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Comparison of electronic properties of quasiperiodic and periodic lattices in two and three dimensions

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The density of states (DOS) in two- and three-dimensional Penrose lattices with sites at vertices of rhombi were calculated in a one-orbital, tight-binding model. The DOS for the two-dimensional model showed much fine structure, indicative of the multitude of gaps thought to exist in quasicrystal spectra. The three-dimensional model showed a much smoother DOS, whose bumps were well matched by those for a periodic Penrose-derived lattice. In all cases, all states were quite delocalized. I conclude that the gross electronic properties of quasilattices are little influenced by their quasiperiodic nature, especially in three dimensions.

I. INTRODUCTION

Quasicrystals have suddenly become of much interest to many investigators, now that some have been found in real samples.[1-3] Much work has been done on their structural properties, but comparitively little on electronics. One-dimensional calculations confirm the intuition that the infinitely dense set of diffraction spots exhibited by quasicrystals gives rise to an equally dense set of energy gaps.[4] What experiments have been done have shown properties very like those of amorphous metals, with no hint of the interesting properties one might think a substance with an infinitely dense set of energy gaps might have. What does quasiperiodic order do to the electronic spectrum in two and three dimensions? In this paper, I report on calculations done on the simplest possible quasiperiodic models, using the simplest method—one-orbital tight binding. These calculations show some of the phenomena expected.

II. METHODS

The lattices used are of the type examined by Elser,[5] in which the basic units are rhombi or rhombohedra, depending on dimension. The lattices were generated using Elser's projection method. Sites were placed at the vertices of the units, and hopping matrix elements assigned to pairs of sites connected by edges. The projection method allows the convenient construction of periodic Penrose-like lattices, built from the same rhombic units as the original. These lattices were natural choices for reference crystalline lattices, and were so used in the calculations. To rule out systematic errors, the same procedures were used for the crystals as for the Penrose lattices, so no advantage was taken of the periodicity of the crystalline case. In two dimensions, the crystalline pattern used was the one pointed out by Elser and Henley[6] as the basis for Al_3Fe. In three dimensions, one can construct a series of cubic lattices by replacing the icosahedral basis set $\{1, \pm\tau, 0\}_{\text{c.p.}}$ with $\{F_n, \pm F_{n+1}, 0\}_{\text{c.p.}}$ where τ is the golden ratio, F_n is the nth Fibbonacci number, and c.p. stands for cyclic permutation. I used as a reference the case where $F_n = 2$, $F_{n+1} = 3$.

The calculations were done on finite excerpts from the lattices described above, terminated with Bethe lattices, as has been done for amorphous semiconductors.[7] The samples contained about 2000 points.

The Hamiltonian is just

$$H = \sum_{i,j} - |i\rangle T_{ij} \langle j| \ , \tag{1}$$

where T_{ij} is 1 for sites joined by edges, and 0 otherwise. The Green's function is formed by adding terms corresponding to the Bethe lattice terminations[7] and inverting the resulting complex $N \times N$ matrix, with N the number of sites. The imaginary part of the diagonal elements gives the local density of states (DOS), and the square of the matrix yields the participation ratio, defined as

$$p(E) = N \frac{\sum_{i=1}^{N} \langle |\psi_i^4| \rangle}{\sum_{i=1}^{N} \langle |\psi_i^2| \rangle^2} \ . \tag{2}$$

This ratio is 1 for a completely delocalized state, and N for a state localized only on one site.

The complex matrices were inverted using the sparse matrix algorithms contained in the AT&T Bell Laboratories PORT-III package. The calculations were done on a VAX 11/780, and consumed several hours of CPU for a 2000-site lattice with 50 values of energy.

III. RESULTS

The DOS for the two-dimensional Penrose tiling, averaged over the inner 1000 sites (out of 2000) is shown in Fig. 1 as the solid line. This DOS is much like that obtained by other workers.[8] The corresponding crystalline DOS is shown in Fig. 1 as the dotted curve. Note the spikiness of the Penrose DOS. Such fine structure in the DOS is consistent with the presence of many gaps. The participation ratio is shown in Fig. 2. Note that only the states of lowest energy have participation ratios significantly different from 1. In both these figures, the energy scale also goes to negative values, but the presence of only even paths in the lattice guarantees that all functions of energy are even, so only the $E > 0$ half is shown.

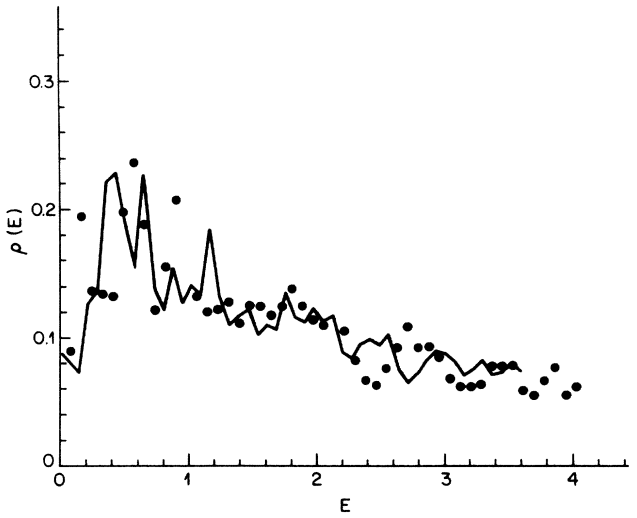

FIG. 1. DOS for periodic (dotted) and quasiperiodic (solid) lattices in two dimensions, averaged over central 1000 sites out of 2000.

