Tight-Binding Electrons on a Penrose Quasiperiodic Lattice: Deflation Construction, Density of States, and Confined States

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Abstract

Quasiperiodic lattices such as the Penrose tiling provide a minimal setting to study electronic states in systems with long-range order but without translational periodicity. In this note I summarize my numerical solution of the tight-binding model on a finite Penrose lattice patch constructed by the deflation method. The lattice is generated from a rhombus tiling following self-similar transformation rules, and its bipartite structure is identified using a breadth-first-search (BFS) coloring. I then define a nearest-neighbor tight-binding Hamiltonian with zero on-site energy and unit hopping on the Penrose graph, construct the corresponding Hamiltonian matrix and diagonalize it using `numpy`. From the eigenvalues I compute the density of states (DOS) and integrated density of states (IDOS), and I analyze the probability density of eigenstates near zero energy. The results show a macroscopic number of zero-energy states and spatially confined wave functions, in close correspondence with the "confined states" and the δ-peak at $E = 0$ reported in previous studies of the Penrose lattice.[1, 2, 3]

1 Introduction

1.1 Periodic crystals and quasiperiodic order

In a conventional crystal, atoms are arranged on a lattice that is *periodic* in space: there exists a set of primitive translation vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ such that the atomic configuration is invariant under integer linear combinations of these vectors. This translational symmetry underlies Bloch's theorem and the usual band-theory description of electrons, where energies $E_n(\mathbf{k})$ are labeled by a band index n and a quasimomentum $\mathbf{k}$ in the Brillouin zone.

For a long time, long-range order was believed to be synonymous with periodicity, and the classical definition of a crystal explicitly required a periodic repetition of a unit cell. This picture was challenged by the discovery of quasicrystals: metallic alloys exhibiting sharp diffraction patterns with, for example, icosahedral or fivefold rotational symmetry, which are incompatible with a periodic Bravais lattice.[4] The seminal work of Shechtman *et al.* showed that solids can display long-range orientational order and essentially discrete diffraction diagrams without translational periodicity, leading to the modern definition of a crystal as any solid with an essentially discrete diffraction pattern.

1.2 Quasicrystals and model quasiperiodic lattices

Mathematically, quasiperiodic structures can be constructed in several ways. Important examples include:

- The one-dimensional Fibonacci chain, obtained by substituting two spacings (*short* and *long*) according to a substitution rule and related to the golden ratio $\varphi = (1+\sqrt{5})/2$.
- The two-dimensional Ammann–Beenker tiling with eightfold rotational symmetry, generated by rhombi related to the silver ratio.
- The two-dimensional Penrose tiling, a non-periodic tiling of the plane using two rhombi ("fat" and "thin") that exhibits local fivefold rotational symmetry and long-range order.[5]

In these systems the underlying geometry is neither periodic nor random. Distances and coordination numbers obey deterministic rules, often involving algebraic irrationals such as the golden ratio. The Penrose tiling is particularly important as a minimal two-dimensional model of a quasiperiodic lattice: it has been used as a toy model for quasicrystals and exhibits many striking features, such as self-similarity under inflation/deflation and a non-trivial distribution of local environments.

1.3 Electronic states on the Penrose lattice: previous work

Electronic properties of tight-binding models on quasiperiodic lattices have been extensively studied in one dimension (e.g., the Fibonacci chain) and in two dimensions on Penrose and related tilings. For the Penrose lattice, Kohmoto and Sutherland considered a tight-binding Hamiltonian on the *vertex model*, where atomic orbitals live on the vertices of the rhombi and electrons hop along edges with a uniform hopping amplitude.[1] They constructed finite Penrose clusters with fivefold symmetry and numerically computed the spectrum and DOS for systems with a few thousand sites. Two key results from this work are:

- The DOS contains a *central peak of zero width* at zero energy, which corresponds to a macroscopically degenerate band of states.
- The remaining spectrum is split into two bands symmetric about $E = 0$ and separated from the zero-energy states by a finite energy gap.

