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# Quantum states of hierarchical systems

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The quantum states of an electron in a hierarchical potential are investigated in the tight-binding approximation. The hierarchy is taken to be in the transition matrix elements, in natural analogy to the classical problem of diffusion in ultrametric structures. The energy spectrum is found to be a Cantor set, and analytical results are presented for its scaling properties. The envelope of the wave function is found to decay algebraically for certain energies and to be constant for others. The results are in excellent agreement with high-precision numerical work.

The hierarchical organization of a number of complex molecules and other condensed-matter structures leads to anomalous properties in their classical transport coefficients. Specifically, for systems with a hierarchical distribution of energy barriers, the phenomenon of ultradiffusion appears as a manifestation of the underlying ultrametric topology.[1-5] This effect is characterized by a power-law decay of the autocorrelation function with a temperature-dependent exponent. Since many hierarchical systems possess electron states which can be probed experimentally, it is of interest to inquire about their quantum states. This communication presents the results of such a study. In particular, we solve the Schrödinger equation in the tight-binding approximation for a system with an ultrametric distribution of transition matrix elements. We discover a number of scaling relations connecting the width of the spectrum to the parameter $R$ which characterizes the ratio between transition matrix elements. Moreover, the whole structure of the spectrum is analogous to that of quasiperiodic crystals, which have been extensively studied in the past few years.[6-11] We also determine the fractal set underlying the spectrum and, most importantly, obtain analytical results for the relevant indices as a function of $R$. These novel results are in excellent agreement with high-precision numerical experiments. Besides showing that ultrametricity and quasiperiodicity are related, this study provides an analytical determination of the quantum signature of hierarchical systems.

We begin by considering the following tight-binding Hamiltonian:

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

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

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

Here, the hierarchy is in the transition matrix elements, and the site energies $U$ are taken as a constant. The model is thus a natural quantum extension of the master equation in ultradiffusion. We assume $R$ to be in the interval $[0,1]$ so that $t_{n,n-1}$ is an almost periodic function of $n$. Also, since $U$ is constant, we may absorb it in the energy $E$ and consider the problem with site energies set to zero.

To analyze the infinite system described by Eq. (1), we consider a series of periodic systems constructed as follows: The period-$2^n$ system has all transition rates equal to $VR^k$, $k > n-1$, replaced by $VR^{n-1}$. For a period of 2, we thus have only two matrix elements, 1 and $V$. We may solve for the band structure of this system using a transfer matrix method. The wave function at cells $2k$ and $2k+1$ is related to that at cells 0 and 1 by a transfer matrix $M_1^k$, where

$$M_1 = \begin{pmatrix} E^2 - \dfrac{V^2}{V} & -\dfrac{E}{V} \\ \dfrac{E}{V} & -\dfrac{1}{V} \end{pmatrix} . \tag{3}$$

Clearly, we have $\det M_1 = 1$; hence, the requirement of $\psi_k$ being bounded gives the condition for the bands,

$$|\mathrm{Tr} M_1| = \left| \frac{E^2 - (1+V^2)}{V} \right| \leq 2 \ . \tag{4}$$

If we now consider a system of period $2^n$, we can carry out a renormalization scheme to reduce it to the period-2 system solved for above. We decimate the pairs of cells surrounding the barrier of height $V$, i.e., cells numbered $4j+1$ and $4j+2$, $j$ an integer. This leads to a recursion relation between the renormalized values $(E', V')$ and the original ones $(E, V)$ given by

$$V' = R(E^2 - V^2), \quad E' = E(E^2 - V^2 - 1)/V \ . \tag{5}$$

Equations (4) and (5) above allow one to determine the band structure for any $n$. Figure 1 shows the resulting

 

