Electronic States on a Penrose Lattice

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We define a hopping Hamiltonian for independent electrons on a two-dimensional quasiperiodic Penrose lattice. This problem is then investigated numerically, 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 central peak of zero width at zero energy, consisting of about 10% of the total number of states. (2) These states are strictly localized; we calculate the wave functions explicitly. (3) The remainder of the states lie in two bands, symmetric about zero energy, separated from the localized states by a finite gap E_0.

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There is much current interest in quasiperiodic structures. These systems are intermediate between the completely periodic perfect crystals and the random or disordered amorphous solids. Undoubtedly, a major push for understanding was given by the experiments of Shechtman *et al.*,[1] which seem to show strong evidence for a quasicrystal in the material $Al_{0.86}Mn_{0.14}$.[2] The theoretical understanding of these structures is based on the nonperiodic tiling of the two-dimensional plane first introduced by Penrose,[3] and described in the beautiful article by Gardner.[4] The papers of de Bruijn are probably the most complete investigation in print.[5,6] The first suggestion that a Penrose tiling might serve as a model for a physical system was made by Mackay.[7,8]

At the same time, the one-dimensional version of these quasiperiodic structures—the Fibonacci lattices—has been treated theoretically by Kohmoto and Banavar[9] and others.[10–14] These investigations are very thorough, and serve as a model of what one would like to do in more dimensions; this paper is only a beginning. Recently Merlin *et al.*[15] have succeeded in growing a quasiperiodic superlattice and have carried out x-ray and Raman measurements on it.

We are aware of two other papers on the electronic states of a Penrose lattice. The first is a paper by Odagaki and Nguyen[16] and the second is a recent letter by Choy,[17] both published after this work was completed. The numerical results both of Odagaki and Nguyen and of Choy are consistent with ours, within the numerical uncertainty of the data. However, the accuracy of our calculation is much greater, so that the significant structure we find—a zero-width central peark separated by finite gaps—appears in Choy's data simply as a relatively broad central peak. And we disagree in interpretation with both of the other studies, as emphasized later in this paper. As we show, the central peak is due to a zero-width band of localized states; it is not a Van Hove singularity.

The Penrose tiles are two-dimensional shapes which tile the plane completely, yet force the resulting pattern to be nonperiodic. The patterns are neither regular nor random. 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 fat 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. Further, there is a constraint on which edges may be adjacent, so that, for instance, we are not allowed to tile the plane with a periodic pattern of thick rhombuses alone.

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. A portion of a typical such Penrose lattice is shown in Fig. 1.

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

$$E\Psi(x,y) = \sum_{nn} \Psi(x',y') = H\Psi,$$

where the summation is over all sites (x',y') which are connected to site (x,y) by a bond. We ignore electron spin.

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, and 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.

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 elec-

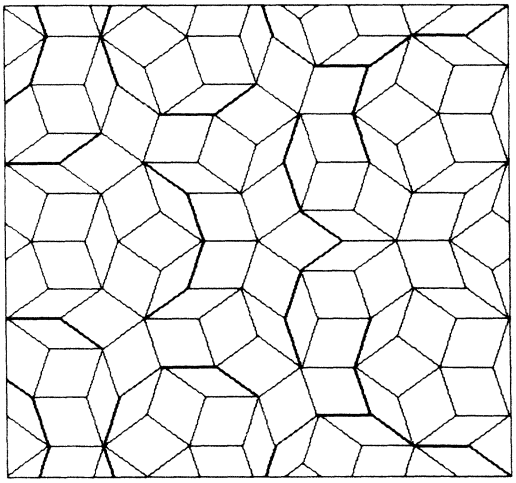

FIG. 1. A section of a Penrose lattice. The center of the pattern is the center of the figure, and the ten tiles at the center are the seed from which the pattern was grown.

