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# Electronic and vibrational modes on a Penrose lattice: Localized states and band structure

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We define a one-parameter family of hopping Hamiltonians with an on-site potential, for independent electrons on a two-dimensional quasiperiodic Penrose lattice. The resulting models include the vibrational modes of the lattice. This problem is then investigated numerically—exploiting the symmetries of the model including scale invariance, up to systems of 3126 sites—and for various boundary conditions. We find the following results for the density of states. (1) There is a peak of zero width at a known energy. (2) We calculate the fraction of states in this central peak, assuming point (5) below. (3) These states are strictly localized; we calculate the wave functions explicitly. (4) The remainder of the states lie in various bands separated by band gaps; this band structure is discussed in the limit of a large on-site potential. (5) There is strong numerical evidence that the energy eigenvalues do not cross, as the on-site potential strength is varied, in the thermodynamic limit.

Since the experiments of Shechtman *et al.*,[1] which seem to show some evidence for a quasicrystal in the material $Al_{0.86}Mn_{0.14}$,[2] there has been an explosion of interest in quasiperiodic structures. The theoretical understanding of these structures is usually based on the nonperiodic tiling of the two-dimensional plane first introduced by Penrose,[3] and described in the beautiful article by Gardner.[4] At the same time, the one-dimensional version of these quasiperiodic structures—the Fibonacci lattices—have been treated theoretically by Kohmoto and Banavar,[5] and others.[6–9] One can expect such structures to be the object of much theoretical and experimental activity[10] in the future, with applications then to follow. In this paper we investigate the electronic and vibrational modes of such a two-dimensional Penrose lattice.

We are aware of three other papers on the electronic or vibrational states of a Penrose lattice. These papers appeared recently and independently. The first is an investigation of Odagaki and Nguyen,[11] on both electronic and vibrational spectra, for uniform and mixed coupling strengths. The second is a recent letter by Choy,[12] on the electronic states with uniform coupling. The third is a paper by the present authors,[13] also on the electronic states with uniform coupling. The numerical results of all studies were consistent, within the accuracy of the respective sample sizes. However, there is a significant disagreement in interpretation, as emphasized in our previous paper. Both Odagaki and Nguyen, and Choy identified the central peak as a Van Hove singularity, while by explicit construction we showed the central peak to be due to a zero width band of strictly localized states.

In this present paper we extend our investigation to include a particular on-site potential in the electronic problem, proportional to the coordination number of the site. The resulting family of models includes as special cases the previous pure hopping problem studied by the authors, a vibrational lattice problem, and, in the limit of very strong on-site potential, a strictly localized electronic problem useful for classification of the states. The numerical calculations are supplemented by exact results, which help in the interpretation

The Penrose tiles are two-dimensional shapes which cover the plane completely, yet force the resulting pattern to be nonperiodic. Our Penrose lattice consists of the vertices of the tiles or sites, and the edges of the tiles or bonds. There are two canonical realizations of the tiles: either a pair of shapes called kite and dart, or a pair of flat and thin rhombuses. A transformation connects the two representations. In this investigation, we employ the rhombus pair, since then the edges, and hence the bonds, are all of the same length, which we take to be unity.

We now define a tight-binding Hamiltonian on this Penrose lattice. It is then reasonable to take the hopping matrix element to be the same for all pairs of sites connected by a bond, and zero otherwise. The hopping matrix element can be set equal to unity. This allows us to concentrate on the effects of the lattice topology alone, without the further complication of variable hopping matrix elements. In addition, we add an on-site interaction proportional to the coordination number $z$ of the site.