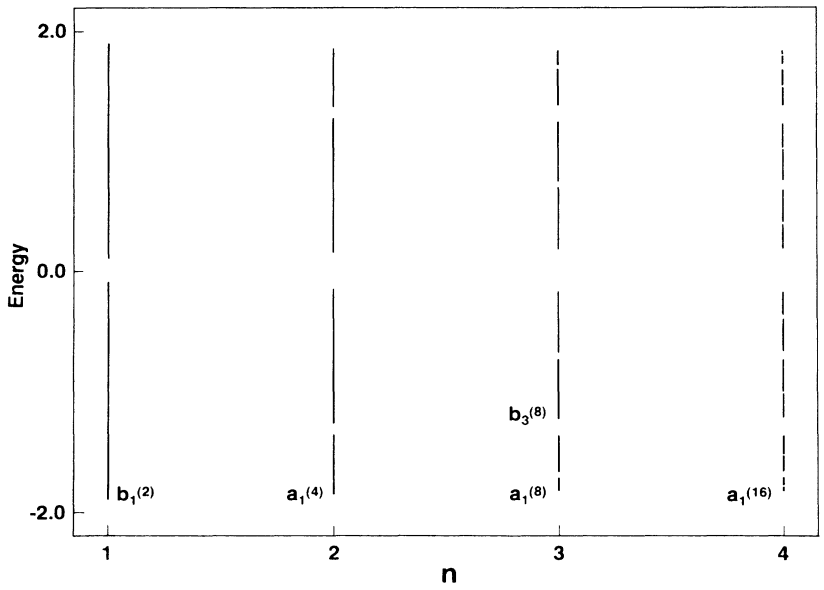


FIG. 1. The energy bands (arb. units) for periodic systems of size $2^n$, $n=1,2,3,4$. We take $V=R=0.9$.

spectra for $n=1,2,3,4$ and $R=0.9$. We will show momentarily that the total bandwidth goes to zero as $n\rightarrow\infty$; hence, Fig. 1 shows directly the construction of the infinite limit Cantor set.

An alternative method for finding the band structure of the period-$2^n$ system, and the one actually employed in the numerical work for Fig. 1, is to make use of Bloch's theorem. If $p=2^n$, then we have $\psi_{j+p}=e^{ikp}\psi_j$ for some wave vector $k$. We choose $k$ to correspond to a band edge; hence, $k=0$ or $k=\pm\pi/p$. The two resulting matrices of order $p$ are easily diagonalized to find the $p$ bands. This was done with great precision for systems of size up to $p=2^{10}$. Clearly, each band will contain the same number of states.

A self-similarity in the energy spectrum is apparent from Fig. 1, and hence it is useful to characterize the corresponding scaling properties. First, we expect that the total bandwidth for the period $p=2^n$ system should scale with $n$ like $B_n\sim p^{-\delta}$, where $\delta$ is some positive constant presumably depending on $R$. From our precision numerical work for the bands, where we are able to calculate the band edges to more than eight significant digits, we find, in fact, the exact expression

$$B_n=4VR^{n-1},\quad n\geq 1,\quad V<1\ . \tag{6}$$

This gives $\delta=-\ln R/\ln 2$. Equation (6) has been verified analytically for $n=1,2$. Figure 2 shows the numerical evidence supporting the expression for $\delta$ as a function of $R$. Furthermore, we discovered that for $n$-ary systems, as opposed to the binary case of Eq. (2), Eq. (6) still holds. This gives $\delta=-\ln R/\ln n$ in the general case.

We may also consider the scaling properties of individual bands. Let $p_n=2^n$. Consider the bands labeled $a_1^{(p_n)}$ in Fig. 1, where $a$ denotes the width of the band. They all appear to be similar, and to contract faster than any other series of bands. Defining

$$k_a\equiv\lim_{n\rightarrow\infty} a_1^{p_n}/a_1^{p_{n+1}}\ , \tag{7}$$

we find numerically, for $R=0.9$, that $k_a\approx 4.59\pm 0.01$. Similarly, the bands labeled $b_{(p_n+1)/3}^{(p_n)}$, $n$ odd, are similar and appear to contract the most slowly. Letting $k_b$ be the analogous scaling ratio of these bands for $R=0.9$, we find that $k_b\approx 4.20\pm 0.02$.