Arai *et al.* analyzed these zero-energy states in more detail for the vertex model on the Penrose lattice.[2] They introduced the concept of "confined states" — eigenstates at $E = 0$ whose amplitudes are strictly localized in finite spatial regions without exponential tails — and "forbidden sites", which are vertices where every zero-energy eigenstate has vanishing amplitude. By exploiting the inflation/deflation structure of strings of rhombi, they showed that the Penrose lattice can be partitioned into finite clusters separated by lines of forbidden sites, and all zero-energy eigenstates are confined within such clusters. They also estimated the fraction of confined states in the thermodynamic limit.

More recently, Koga and Tsunetsugu studied the Hubbard model on the Penrose vertex lattice.[3] In the non-interacting limit their DOS reproduces a δ-function peak at $E = 0$ with a finite gap to the continuum bands, and they showed that all confined states lie at the Fermi energy for half-filling. Turning on an infinitesimally small on-site repulsion U lifts the macroscopic degeneracy and produces an antiferromagnetic ground state whose structure is dictated by the distribution of confined states.

1.4 Aim of this work

In this note I present my own numerical solution of the non-interacting tight-binding model on a Penrose lattice, focusing on:

- The explicit construction of a finite Penrose cluster using the *deflation method*, following self-similar edge transformation rules.[6]
- The formulation of the tight-binding Hamiltonian on the resulting graph, with on-site energy set to zero and hopping amplitude $t = 1$ along edges.
- The computation of the DOS and IDOS from the full spectrum obtained by direct diagonalization using `numpy`.
- The structure of zero-energy eigenstates and their interpretation in terms of confined states and forbidden regions.[2, 3]

My implementation is contained in the repository `achmadj/HU`, and this note provides a research-style explanation of the underlying methods and physical interpretation of the numerical results.

2 Methodology

2.1 Construction of a Penrose lattice via the deflation method

2.1.1 Penrose rhombus tiling and golden ratio scaling

The Penrose lattice can be realized as a tiling of the plane by two types of rhombus tiles with equal edge length:

- A *fat* rhombus with acute angle 72° and obtuse angle 108°.
- A *thin* rhombus with acute angle 36° and obtuse angle 144°.

The tiling is subject to local matching rules, which are conveniently encoded by decorating the edges with arrows (single or double) and requiring that neighboring tiles match arrow directions.[5] The vertices of the tiles form the sites of the Penrose lattice, and the edges become the bonds along which electrons can hop in the tight-binding model.

A particularly convenient way to generate large Penrose clusters numerically is the *deflation method.*[6] Instead of inflating small tiles into larger ones, we recursively apply a self-similar transformation that replaces each edge (or each tile) by a small cluster of edges and vertices scaled by the inverse golden ratio. For the rhombus Penrose tiling the characteristic scale factor is the golden ratio

$$\varphi = \frac{1 + \sqrt{5}}{2}\,, \tag{1}$$

and one deflation step reduces the edge length by a factor φ^{-1}. After each step, we rescale all coordinates by φ so that the shortest edge length remains normalized to unity.

2.1.2 Edge-based deflation rule

Following Inoue's summary of the deflation method,[6] the transformation can be reduced to an operation on a single oriented edge. Consider an edge with starting vertex i and ending vertex j, with position vectors $\mathbf{r}_i, \mathbf{r}_j \in \mathbb{R}^2$ and edge vector

$$\mathbf{e}_{ij} = \mathbf{r}_j - \mathbf{r}_i \,. \tag{2}$$

Introduce the rotation matrix

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \tag{3}$$

and the golden ratio φ defined above. For each edge we generate five new vertices k, l, m, g, h whose positions are given schematically by

$$\mathbf{r}_k = \mathbf{r}_j - \varphi^{-1}\mathbf{e}_{ij}, \tag{4a}$$
$$\mathbf{r}_l = \mathbf{r}_i + \varphi^{-1}R(-72^\circ)\mathbf{e}_{ij}, \tag{4b}$$
$$\mathbf{r}_m = \mathbf{r}_i + \varphi^{-1}R(+72^\circ)\mathbf{e}_{ij}, \tag{4c}$$
$$\mathbf{r}_g = \mathbf{r}_i + \varphi^{-1}R(-36^\circ)\mathbf{e}_{ij}, \tag{4d}$$
$$\mathbf{r}_h = \mathbf{r}_i + \varphi^{-1}R(+36^\circ)\mathbf{e}_{ij}. \tag{4e}$$

These new vertices are then connected by a prescribed pattern of edges (which depends on whether the original edge carries a single or double arrow) so that fat and thin rhombi are generated at the smaller scale. The arrow type of each new edge is assigned according to the Penrose matching rules.