The corresponding time-independent Schrödinger equation for the energy eigenfunction $\Psi(\mathbf{x})$ with energy $E$ is then

$$E\Psi(\mathbf{x}) = -\sum_{\mathrm{NN}} [\Psi(\mathbf{x}') - a\Psi(\mathbf{x})] = H\Psi ,$$

where the summation is over all nearest-neighbor sites $\mathbf{x}'$ which are connected to site $\mathbf{x}$ by a bond. We ignore electron spin. If we define $z(\mathbf{x})$ to be the coordination number of site $\mathbf{x}$, then we can rewrite the Schrödinger equation as

$$E\Psi(\mathbf{x}) = -\sum_{\mathrm{NN}} \Psi(\mathbf{x}') + az(\mathbf{x})\Psi(\mathbf{x}) .$$

We note the following special cases: (1) If $a=0$, this is the previous electronic problem with a pure hopping Hamiltonian. (2) If $a=1$, then this is the problem of the vibrational modes of the Penrose lattice with springs of unit strength between sites with bonds. $\Psi(\mathbf{x})$ is the displacement of site $\mathbf{x}$, and the frequency of vibration $w$ is given by $E=w^2$. (3) If $a \approx \infty$, then $E \approx az(\mathbf{x})$, so that $E/a$ is equal to the coordination numbers $z$, with corrections of order $1/a$. The fractions of states with these energies are given by $f(z)$, the fraction of sites with coordination number $z$.

We would like to be able to make statements about the spectrum and eigenfunctions of the Hamiltonian for the single infinite Penrose lattice. However, we cannot solve this problem exactly, so we are forced to try and extrapolate the properties of the infinite lattice from a succession of larger and larger finite systems. This necessarily introduces boundary effects, whose influence we hope to minimize by a judicious extrapolation scheme. Our scheme is to take a seed, then expand the seed to ever larger lattices by the inflation or scaling transformation. From this finite lattice we cut larger and larger decagons, each decagon larger than the previous by a scale factor equal to the golden mean, $f=(\sqrt{5}+1)/2$. The decagon preserves the maximum symmetry of the lattice, while minimizing the surface to volume ratio. Since we cut all bonds crossing the decagon, this is equivalent to requiring the wave function to vanish on the surface of the decagon.

The other way in which boundary conditions may enter the problem is through the choice of initial seed for the lattice. We choose a seed which has the full dihedral $D_5$ symmetry. In these preliminary studies we are able to inflate the pattern six times, for a total lattice of 3126 sites.

One important feature of the spectrum can easily be shown. Since the lattice sites occur at the four corners of the rhombus shaped tiles, the lattice can be divided into two sublattices, say $A$ and $B$, such that the electron only hops from an $A$ site to a $B$ site, or back. We then say the lattice is bipartite. By changing the sign of the wave function on the $B$ sublattice—a unitary transformation—we change all the hopping matrix elements from 1 to $-1$. If, in addition, we change the sign of $a$, we change the sign of the Hamiltonian $H$. Thus $H(-a)$ and $-H(a)$ have the same spectrum. For the special point $a=0$, the spectrum is invariant if we reflect the energy $E$ about the origin.

Since the seed placed at the origin is invariant under the dihedral group $D_5$ about the origin, and since the inflation transformation commutes with $D_5$, our series of lattices have the full $D_5$ symmetry, as does the Hamiltonian of the electron system. The dihedral group $D_5$ includes the group of rotations by $2\pi/5$, so we may classify the states by their behavior under such a rotation. If $r$ is the eigenvalue of a rotation $R$ by an angle $2\pi/5$ counterclockwise about the origin, then since $r^5=1$, $r$ is a fifth root of unity, or $r=\exp(2\pi i n/5)$, where $n \in \{-2,-1,0,1,2\}$. This quantum number serves to label the states. The spectrum is invariant if we replace $n$ by $-n$.

Further, for the rotationally invariant state with $n=0$ we can in addition classify the states as either even or odd under reflection about one of the dihedral planes. The wave function for $n=0$, odd vanishes on all the dihedral planes. On the other hand, all wave functions vanish at the origin, except $n=0$, even. In this study we restrict ourselves to the $n=0$ sector with the wave function either even or odd; this allows much simplification and economy in the calculations. However, it is possible to take a $2\pi/5$ wedge, and apply a boundary condition equivalent to $n=\frac{5}{2}$. This we do, for it provides a bound on the $n \neq 0$ sectors.

In Fig. 1 we show the integrated density of states normalized to the total number of states, as a function of energy, for several values of the on-site potential $a$. The lattice has been inflated five times, but a larger lattice would be indistinguishable. The case $a=0$ was completely discussed in Ref. 13. The eigenvalues were found using an IMSL library routine on a Digital Equipment Corporation VAX11/785 computer. The accuracy of the calculations is much greater than the resolution of the figures used to display the results.

