - R$ for $R < 2$, while for $R > 2$, A cannot be determined by this method. For $R = 2$ we expect logarithmic corrections to scaling. Indeed, in this case one finds easily
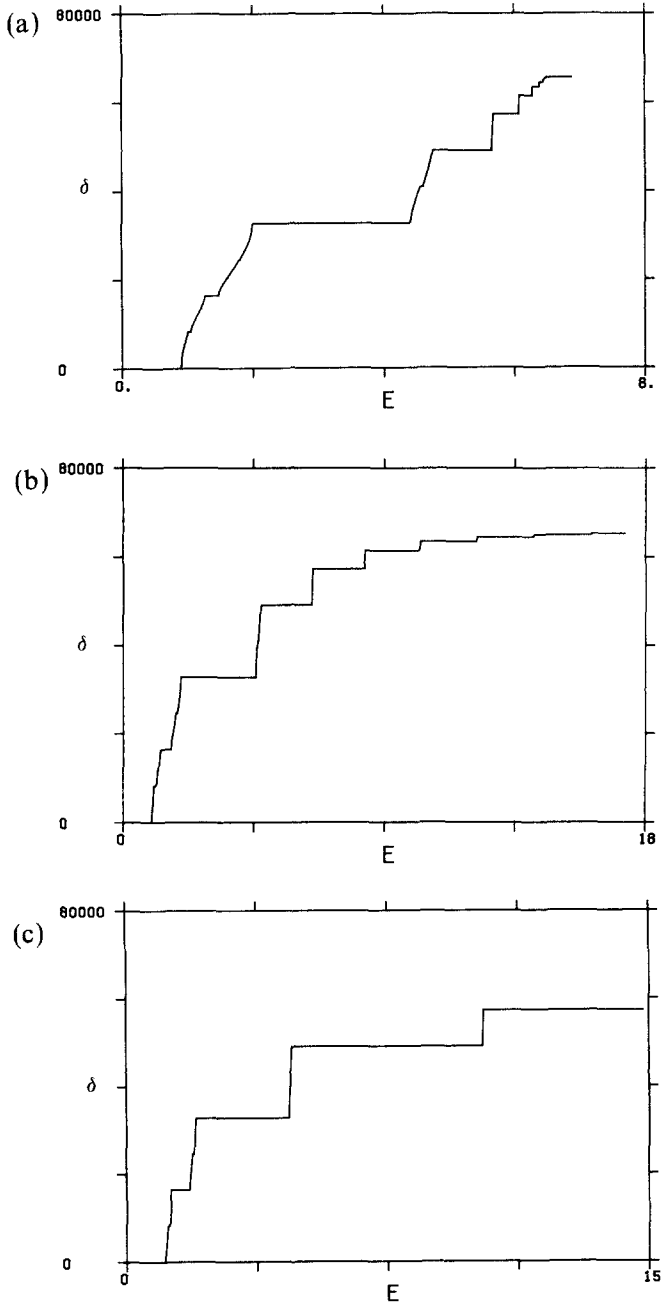
$$f(X) = \frac{X+2}{|\log(X+2)|} 4 \log 2 \tag{26}$$

Fig. 2.   Plot of δ versus E for $N = 2^{16}$ and $V = 2$ and (a) $R = 1/2$, (b) $R = 1$, (c) $R = 3$.

Since the invariant set $Y = f(X)$ represents the limit of the left preimages of the axis $X = 0$, the band-edge energy is obtained solving the equation $f(E_{be} - 2) = V_1$. This can be done explicitly only for $V_1 \to 0$ using the asymptotic form of $f(X)$ around $X = -2$. One obtains

$$E_{be} \sim V_1^{1/z} \tag{27}$$

apart from the logarithmic corrections present for $R = 2$. This result has been checked numerically for $R = 1/2$ and for $R = 4$ and it is shown in Fig. 3. It is also straightforward to calculate the scaling correction to Eq. (27), imposing that $f(X) = A(X + 2)^z [1 + B(X + 2)^\omega]$. Following the previous procedure, one obtains

$$E_{be} \sim V_1^{1/z} \left[1 - \frac{B}{z} \left(\frac{V_1}{RA} \right)^{\omega/z - 1} \right] \tag{27a}$$

where

$$\omega = \frac{\log R}{\log 2}, \qquad B = \frac{AR \log(2R)}{(R - 2) \log 4}, \qquad 2 < R < 8$$

$$\omega = \frac{\log(8R)}{\log 4}, \qquad B = \frac{z - 2}{12}, \qquad R > 8 \tag{27b}$$