In practice, the implementation proceeds as follows:

1. Store the current lattice as:
   - A dictionary of vertices $\{\mathbf{r}_i\}_{i=1}^{N} \subset \mathbb{R}^2$.
   - A dictionary of directed edges $(i, j) \mapsto$ `arrow_type` $\in \{1, 2\}$, where 1 and 2 denote single and double arrows.
2. For each directed edge (i, j):
   (a) Compute $\mathbf{e}_{ij}$ and the new vertex positions $\mathbf{r}_k, \mathbf{r}_l, \mathbf{r}_m, \mathbf{r}_g, \mathbf{r}_h$.
   (b) Insert these vertices into the vertex dictionary. If a newly generated vertex lies within a numerical tolerance of an existing vertex, merge them to avoid duplicates.
   (c) Add the corresponding new edges between i, j, k, l, m, g, h with the appropriate arrow types, according to the deflation rule for a single or double arrow.
3. Replace the old edge set by the new one and rescale all coordinates $\mathbf{r}_i \leftarrow \varphi\,\mathbf{r}_i$ so that the shortest bond length remains of order one.
4. Repeat the procedure for the desired number of deflation steps.

The growth of the Penrose cluster through repeated deflation steps is illustrated in Fig. 1. Starting from a small seed, each iteration increases the number of vertices and reveals the self-similar fivefold structure of the tiling.