The first feature of these spectra that we notice is a step of uniform height at the energy $E=3a$. This step corresponds to an infinite degeneracy, which can be understood as follows. In Ref. 13 we found states with energy $E=0$, strictly localized on certain lattice configurations. All of the sites on which these wave functions are nonzero in fact have coordination number three, with the only exception being configurations which intersect the boundary. Thus these bulk states persist as eigenstates for $a \neq 0$ with energy $E=3a$. (This is not the case for the edge states, however.) Shortly, we will give an exact calculation of the fraction $N_0/N$ of such localized states.

One further feature deserves special mention. When $a=1$, the case of uniform displacement is obviously a normal mode of the vibrational problem, with frequency $w=0$ or $E=0$. For $w \approx 0$ or $E \approx 0$ we might expect that $\Psi(\mathbf{x})$ is only a slowly varying function of $\mathbf{x}$. Thus, if we write $\mathbf{x}'=\mathbf{x}+\Delta$ for $\mathbf{x}'$ a nearest neighbor of $\mathbf{x}$, with $\Delta$ a unit vector pointing from $\mathbf{x}$ to $\mathbf{x}'$, we can expand $\Psi(\mathbf{x}')$ in a Taylor expansion, so

$$\Psi(\mathbf{x}') \approx \Psi(\mathbf{x}) + \Delta_j \partial_j \Psi(\mathbf{x}) + \tfrac{1}{2} \Delta_j \Delta_k \partial_j \partial_k \Psi(\mathbf{x}) \; .$$

Then the Schrödinger equation becomes

$$E\Psi(\mathbf{x}) \approx -\tfrac{1}{2} \left[ \sum_{\mathrm{NN}} \Delta_j \Delta_k \right] \partial_j \partial_k \Psi(\mathbf{x}) - \left[ \sum_{\mathrm{NN}} \Delta_j \right] \partial_j \Psi(\mathbf{x}) \; .$$

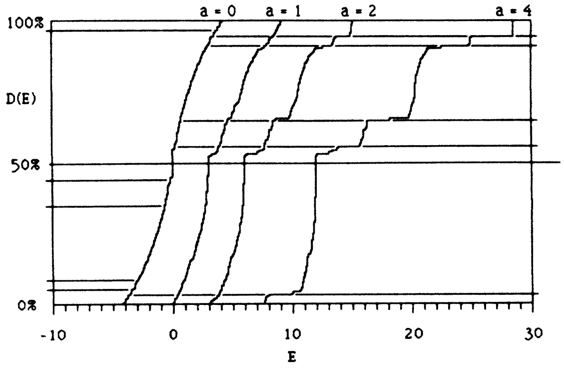

FIG. 1. The integrated density of states $D(E)$, normalized to unity, shown as a function of energy $E$ for various values of the on-site potential $a$. This is for a lattice inflated five times, with 1211 sites. The horizontal lines indicate the fraction of sites with different coordination numbers. The right-hand set of horizontal lines marks the coordination numbers for $a \to +\infty$, with $z=7$ at the top, while $z=2$ is at the bottom. The left-hand set of horizontal lines marks the coordination numbers for $a \to -\infty$, and the order of the coordination numbers is reversed from the right-hand side.

When we average the equation—permissible if all quantities are slowly varying—we find the second term on the right-hand side of the equation to be zero, by the isotropy of space, while the factor in large parentheses in the first term must be proportional to the unit tensor for the same reason. Taking the trace, the proportionality constant is found to be $\langle z \rangle /2=2$, since the average coordination number is $\langle z \rangle =4$.

Thus, we expect that for $a=1$ and small $E$ or $w^2$ the displacements or wave functions approximately obey the wave equation

$$\partial_j\partial_j\Psi(\mathbf{x})+w^2\Psi(\mathbf{x})=0 ,$$

with the velocity of sound equal to unity. By a standard calculation, we find that the integrated density of states $D(E)$ is given by

$$D(E)=E/4\pi(A/N) .$$

The quantity $A/N$ is the area per site, easily calculated to be

$$[(4f^2-1)^{1/2}+(4-f^2)^{1/2}]/2(1+f)=0.8124\ldots$$

(Ref. 13).