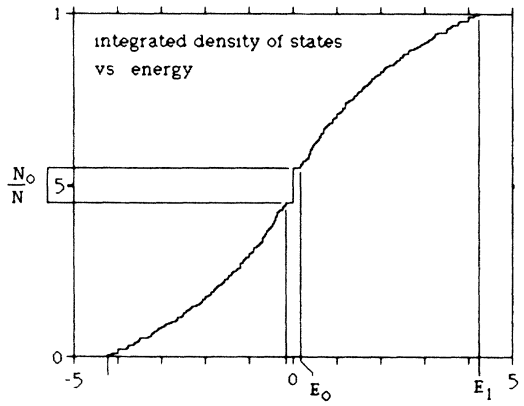

FIG. 2. The integrated density of states, normalized to unity, as a function of energy. This is for the lattice inflated five times, with 1211 lattice sites. The quantities N_0/N, E_0, and E_1 are shown here.

tron only hops from an A site to a B site, or back. We then say that the lattice is bipartite. By changing the sign of the wave function on the B sublattice—obviously a unitary transformation—we change all the hopping-matrix elements from 1 to -1, and thus change the sign of the Hamiltonian H. Thus H and $-H$ have the same spectrum, and the spectrum of our original model is invariant if we reflect the energy E about the origin. Further, by an ordering of the basis states so that first the electron is on A sites, then on B sites, the Hamiltonian reduces to an $N/2\times N/2$ block form, where N is the number of sites. The two diagonal blocks are zero, so that we need only diagonalize a matrix of half the size of the Hamiltonian.

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 that 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 $r=\exp(2\pi in/5)$, where n is an integer equal to -2, -1, 0, 1, or 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. 2, we show the integrated density of states, normalized to the total number of states, for the lattice inflated five times. These figures are for the series of lattices seeded by one of the two symmetrical seeds; the series seeded by the other would look identical, at the resolution of this figure, as would inflation six times, or the sectors with $n\neq 0$.

We note the following features of the integrated density of states: (1) There is a prominent central step at zero energy with a size becoming independent of the lattice size, corresponding to a nonzero degeneracy proportional to the crystal size in the thermodynamic limit. We denote the step height by the ratio N_0/N, with N_0 the number of zero-energy states, and N the total number of states. (Remember, we are working only in the $n=0$ sector; however, in the thermodynamic limit, the ratio for the total states becomes the same.) These zero-energy states will be explained at length in the next section. (2) There is a sharp cutoff at a maximum and minimum energy $\pm E_1$; this reflects a certain most probable coordination number as explained in the next paragraph. (3) There is a gap in the density of states of width $2E_0$, centered on the central peak. (4) There may be further gaps or structure in the spectrum, particularly near $\pm E_1$, but the numerical calculations are not able to eliminate the possibility that these might be simply finite-size effects. These conclusions, of course, would not necessarily hold, however, if we were to have non-uniform hopping matrix elements.

We may estimate and understand the maximum energy as follows. The variational principle easily supplies us with a lower bound for E_1. For instance, if we take as a trial wave function one which is uniform,

then we obtain $E_1 \geq \langle z \rangle$, where $\langle z \rangle$ is the average coordinate number, equal to four since our lattice has N sites and $2N$ bonds. Better yet, the wave function for each of our finite lattices can serve as a trial function for the infinite lattice, so that our sequence of numerical calculations on larger and larger finite lattices increases monotonically to the infinite value E_1.

From finite-sized scaling, we estimate these various parameters of the spectrum to be

$$N_0/N = 0.09 \pm 0.01, \quad E_0 = 0.163 \pm 0.007,$$

$$E_1 = 4.236 \pm 0.002.$$

These are the values estimated for the infinite lattice, including all sectors. In addition, for a large but finite lattice, inflated s times, we find the results for E_1 well fitted by the formula

$$E_1 \approx f^3 - f^{-2(s-1)} + \ldots, \quad f = (\sqrt{5}+1)/2.$$

Other structure in the integrated density of states might be finite-size effects, so that the curve may become smooth as the lattice becomes larger.

We now concentrate our attention on the highly degenerate zero-energy eigenstates. We will show that this is a strict degeneracy, proportional to the total number of states, and thus to the size of the lattice. Further, we claim that these electronic states are strictly localized in that the wave function is zero outside of a finite region, and their existence and location depend only upon the local lattice topology.

As we increase the lattice size, the first occurrence of a zero-energy eigenstate is after the first inflation. We show these lattices in Figs. 3(a) and 3(b). We claim that the zero-energy eigenstate is nonzero only on the ring of ten sites about the origin, shown by the dark circles in each of the figures. On these ten sites, the wave function has a constant amplitude, but alternates signs, as we go around the ring. Then the wave function cancels in pairs on neighboring sites, and thus obeys the Schrödinger equation.