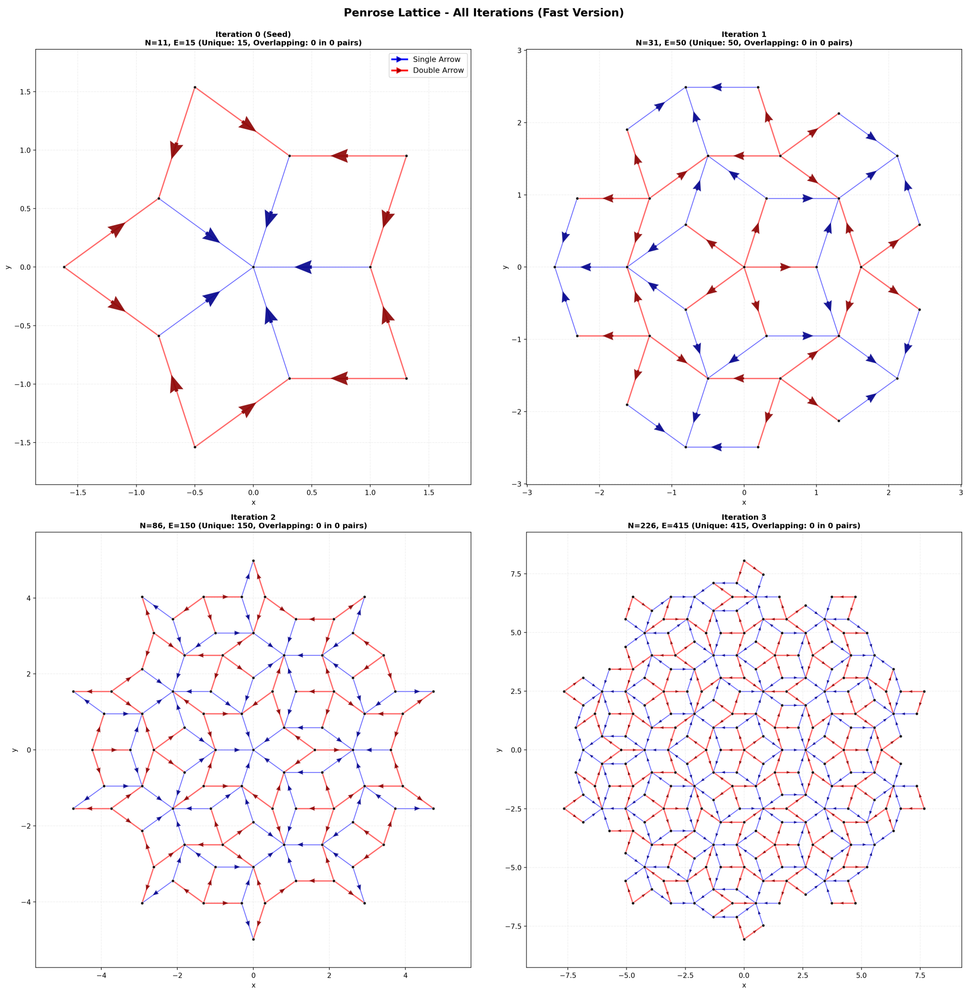

Figure 1: Penrose clusters after successive deflation iterations, from the initial small seed to larger patches with approximate fivefold symmetry. Each iteration adds new vertices and edges according to the deflation rules, and the overall shape approaches a roughly circular quasiperiodic cluster.

2.1.3 Graph structure and bipartite coloring

Once the deflation process is complete, I discard the arrow information and keep only the *undirected* adjacency structure of the graph: two vertices i and j are considered nearest neighbors if they are connected by at least one edge in the tiling. This yields a simple graph $G = (V, E)$ with

- Vertex set $V = \{1, 2, \dots, N\}$,
- Edge set $E = \{\{i, j\} \mid i, j \in V,\ i \neq j,\ \text{edge between } i, j\}$.

An important property of the Penrose vertex model is that the graph is *bipartite*: vertices can be divided into two sublattices A and B such that all edges connect an A site to a B site, and there are no edges within A or within B.[1] To verify this and to assign a sublattice label to each vertex, I use a breadth-first-search (BFS) coloring algorithm: starting from an arbitrary site, I color it "A", then color all its neighbors "B", all neighbors of those as "A", and so on. If a conflict ever appears (an edge connecting two sites of the same color) the graph would not be bipartite, but for a correctly generated Penrose tiling this does not happen.

Figure 2 shows the result of the BFS bipartite coloring for the first iteration cluster: sites on the two sublattices are clearly separated and every bond connects a red site to a blue site. This bipartite structure implies that the tight-binding spectrum will be symmetric around $E = 0$, as discussed in Sec. 3.

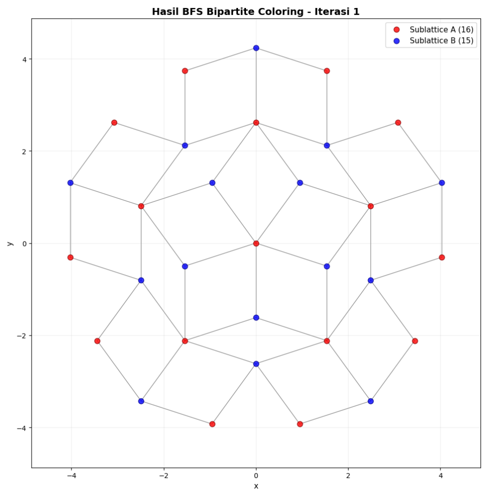

Figure 2: BFS bipartite coloring for the first Penrose iteration (see also the code-generated image `bipartite_coloring.png`). Red and blue dots represent the two sublattices, and each gray bond connects opposite colors, confirming that the Penrose vertex graph is bipartite.

2.2 Tight-binding model on the Penrose lattice

In the single-particle (first-quantized) picture, a state of an electron on the Penrose lattice is described by a complex column vector

$$\boldsymbol{\psi} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}, \tag{5}$$

where ψ_i is the probability amplitude on site i and N is the total number of vertices in the Penrose cluster. The tight-binding Hamiltonian acts on $\boldsymbol{\psi}$ through the eigenvalue equation

$$H\boldsymbol{\psi} = E\boldsymbol{\psi}, \tag{6}$$

with H represented in the site basis $\{|i\rangle\}$ by the $N \times N$ matrix

$$H = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ t_{21} & t_{22} & \cdots & t_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ t_{N1} & t_{N2} & \cdots & t_{NN} \end{pmatrix}. \tag{7}$$

For the model used in this work, the matrix elements t_{ij} are defined by

$$t_{ij} = \begin{cases} 0, & i = j \quad \text{(on-site energy set to zero)}, \\ -1, & i \neq j \text{ and sites } i, j \text{ are nearest neighbours}, \\ 0, & \text{otherwise}. \end{cases} \tag{8}$$