A further interesting point is to see how the density of states ρ and the Liapunov exponent λ scale with E at the band edge. Of course, the two functions can be in general highly singular and different from zero only on a very complicated set (for instance, Fig. 2 suggests that this is the case). Therefore our results for these scaling laws apply to these functions as averaged over a suitable infinitesimal interval of energy.

A standard method to obtain ρ for the eigenvalue problem (3) amounts to studying the associated equation for the Green's function (resolvent) $P_{x_0, x}$,

$$\alpha(E, Y; x) P_{x_0, x} = P_{x_0, x + 1} + P_{x_0, x - 1} + \delta_{x_0, x} \tag{28}$$

which is well defined at least for $E < E_{be}$ and where $\delta_{x_0, x}$ is the Kronecker delta function. The analytic continuation to $E > E_{be}$ of the solution $P_{x_0, x}(E, Y)$ is related to ρ and to the Liapunov exponent $\lambda(E, Y)$ through the equations

$$\rho = \lim_{N \to \infty} \frac{1}{N} \mathrm{Tr}\, \delta(H - E) = \frac{1}{\pi} \mathrm{Im}\, P(E + i0^+, Y) \tag{29}$$

$$\frac{\partial \lambda}{\partial E} = \mathrm{Re}\, P(E + i0^+) \tag{30}$$

where $P(E, Y) = \lim_{N \to \infty} (1/N) \sum_{x_0} P_{x_0, x_0}(E)$. This problem can be mapped into a statistical problem where $P_{x_0, x}$ is the two-point correlation function of a Gaussian model with reduced Hamiltonian

$$H = \sum_x \frac{\alpha(x)}{2} \varphi_x^2 - \sum_x \varphi_x \varphi_{x+1} \tag{31}$$
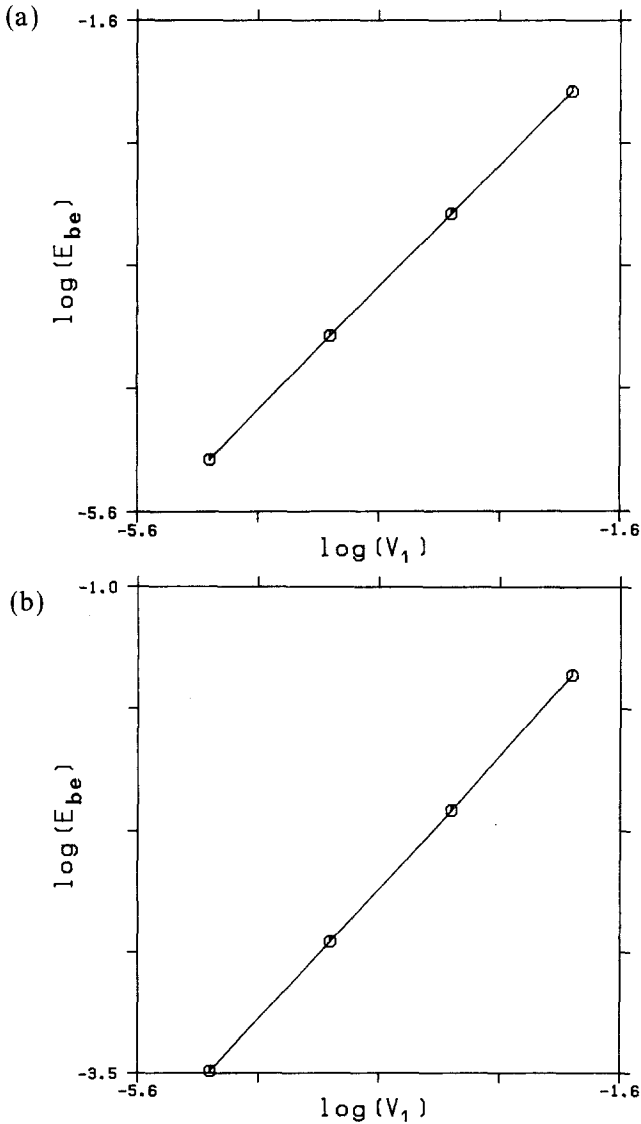
Fig. 3.   Plot of $\log(E_{be})$ versus $\log(V_1)$ for $N = 2^{16}$ and (a) $R = 1/2$, (b) $R = 4$.