To be more specific, we verify that this wave function is an eigenstate as follows: If we number the sites clockwise around the ring by the integer n, then the wave function can be taken to be $(-1)^n$. An electron on a dark ring site n can hop off the ring to a nearby site not on the ring. From there it can hop back to exactly one other ring site, which is at either $n+1$ or $n-1$. However, the wave function on this neighboring ring site is exactly out of phase with the wave function on the original ring site. Hence, in the discrete Schrödinger equation we have a cancellation, and thus the wave function is an eigenfunction with zero energy.

As we enlarge the lattice size, this particular configuration remains unchanged with its own unique local topology, and thus it remains an eigenstate for all larger lattices. Since the wave function is nonzero only within a region of radius R, we take this to be the radius of the localized state.

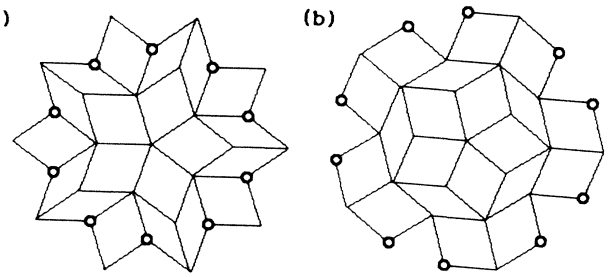

FIG. 3. (a),(b) The first occurrence of a localized state in the two symmetrical lattices. The seeds have been inflated once. The localized states vanish everywhere except on the ten sites shown by heavy circles. These states persist in the infinite lattice, at all regions with the same local structure.

It is a theorem for Penrose lattices, quoted in the article of Gardner and originally due to Conway, that if we start at a point in the Penrose lattice with a local configuration of diameter D, then we can always find the identical configuration within a distance $2D$, and usually we need only go to a distance D. This theorem insures that in the infinite Penrose lattice, our localized or bound states are distributed with a finite, nonzero density inversely proportional to their area, or proportional to $1/R^2$. (The proportionality constant does depend upon the particular configuration.) Further, since most bound states will not include the origin, they will show up with equal strength in each of the n sectors, not just the $n=0$ sector we have numerically investigated.

Finally, it can be shown that when we inflate a configuration supporting a bound state, we obtain an inflated configuration, also supporting a bound state, with a radius equal to the golden mean f times the original radius R. Thus the bound states occur in families with radii $R_n = f^n R_0$. We now estimate the proportion of localized to total states as follows. Let us assume that the theorem quoted gives an estimate of the density of a given configuration to be of the order

$$[2 \times (\text{area of configuration})]^{-1} = 1/2\pi R^2.$$

Then for a family of bound states we have

$$N_0/N \approx \sum_n (\text{area per site})/2\pi R_n^2.$$

The area per site is simply the average area per tile, and since fat and thin rhombuses are in the ratio of the golden mean, this is easily calculated to be 0.8124. This gives us, for our estimate,

$$N_0/N \approx (0.8124/2\pi R_0^2) \sum_n f^{2n} = (0.8124/2\pi R_0^2) f^2/(f^2-1).$$

Taking $R_0 \approx f$, we obtain the crude estimate $N_0/N \approx 0.08$.

We make the following further remarks about the bound states: (1) As radius of the localized state becomes large, the states become one dimensional in the limit of infinite radius. In fact, we can grow configurations which support one-dimensional states by starting with another seed—the so-called king. This is the tiling shown on the cover of Scientific American, and Gardner calls the configurations supporting these one-dimensional states "worms." These one-dimensional states have the Fibonacci structure, and are thus treated by the method of Kohmoto and Banavar.[9] (2) The peak in the density of states due to these localized states is a strict delta function. It is evidently this peak which was mistakenly identified tentatively as a Van Hove singularity in the papers of Odagaki and Nguyen and of Choy. (3) The existence of these localized states is not directly a consequence of the quasiperiodicity of the lattice. They also occur in certain examples of periodic lattices,[18] amorphous solids,[19] and quantum percolation.[20,21] (4) The finite-size behavior for the quantity N_0/N is complicated by the competing threshold and boundary effects. (5) Qualitatively, the gap E_0 in the spectrum is due to the depletion of states into the central peak.

We add that since the paper was submitted, we have been able to make an exact calculation of the fraction of localized states in the thermodynamic limit, and find that $N_0/N = 13 - 8f = 0.0557\ldots$. Also, we have added an on-site potential proportional to the coordination number, and find that the localized states persist. Further, this model allows us to identify some additional structure in the spectrum.[22]

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