In practice, I construct the matrix H directly from the edge list of the Penrose graph: after assigning site indices $i = 1, \ldots, N$, every undirected edge $\{i, j\}$ is translated into the pair of entries $t_{ij} = t_{ji} = -1$, while all diagonal elements t_{ii} and all non-neighbour pairs remain zero. The resulting Hermitian matrix H is diagonalized using `numpy.linalg.eigh`, which yields the complete set of eigenvalues $\{E_n\}$ and normalized eigenvectors $\{\boldsymbol{\psi}^{(n)}\}$. These are then used to compute the density of states, integrated density of states, and real- space probability densities discussed in Sec. 3. Because the underlying graph is bipartite (Sec. 2.1), the spectrum of H is symmetric about $E = 0$.[1]

2.3 Density of states and integrated density of states

Given the discrete spectrum $\{E_n\}_{n=1}^{N}$ of a finite system, the *density of states* (DOS) is formally defined as

$$\rho(E) = \frac{1}{N} \sum_{n=1}^{N} \delta(E - E_n), \tag{9}$$

where δ is the Dirac delta function. The DOS gives the number of single-particle states per site and per unit energy.

The *integrated density of states* (IDOS) is

$$N_0(E) = \int_{-\infty}^{E} \rho(E')\, \mathrm{d}E' = \frac{1}{N} \sum_{n=1}^{N} \Theta(E - E_n), \tag{10}$$

where Θ is the Heaviside step function. By construction, $N_0(E)/N \in [0, 1]$ is the fraction of single-particle states with energy less than or equal to E. The DOS and IDOS are related by

$$\rho(E) = \frac{\mathrm{d}}{\mathrm{d}E}\left[\frac{N_0(E)}{N}\right]. \tag{11}$$

In numerical calculations on a finite system, the delta functions in Eq. (9) are approximated by narrow Gaussians of width σ, and the DOS is evaluated on a grid of energy points. The IDOS $N_0(E)/N$ can then be obtained either by integrating the smoothed DOS or, more accurately, by directly counting the fraction of eigenvalues E_n that satisfy $E_n \leq E$ for each value of E.

3 Results and discussion

3.1 Energy spectrum and density of states

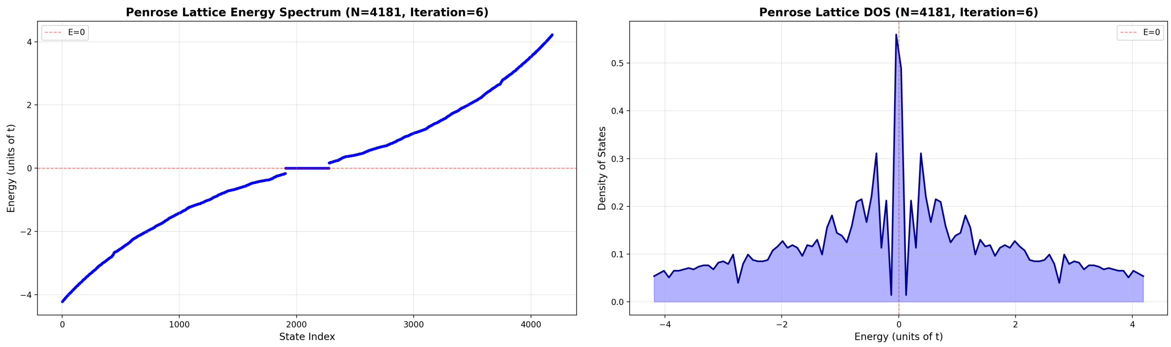

Figure 3: (Left) Single-particle energy spectrum of the tight-binding model on a finite Penrose cluster, showing symmetry around $E = 0$ and a macroscopic number of eigenvalues near zero energy. (Right) Smoothed density of states $\rho(E)$ obtained by Gaussian broadening of the eigenvalues. The sharp central peak at $E = 0$ and the two side bands are characteristic of the Penrose vertex model and agree qualitatively with previous results.[1, 3]

For Penrose clusters generated by four or five deflation steps I obtain spectra that are symmetric about $E = 0$, as expected from the bipartite structure of the lattice.[1] Several characteristic features are observed:

- The spectrum is bounded within a finite energy range $[-E_{\max}, E_{\max}]$ with $E_{\max}$ of order 4 for $t = 1$.
- There is a large accumulation of eigenvalues around $E = 0$; many eigenvalues are numerically indistinguishable from zero within machine precision.
- Away from $E = 0$, the eigenvalues fill two broad bands (one around negative energies and one around positive energies), separated from the zero-energy states by a gap of finite width, in agreement with earlier calculations on the Penrose vertex model.[1, 3]

The smoothed DOS $\rho(E)$ shows two broad bands symmetric about $E = 0$ and a very sharp central peak at $E = 0$. In the infinite-size limit this central peak corresponds to a δ-function of weight p_{conf}, the fraction of states at exactly zero energy.[2, 3] Figure 3 presents my numerical energy spectrum and DOS for a representative Penrose cluster; the overall shape, including the sharp peak at $E = 0$ and the gap separating it from the continuum, follows closely the results reported in Refs. [1, 3].

Physically, the presence of a δ-like central peak implies that the non-interacting system has a macroscopically degenerate manifold of single-particle states at $E = 0$. At half-filling, this corresponds to a highly degenerate ground state, which is known to be lifted by even infinitesimal electron–electron interactions such as a Hubbard repulsion.[3]

3.2 Integrated density of states

The IDOS $N_0(E)/N$ provides a complementary view of the spectrum. For the Penrose tight-binding model, my numerical IDOS exhibits the following features:

- For $E \ll 0$, $N_0(E)/N$ is close to 0 and increases monotonically as E enters the lower band.
- As E approaches 0 from below, $N_0(E)/N$ rises through a sequence of small steps (due to the quasi-discrete band structure).
- At $E = 0$, there is a *macroscopic jump* in the IDOS: all states at exactly zero energy contribute simultaneously, increasing $N_0(E)/N$ by approximately the fraction of confined states p_{conf}.[2]
- For $E > 0$, $N_0(E)/N$ continues to increase through the upper band and saturates to 1 as E exceeds the maximum eigenvalue.

Figure 4 shows the numerically obtained IDOS for a typical cluster. The vertical step at $E = 0$ is the IDOS signature of the central δ-peak in the DOS: its height measures directly the fraction of localized zero-energy states, in agreement with the confined-state analysis of Arai *et al.* and with the Hubbard-model study of Koga and Tsunetsugu.[2, 3]

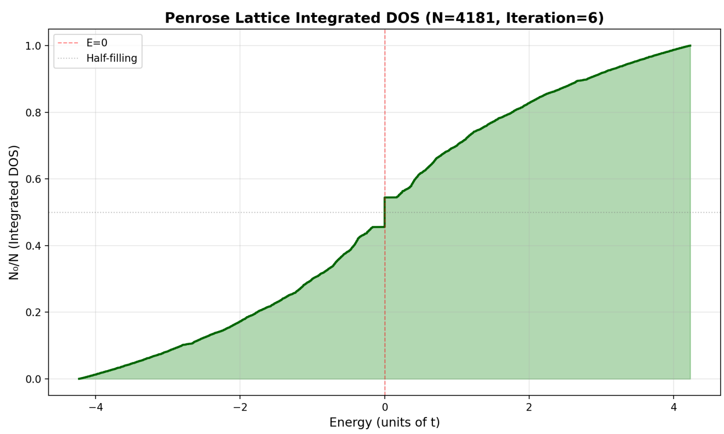

Figure 4: Integrated density of states $N_0(E)/N$ for the tight-binding model on a finite Penrose cluster. The step-like shape reflects the discrete energy levels; the large jump at $E = 0$ corresponds to a macroscopic number of zero-energy states and becomes a finite discontinuity in the thermodynamic limit.[2, 3]

3.3 Zero-energy probability density and confined states

To understand the spatial structure of the zero-energy states I inspect the probability density $|\psi_i^{(0)}|^2$ for eigenvectors with $E \approx 0$. Figure 5 shows an example of such a wavefunction: each vertex of the Penrose lattice is drawn at its geometric position and colored according to the local probability density.