Thus, if the previous reasoning is correct, we should find for $a=1$ that the integrated density of states $D(E)$ approaches zero linearly as $E$ approaches zero, with slope $0.06465\ldots$. If we examine the data, as shown in Fig. 1, we see that indeed the relationship is linear for small $E$. However, the slope is closer to 0.1. The discrepancy could arise from the fact that although the wave function is slowly varying, there is still a long-range correlation with the coordination numbers $z(\mathbf{x})$, so that for these states with $E$ not strictly zero the average coordination number differs from the lattice average 4. Gaps in the spectrum are most easily seen by plotting the energies of all eigenvalues as a function of the on-site potential $a$; this is done at successive magnifications in Fig. 2, for a lattice inflated five times.

For very large absolute values of the on-site potential $a$, the wave functions become localized on individual sites with energy equal to the coordination number of the site, up to corrections of order unity. The multiplicities for energies $E\approx za$ are the numbers of sites $N(z)$ with coordination number $z$. The bulk values $f(z)=N(z)/N$ can be calculated from the inflation transformation, and we find

$$f(3)=f^{-2}+f^{-4}=7-4f\approx 0.5279\ldots ,$$

$$f(4)=f^{-5}=-8+5f\approx 0.0902\ldots ,$$

$$f(5)=f^{-3}+f^{-6}=10-6f\approx 0.2918\ldots ,$$

$$f(6)=f^{-7}=13f-21\approx 0.0344\ldots ,$$

$$f(7)=f^{-6}=13-8f\approx 0.0557\ldots .$$

These values fit very well the large $a$ data. This is most clearly seen in Fig. 3, where we plot $E/a$ as a function of $1/a$.

We can calculate corrections to these limiting values by degenerate perturbation theory, using the hopping term as a correction of order $1/a$. To first order in $1/a$ we need only consider sites of the same coordination number which are nearest neighbors. This can happen only for particular configurations of six sites consisting of a central site with coordination number $z=5$ surrounded by exactly five nearest-neighbor sites also with coordination number $z=5$. Let $N_*$ be the number of such configurations; then these particular configurations occur with frequency

$$N_*/N=f^{-6}=13-8f\approx 0.0557\ldots .$$

Explicit diagonalization of the resulting $6\times 6$ matrix gives us four states with $E/a\approx 5$, one state with $E/a\approx 5+\sqrt{5}/a$, and one state with $E/a\approx 5-\sqrt{5}/a$. These are the only corrections to $E/a$ of order $1/a$ in the thermodynamic limit. Such satellite states to the $z=5$ band are easily seen in Fig. 3.

Of course, for our finite sample, there are edge states roughly $\sqrt{N}$ in number, which deviate from the bulk properties. In Figs. 2 and 3, the band with $z=2$ and the satellite bands with $1/a$ splitting from the $z=3$ band are clear examples of edge effects, which can be explicitly calculated. Also, the data indicate a "no-crossing" rule for the bulk energy eigenvalues as the on-site potential $a$ is varied. The few levels that do cross other levels we identify as edge effects because (i) they are only $\sqrt{N}$ in number, and (ii) for large $|a|$, they can be explicitly identified with edge sites—for instance, $z=2$.

Given this conjecture, or empirical fact, of no crossing for the bulk states, we can exactly calculate the fraction $f_0=N_0/N$ of localized states with $E=3a$, as follows. The localized states have $z=3$ for all $a$. For large positive $a$, the states with lowest energy have the lowest coordination number, while for large negative $a$, the states with lowest energy have the highest coordination number. At $a=0$ the localized states exactly divide the spectrum, and thus by the no-crossing rule exactly divide the spectrum at any $a$. Thus,

$$f(3)=\tfrac{1}{2}+f_0/2 ,$$

or

$$f_0=2f(3)-1=f^{-6}=13-8f\approx 0.0557\ldots .$$

This differs slightly from our numerical estimate of Ref. 13 because of an underestimate of edge states, which are still localized but no longer degenerate for $a\neq 0$.