To study the spectrum in more detail, we follow the method of Halsey *et al.*,[12] and calculate the fractal spec-

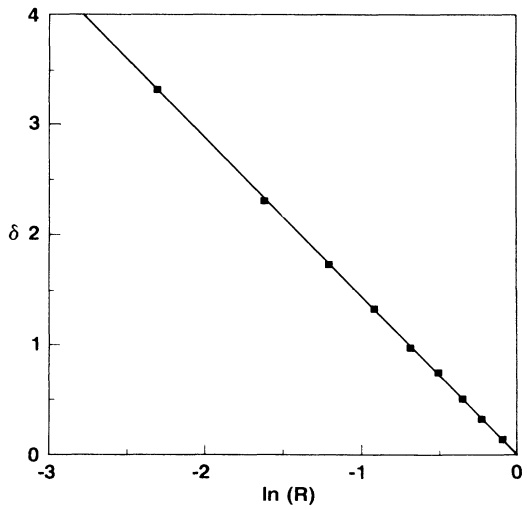


FIG. 2. The solid squares are the numerically determined values of $\delta$ plotted vs $\ln R$, for $R=0.1,0.2,\ldots,0.9$, with $V=R$. The line is the least-squares best fit, with slope $-1.44\approx -1/\ln 2$, in agreement with the result following Eq. (6).

trum of the resulting Cantor set. To do so, we consider the partition function

$$\Gamma_n(q,\tau)=\sum_{i=1}^{2^n}\frac{P_i^q}{(\Delta E_i)^\tau} . \tag{8}$$

Here, $P_i$ is the probability of a state belonging to the $i$th band; since all bands have equal numbers of states in them and there are $2^n$ bands, we have $P_i=2^{-n}$. We determine a relationship between $\tau$ and $q$ by requiring $\Gamma_n(q,\tau)=1$ in the large-$n$ limit. The behavior of $\tau$ and $q$ is related to the scaling properties of the spectrum as follows. Let $N(E)$ be the integrated density of states. Define the scaling exponent $\alpha_E$ by $|N(E+\Delta E)-N(E)|\sim(\Delta E)^{\alpha_E}$. The scaling parameters $\alpha$ belonging to various parts of the spectrum are given by $d\tau/dq$. One can then calculate the fractal dimension $f(\alpha)$ of those points which scale with $\alpha$ from $f(\alpha)=-\tau+q\alpha$.

We have carried out this calculation numerically, with the resulting curve plotted, again for $R=0.9$, in Fig. 3. To improve the numerical efficiency, we determined $\tau(q)$ through the equivalent condition $\Gamma_n/\Gamma_{n'}=1$, with $n=9$ and $n'=10$. Note in particular that the maximum value of $f$ corresponds to the fractal dimension $D_0$ of the set. We may account for the zeros of $f$ from knowledge of the largest and smallest scaling constants in the spectrum. From above, we expect $\alpha_{\min}=\ln 2/\ln k_a$ and $\alpha_{\max}=\ln 2/\ln\sqrt{k_b}$ (since the $b$ sequence has period two). For $R=0.9$, this gives $\alpha_{\min}=0.45\pm0.01$ and $\alpha_{\max}=0.97\pm0.01$, in agreement with Fig. 3.

The above numerical results may be explained analytically. First, let us consider the fractal dimension $D_0$. Let $N(n,l)$ denote the number of segments of $l$ it takes to cover all the bands for period $2^n$. Then by definition, $N(n,l)\sim l^{-D_0}$. The total bandwidth $B_n$ thus scales like $l^{1-D_0}$, but we also have $B_n\sim 2^{-n\delta}$ and $N(n,l)\sim 2^n$. Thus,

$$D_0=1/(1+\delta)=\ln 2/\ln(2/R) . \tag{9}$$

For $R=0.9$, this gives $D_0=0.8681$, in excellent agreement with Fig. 3. One should note that Eq. (9) gives a value for $D_0$ which is the same as the exponent for the power-law decay of the autocorrelation function in ultradiffusion.[1]