i.e.,

$$P_{x_0, x} = \langle \varphi_{x_0} \varphi_x \rangle = Z_N^{-1} \int_{-\infty}^{+\infty} \prod_{x=1}^{N} d\varphi_x \exp(-H) \, \varphi_{x_0} \varphi_x \tag{32}$$

with the partition function Z_N given as usual by

$$Z_N = \int_{-\infty}^{+\infty} \prod_{x=1}^{N} d\varphi_x \exp(-H)$$

Recalling the definition of $\alpha(x)$ given in Eq. (4), one obtains immediately the average over sites of $P_{x_0, x}$:

$$P(E, Y) = 2 \lim_{N \to \infty} \frac{1}{N} \frac{\partial}{\partial E} \log Z_N(E, Y) \tag{33}$$

A renormalization group procedure based on the decimation of odd sites[11,12] gives for the model (31) again the recursion equations (19) together with the scaling of the "free energy density" $F = \lim_{N \to \infty} (1/N) \log Z_N$

$$F(E, Y) = \tfrac{1}{4} \log(2\pi) + \tfrac{1}{2} F(E', Y') \tag{34}$$

The fixed points of (19) are

$$u = (X_u^*, Y_u^*) = (-2, 0),$$

$$v = (X_v^*, Y_v^*) = \left(-\frac{1}{R}, \frac{(2R^2 + R - 1)}{R} \right)$$

$$w = (X_w^*, Y_w^*) = (1, 0)$$

As we shall see, only u and v are relevant for the scaling at the band edge. Looking at Table I, one realizes that for $R < 1/2$, u has a domain of

Table I. Eigenvalues and Eigenvectors of the Jacobian Map (19) at the Fixed Points u and v[a]

Fixed point	Eigenvalues	Eigenvectors
u	$\lambda_u^+ = 4$	$(1, 0)$
	$\lambda_u^- = 2R$	$(1, 2 - R)$
v	$\lambda_v^+ = \dfrac{S + (S^2 - 8R)^{1/2}}{2R}$	$\left(1, \dfrac{2R^2 + 1 - (S^2 - 8R)^{1/2}}{2} \right)$
	$\lambda_v^- = \dfrac{S - (S^2 - 8R)^{1/2}}{2R}$	$\left(1, \dfrac{2R^2 + 1 + (S^2 - 8R)^{1/2}}{2} \right)$

[a] $S = 2R^2 + 2R + 1$.

attraction which is an invariant line intersecting u with slope $(2 - R)$. At $R = 1/2$, v crosses u and for $R > 1/2$ it enters the positive Y plane, where it acquires a domain of attraction which is an invariant line. It is tempting to conjecture that this invariant line joins together u and v and is the same invariant line $Y = f(X)$ we have been speaking of above. We have direct numerical evidence that this is the case for different relevant values of R. Furthermore, an immediate consequence should be that for $V_1 = Y_v^*$ in Eq. (18), the value of E_{be} should be given by $E_{be} = 2 + X_v^* = 2 - 1/R$ for $R > 1/2$. A high-precision estimate of E_{be} for this value of V_1 gives a perfect agreement with our prediction, making us confident that indeed the conjecture is plausible.