The no-crossing rule itself is quite interesting, for it indicates a significant difference from the periodic lattice, which in two-dimensions would exhibit band overlap and thus level crossing. In addition, the "non crossing" forces a multitude of gaps at intermediate potential $a$, labeled by the behavior at large $|a|$. For instance, the gap about the central peak of localized states for $a=0$, emphasized in Ref. 13, can be seen from Fig. 2 to be a remnant of the gap between the states with coordination numbers 3 and 4, for large $|a|$. Other structures can be similarly identified.

The important unanswered question is what is the nature of the spectrum of the Schrödinger operators—absolutely continuous, singular continuous, or pointlike. The type of spectrum uniquely determines the nature of the wave functions. An absolutely continuous spectrum

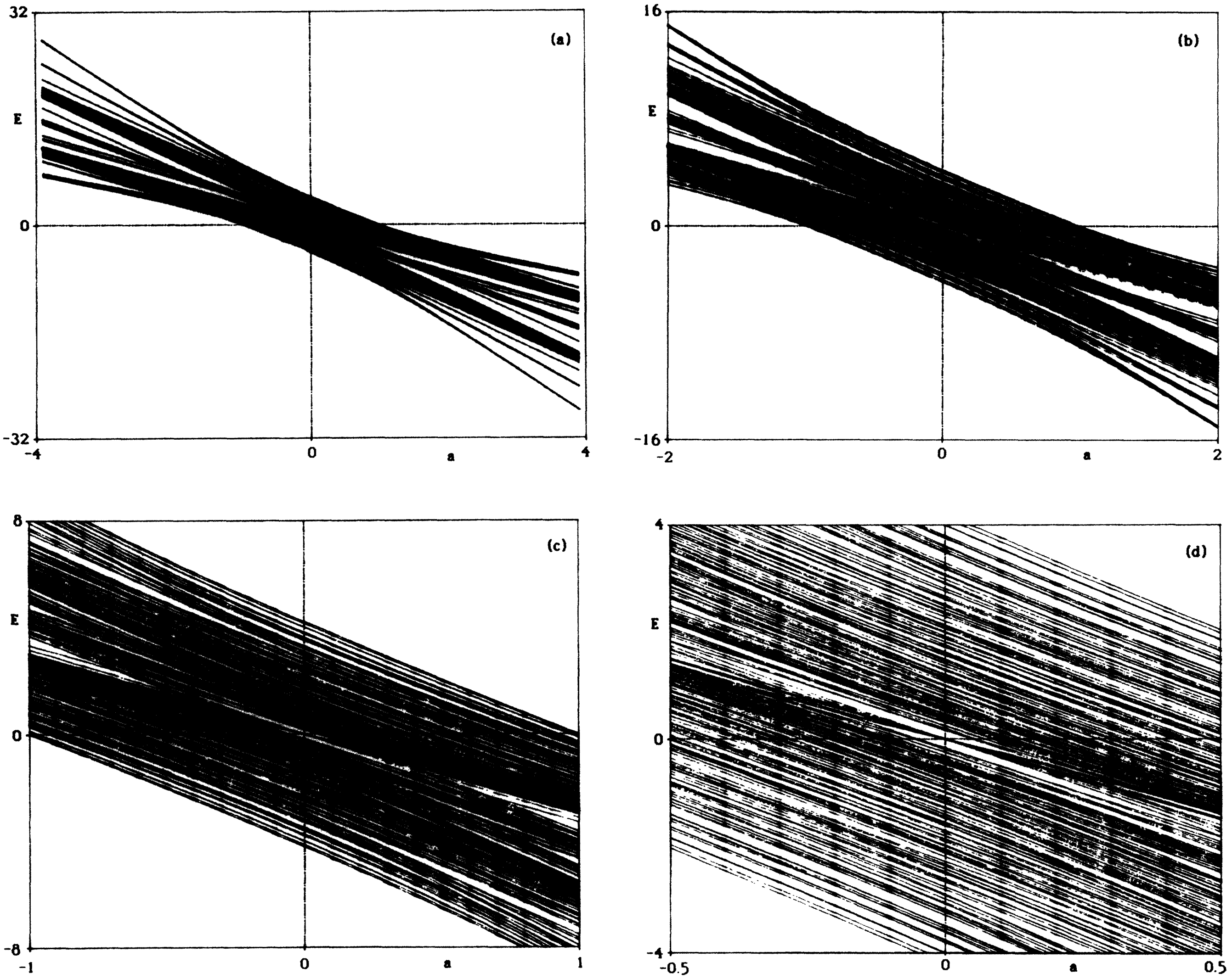

FIG. 2. Plot of the energy eigenvalues $E$ for the lattice of Fig. 1 as a function of the on-site potential $a$. In each successive figure we enlarge the plot by a factor of 2. The gaps are clearly evident in these figures.