Next, we examine the fixed points of the recursion relations in Eq. (5), define $E_n$ and $V_n$ to be the $n$th iterates of $E$ and $V$, and let $T_{n+1}=(E_n^2-V_n^2-1)/V_n$. We see then from Eq. (4) that $(E,V)$ is in the spectrum of the period-$2^{n+1}$ system provided that $|T_{n+1}|\le 2$. We may use this definition of $T_n$ to eliminate $E_n$ from the recursion relations, obtaining the following set in terms of $T$ and $V$ only:

$$\begin{aligned} RT_{n+2}&=T_{n+1}^2+(1-R^2)V_nT_{n+1}-(1+R^2) ,\\ V_{n+1}&=R(1+V_nT_{n+1}) . \end{aligned} \tag{10}$$

Then $E_n^2=1+V_n^2+T_{n+1}V_n$. We emphasize that these recursion relations are entirely equivalent to those above, except that we have now avoided any difficulties which occurred in Eq. (5) when some iterate $V_n=0$.

The fixed points of Eq. (10) are easily identified. First, we have the point $T_1^*=1$, $V_1^*=R/(1-R)$, and $E_1^{*2}=(1-R+R^2)/(1-R)^2$. The eigenvalues of the matrix $\partial(V',T')/\partial(V,T)$ are

$$\lambda_{1,2}^{(1)}=\left[\frac{1}{2}+\frac{1}{R}+R\right]\pm\left[\left[\frac{1}{2}+\frac{1}{R}+R\right]^2-2\right]^{1/2} . \tag{11}$$

Note that regardless of $R$, $\lambda_{\max}>1$; hence, the fixed point is repulsive. This is consistent with the Cantor property of the spectrum in the infinite limit. Second, we have the fixed point $T_2^*=-1$, $V_2^*=R/(1+R)$, and $E_2^{*2}=(1+R+R^2)/(1+R)^2$. The corresponding eigenvalues are

$$\lambda_{1,2}^{(2)}=\left[\frac{1}{2}-\frac{1}{R}-R\right]\pm\left[\left[\frac{1}{2}-\frac{1}{R}-R\right]^2-2\right]^{1/2} . \tag{12}$$

Again, for any value of $R$ we have $|\lambda|_{\max}>1$, and thus this fixed point is also repulsive. Third, there is the fixed point $T_3^*=(1+R^2)/R$, $V_3^*=-1/R$, and $E_3^*=0$.

Because $|T_3^*|>2$, only the first two fixed points listed above are relevant to the scaling properties of the spectrum. Moreover, note that for any value of $R\in[0,1]$, we have $0<\lambda_1^{(1)}<1<\lambda_2^{(1)}$ and $\lambda_2^{(2)}<-1<\lambda_1^{(2)}<0$. Thus the first fixed point is hyperbolic and the second hyperbolic with reflection. From examination of the $(T,V)$ phase-space diagram, we find that there are two heteroclinic points where the stable invariant manifold of one fixed point intersects the unstable invariant manifold of the other. As is well known, the existence of one heteroclinic point implies the existence of an infinity of them, implying that the stable invariant curves for the two fixed points must be extremely complicated, twisted objects. The intersections of these curves with the segment $V=V_0$, $T\in[-2,2]$ provide the set of initial $T$ (and hence $E$)