Several characteristic features emerge, consistent with the confined-state picture developed in Refs. [2, 3]:

- The support of a zero-energy eigenstate is typically restricted to a finite cluster of sites, surrounded by regions where the amplitude is numerically zero. These finite "islands" are separated from each other by lines of sites on which *every* zero-energy eigenstate vanishes (forbidden sites).
- The positions of these forbidden sites form ladder-like structures that trace strings of rhombi across the lattice. They partition the lattice into finite regions; within each region the Schrödinger equation at $E = 0$ is decoupled from the rest, giving rise to strictly localized confined states.
- Within each finite region, the amplitude of a zero-energy state typically resides on only one of the two sublattices defined by the BFS coloring (Sec. 2.1), reflecting the bipartite nature of the Hamiltonian.[1]

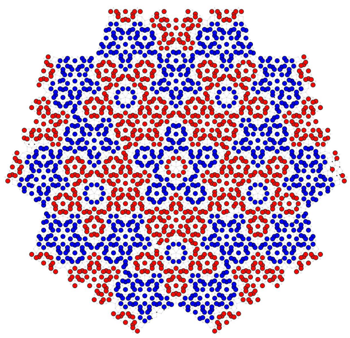

Figure 5: Example of a zero-energy eigenstate on the Penrose lattice. Dot positions correspond to the Penrose vertices; the dot size (and/or color) encodes the local probability density $|\psi_i^{(0)}|^2$. The wavefunction is confined to a finite region, separated by lines of vertices where the amplitude vanishes (forbidden sites). Very similar confined clusters and forbidden ladders are reported in Refs. [2, 3].

From a physical perspective, the existence of confined states at $E = 0$ has several important implications:[2, 3]

- At half-filling and without interactions, the ground state is highly degenerate: within each confined cluster, the zero-energy orbital can be either occupied or empty without changing the total energy (modulo global constraints and spin degrees of freedom).
- In the presence of interactions (e.g. a Hubbard repulsion), these confined clusters become the building blocks of magnetic order. In the weak-coupling limit, local moments develop first in the confined clusters, and the spatial pattern of antiferromagnetic order is controlled by their geometry.[3]

- The confined nature of the zero-energy states suggests that transport at energies near $E = 0$ is strongly suppressed, with conduction dominated by extended states in the continua above and below the central gap.

4 Conclusion

In summary, my numerical solution of the tight-binding model on the Penrose lattice proceeds in three main steps:

1. Construct a finite Penrose cluster using the deflation method, starting from a small seed and iteratively applying self-similar edge transformations involving the golden ratio and specific rotation angles.[6]

2. Extract the underlying graph, verify its bipartite nature by BFS coloring, and build the Hamiltonian matrix H with zero on-site energies and unit nearest-neighbor hoppings.

3. Diagonalize H using `numpy` to obtain the full spectrum and eigenvectors, from which the DOS, IDOS, and spatial probability densities are computed.

The resulting DOS and IDOS exhibit the characteristic features reported in the literature: a δ-like peak at $E = 0$ corresponding to a macroscopic fraction of confined states, separated by a finite gap from two bands of extended states.[1, 2, 3] The wavefunctions at $E \approx 0$ are strictly localized in finite regions separated by forbidden ladders, in agreement with the confined-state picture.

References

[1] Mahito Kohmoto and Bill Sutherland. Electronic states on a penrose lattice. *Physical Review Letters*, 56(24):2740–2743, 1986.

[2] Masao Arai, Tetsuya Tokihiro, Tohru Fujiwara, and Mahito Kohmoto. Strictly localized states on a two-dimensional penrose lattice. *Physical Review B*, 38(3):1621–1626, 1988.

[3] Akihisa Koga and Hirokazu Tsunetsugu. Antiferromagnetic order in the hubbard model on the penrose lattice. *Physical Review B*, 96(21):214402, 2017.

[4] Dan Shechtman, Ilan Blech, Denis Gratias, and John W. Cahn. Metallic phase with long-range orientational order and no translational symmetry. *Physical Review Letters*, 53(20):1951–1953, 1984.

[5] Roger Penrose. The role of aesthetics in pure and applied mathematical research. *Bull. Inst. Math. Appl.*, 10:266–271, 1974.

[6] Takashi Inoue. How to construct quasiperiodic lattices using the deflation method, 2025. Unpublished lecture notes.