implies extended and nonnormalizable wave functions, while a point spectrum gives localized states. The nature of states corresponding to a singular continuous spectrum has not yet been understood completely; however they should be very interesting and possibly fractal, self-similar, chaotic, etc.[5,14–16] These wave functions may be typical near the metal-insulator transition.

We have explicitly shown that the spectra for the Schrödinger operators on the Penrose lattice contain a single infinitely degenerate point. However, the present numerical analysis is not sufficient to say much about the rest of the spectra. For the one-dimensional quasiperiodic system proposed by Kohmoto *et al.*[6] and Ostlund *et al.*,[7] the spectrum has been conjectured to be purely singular continuous.[8] More recently, Delyon and Petritis[17] proved rigorously the absence of localization for a class of one-dimensional models which take a finite number of values for the potentials.

Since the present model in two dimensions also takes only a finite number of potential values, it is likely to have no localized states, except for the infinitely degenerate iso-

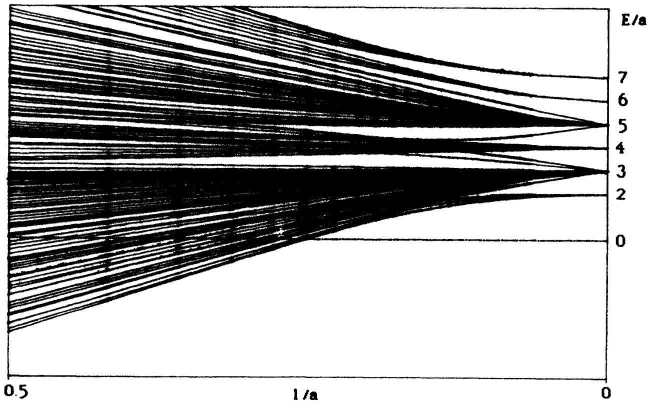

FIG. 3. Similar plot to Fig. 2. However, we instead show the energy eigenvalues divided by the on-site potential strength $a$, $E/a$, as a function of the inverse on-site potential strength $1/a$. This clearly shows the limit of large on-site potential, as discussed in the paper.

lated point. Note that states have a greater tendency to be extended—delocalized—in higher dimensions. An additional point unfavorable to localization is the existence of long-range orientational order. The rotational invariance of the Penrose lattice allows the possibility of localization only in the radial direction.

In Ref. 18, a special self-similar wave function is explicitly obtained for the electronic problem. It is likely that this type of wave function would give a singular continuous contribution to the spectrum. The important questions are as follows: How abundant is this or some other type of *critical wave function* in the spectrum? Do there exist transitions between different types of wave functions as $a$ is varied? If so, how are these transition points distributed in the spectrum? Further analytical and numerical studies are required to answer these questions, and to determine whether there are an infinite number of gaps in the energy spectrum, distributed densely—a Cantor set spectrum. Perhaps more powerful techniques to characterize spectra and wave functions will be required.