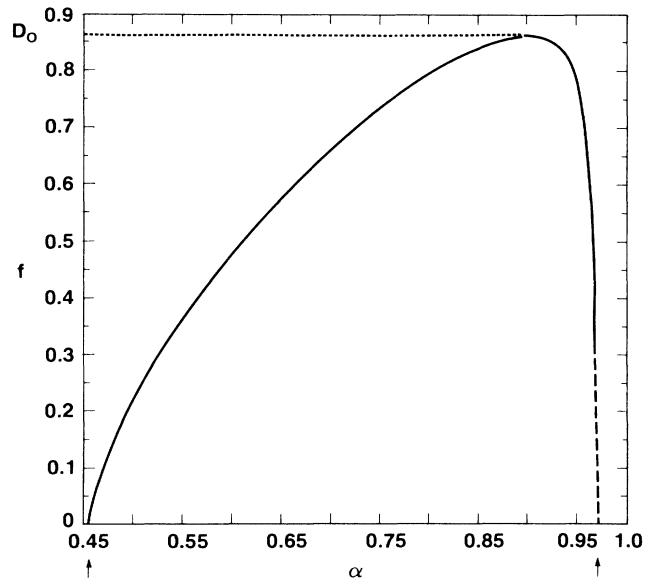


FIG. 3. The numerically determined fractal spectrum $f$ plotted as a function of $\alpha$, drawn with a smooth curve connecting the data points. We take $V=R=0.9$. The arrows and horizontal line correspond to the analytical values. The dashed portion of the curve is extrapolated.

values which will relax to the fixed points. Furthermore, small intervals around these points will scale with $|\lambda|^{(i)}_{\max}, i=1,2$. Note from Fig. 3 that initial $T$ values which iterate to the fixed points correspond to sets of fractal measure zero (the edges of the fractal spectrum) and hence compose only a part of the total energy spectrum.

The sequence of bands labeled $a$ in Fig. 1 belongs to the first fixed point. Thus, we expect a scaling value of $\ln 2/\ln|\lambda|^{(1)}_{\max}$. For $R=0.9$, this gives $\ln 2/\ln 4.5861 = 0.4551$. This is in excellent agreement with both Fig. 3 and with the numerical value of $k_a$ found above. The bands labeled $b$ in Fig. 1 belong to the second fixed point, and hence we expect a scaling value of $\ln 2/\ln|\lambda|^{(2)}_{\max}$. For $R=0.09$, this expression yields $\ln 2/\ln 2.0435 = 0.9699$. Again, we have excellent agreement with the numerical results. Note that the second fixed point of Eq. (10) corresponds to a two-cycle $V_2^* \to V_2^*$, $E_2^* \to -E_2^*$ in Eq. (5), accounting for the observed period-2 structure in Fig. 1.

It is interesting to note that the one-step recursion relations (10) can be cast in terms of a single two-step relation involving $T$ alone:

$$T_{n+2} = \left[R+\frac{1}{R}\right] T_{n+1}^2 + (2-T_n^2)T_{n+1} - \left[R+\frac{1}{R}\right] . \tag{13}$$

We suggest that bounded chaotic solutions to Eq. (13) may account for the uncountable set of energies in the spectrum which do not iterate to one of the fixed points listed above.

The presence of a Cantor set in the energy spectrum suggests, as in the quasiperiodic case,[11] that we have eigenstates that are intermediate between localized and extended. To study them, we consider the transfer matrix $M_k$ for the system of period $p_k = 2^k$. Then we have $M_{k+1} = AM_k^2$, where the matrix $A$ has elements $A_{11}=R$, $A_{12}=E(1-R^2)/R$, $A_{21}=0$, and $A_{22}=1/R$. $M_1$ is given by Eq. (3). From examination of this recursion relation at the fixed points, we find that (1) for the first fixed point the envelope of the wave function has power-law decay from the maximum with an exponent depending on $R$, and (2) for the second fixed point the envelope is a constant. Details will be published elsewhere.

In summary, we have investigated a simple quantum model which is a natural extension of the problem of classical diffusion in hierarchical systems. We have examined in detail the structure and scaling properties of the energy spectrum, and have been able to account analytically for the most relevant features. We have also briefly described the shape of the wave functions at the fixed points. The observed properties quite closely mimic the behavior found in quasiperiodic systems.

In closing, we should mention that after completion of this work we became aware that a related problem, that of electronic states in hierarchical heterostructures, has been recently solved.[13] It corresponds to a hierarchical distribution in the site potential energies, as opposed to the present case where the hierarchy is in the transition matrix elements. The authors find for $R<1$ a narrow band structure instead of the Cantor set uncovered in this study.

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