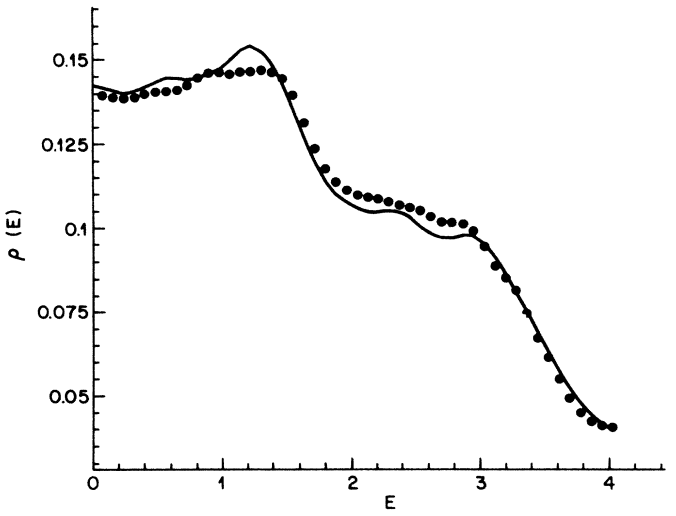

FIG. 3. DOS for periodic (dotted) and quasiperiodic (solid) lattices in 3D, averaged over central 1000 sites out of 2000.

The DOS for the three-dimensional (3D) tilings are shown in Fig. 3. Here, the match between the crystal and the Penrose samples is very close, and the DOS is quite smooth, presumably because there are so many possible gaps in 3D that they all average out. The participation ratio is shown in Fig. 4 for the Penrose lattice, and again, all values are very close to 1. This result shows that in each state, an electron has roughly equal probability of appearing on any site, so there are no bottlenecks through which electric current must pass.

IV. DISCUSSION

We see that the DOS for the 3D problem is almost featureless, as if the model had been amorphous, rather than Penrose. Any interesting structure must be at a level more subtle than the DOS. While the calculation does not have anything to say directly about transport properties, the fact that all the states seem to be delocalized would suggest that the properties of the Penrose lattice are not much different than those of an ordered lattice, which also has delocalized states.

There is evidence that icosahedral Al-Mn-Si is built around the same structural units as the so-called α phase of Al-Mn-Si.[9] If so, then the obvious prediction is that the icosahedral and α phases should have comparable resistivities.

The results indicate that for three dimensions, any "strangeness" about the electronic properties of quasicrystals will only be seen by probes sensitive to the direction of the electron momentum. Most such probes will have to wait for the availability of single-domain specimens. In two dimensions, features should still be visible in the DOS. Perhaps the properties of the T-phase will prove interesting.

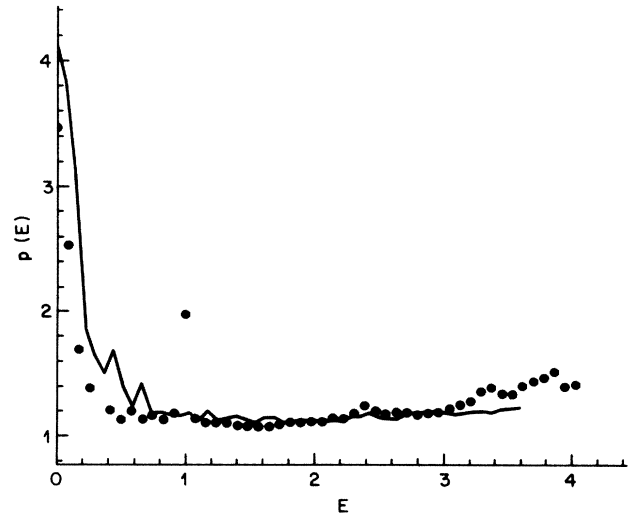

FIG. 2. Participation ratio for 2D lattices, as in Fig. 1.

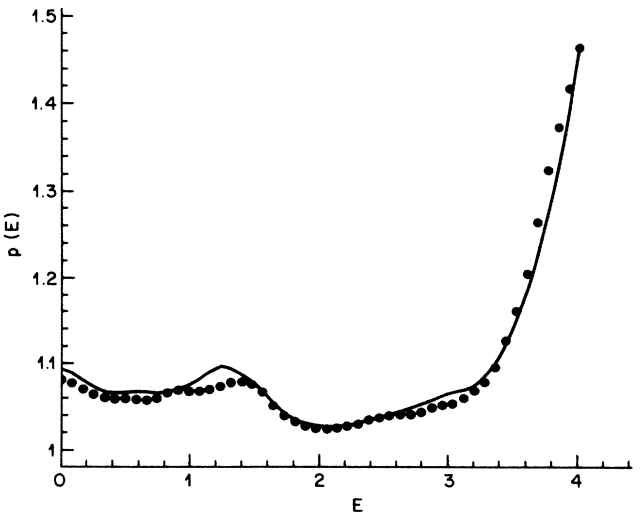

FIG. 4. Participation ratio corresponding to Fig. 3.

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