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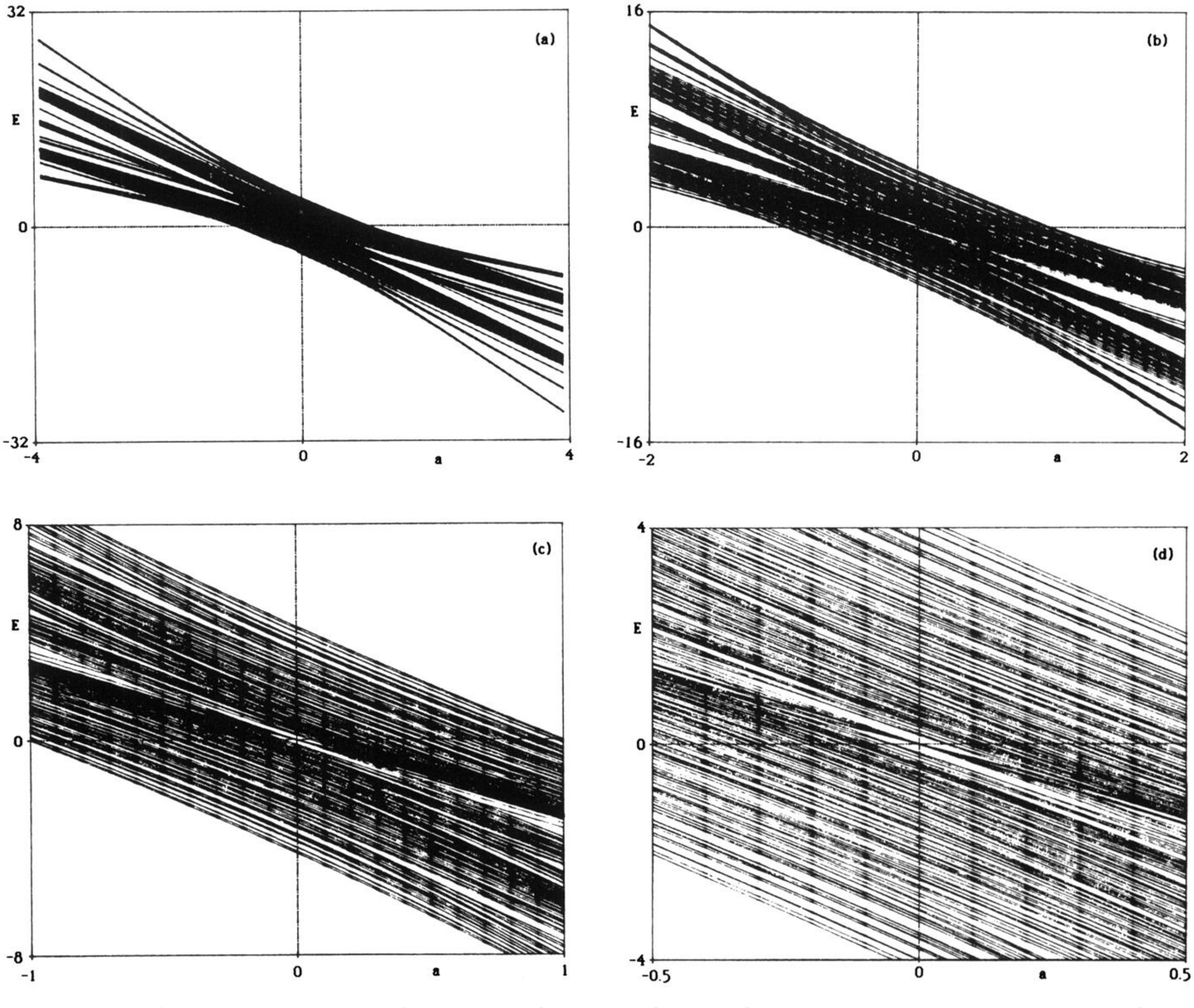

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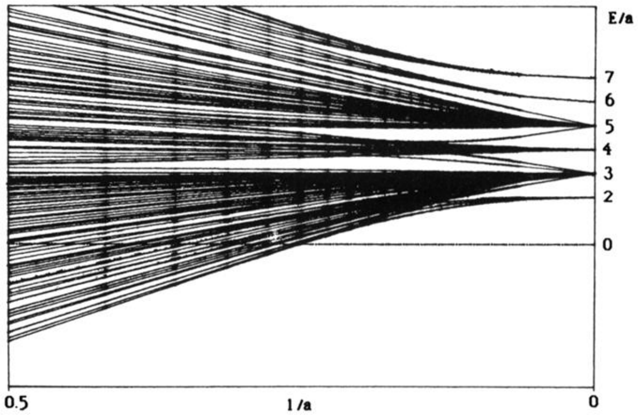

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