Let us come back to Eq. (34), which implies that

$$\nabla F(E, Y) = \tfrac{1}{2} T(E, Y) \nabla F(E', Y') \tag{35}$$

where

$$T(E, Y) = \begin{pmatrix} \partial E'/\partial E & \partial Y'/\partial E \\ \partial E'/\partial Y & \partial Y'/\partial Y \end{pmatrix} \tag{36}$$

If the above conjecture holds, starting with $Y = V_1$ and $E = E_{be}(V_1) - \varepsilon$, the resulting renormalization group trajectory will spend an increasing "time" near the fixed point u or v for $R < 1/2$ and $R > 1/2$, respectively, as ε approaches zero. Thus, we can write

$$(E^{(n)}, Y^{(n)}) \sim \varepsilon \lambda_{max}^n \mathbf{w} \tag{37}$$

where λ_{max} is the maximum eigenvalue in u and v for $R < 1/2$ and $R > 1/2$, respectively, and $\mathbf{w}$ the corresponding eigenvector (see Table I). Equation (37) will hold for $n \in (n_0, n(\varepsilon))$, where n_0 is fixed and depends on the transient (i.e., on V_1), while $n(\varepsilon) \to \infty$ as $\varepsilon \to 0$. In this range of values of n one has

$$P(E, Y) = (1, 0) \nabla F(E, Y) \sim \left(\frac{\lambda_{max}}{2}\right)^n g(\varepsilon \lambda_{max}^n) \tag{38}$$

where g is a suitable function. Taking $n(\varepsilon)$ such that $\varepsilon \lambda_{max}^{n(\varepsilon)} = \varepsilon_0 \ll 1$ with ε_0 fixed, Eq. (38) implies

$$P(E_{be} - \varepsilon, Y) \sim \varepsilon^{(\varphi - 1)} \tag{39}$$

with

$$\varphi = \frac{\log 2}{\log \lambda_{max}} = \begin{cases} 1/2, & R \leqslant 1/2 \\ \log 2/\log \lambda_v^+, & R \geqslant 1/2 \end{cases} \tag{40}$$

The analytic continuation in Eq. (29) gives the same scaling of Eq. (39) for the density of states, while for the integrated density of states $\eta(E, Y)$ we have

$$\eta(E_{be} + \varepsilon, Y) \sim \varepsilon^{\varphi} \tag{41}$$

and for the Liapunov exponent

$$\lambda(E_{be} + \varepsilon, Y) \sim \varepsilon^{\varphi} \cos(\pi\varphi) + \text{const} \tag{42}$$

Equation (41) has been checked numerically for different relevant values of R, showing a perfect agreement with the theoretical prediction. Even if these results are interesting for the "averaged" functions and can be verified numerically, it is important to remark that no conclusions can be drawn on the value of the Liapunov exponent in the spectrum.

5. CONCLUSIONS

In this paper we have obtained rigorous closed expressions for the eigenvalue problem of a hierarchical model defined on a semi-infinite chain with Dirichlet boundary conditions. The eigenvalues accumulate in a very rich Cantor set structure; one can prove that the essential spectrum of the semi-infinite chain is the same as for the infinite one. We have also derived the scaling law of the lowest band-edge energy in terms of the potential amplitude V_1. The scaling exponents change at $R = 2$ and at $R = 8$. Similar scaling laws may exist at any band edge in the spectrum. Scaling laws for the density of states and for the Liapunov exponent change at $R = 1/2$. Analogous changes for other properties of the spectrum could be expected for any value of R which is a power of 2.

Let us stress that the renormalization group method cannot allow one to draw strict conclusions on the value of the Liapunov exponent λ, even at $E = E_{be}$, although we have strong numerical evidence that $\lambda = 0$ in the spectrum. The study of the properties of the eigenstates must be performed by other methods. Bellissard[1] has recently proven that for $R > 2$ this model has a "singular" continuous spectrum. Other authors[10] have reached analogous conclusions by using resolvent techniques. The effective calculation of the singular wave functions remains an open problem.

For $R < 1$ we have numerical evidence that the Lebesgue measure of the spectrum is positive and therefore we conjecture that the spectrum has an absolutely continuous component. For a similar model which shows an absolutely continuous component of the spectrum see ref. 13.

Finally, we think that important hints may come from a more detailed analysis of the dynamical system (19), which we have associated with the properties of the spectrum.

ACKNOWLEDGMENTS

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