Exact results on electronic wavefunctions of 2D quasicrystals

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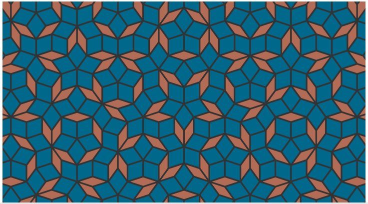


Electrons on quasicrystals

- In 1D (quasiperiodic chains): electronic spectrum and wavefunctions are well known.
- In 2D and 3D: many numerical investigations, but almost no exact results.

$\rightarrow$ recent (big!) improvement: Kalugin, Katz (2014) guessed the groundstate of a large class of 2D models.

- What does this groundstate look like?
- Which new insights does it bring us?

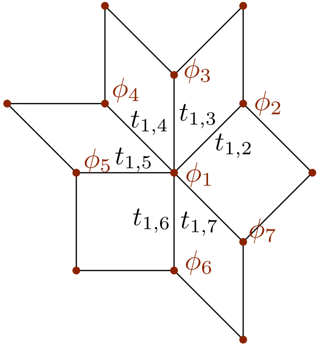
Toy models of quasicrystals

We want to model:

- a single electron (ie we do not consider interactions)
- on a quasiperiodic tiling, in 1D or in 2D
- in the simplest possible way : tight-binding model with nearest neighbors hoppings only

$$i\frac{\partial \phi_m}{\partial t}(t) = \sum_{n \text{ NN } m} t_{m,n}\phi_n(t)$$

$|\phi_m(t)|^2 =$ proba to be on atom m at time t.



Solve for the stationary states (or eigenstates):

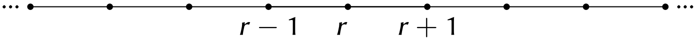
$$E\psi_m = \sum_{n \text{ NN } m} t_{m,n}\psi_n$$

Outline

Periodic and disordered models

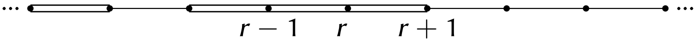
- Eigenstates on periodic materials:
  - Plane waves
  - **uniform** probability $\rightarrow$ **extended states**

$$|\psi(r)|^2 = \text{cst}$$



- Eigenstates on disordered materials:
  - Evanescent waves
  - **exponentially decreasing** probability $\rightarrow$ **localized states**

$$|\psi(r)|^2 = e^{-r/\xi}$$



What about quasiperiodic materials?

We will see on examples their electrons are somewhat **in between**: the wavefunctions have power law decays, they are **critical**

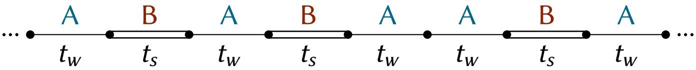
The Fibonacci chain

The geometrical model: a chain of two letters generated by the substitution

$$M : \begin{cases} A \rightarrow & AB \\ B \rightarrow & A \end{cases}$$

$$M^{\infty}(A) = \dots ABABAABAABABAABABA \dots$$

The corresponding chain of atoms:



The Schrödinger equation for the eigenstate of energy E:

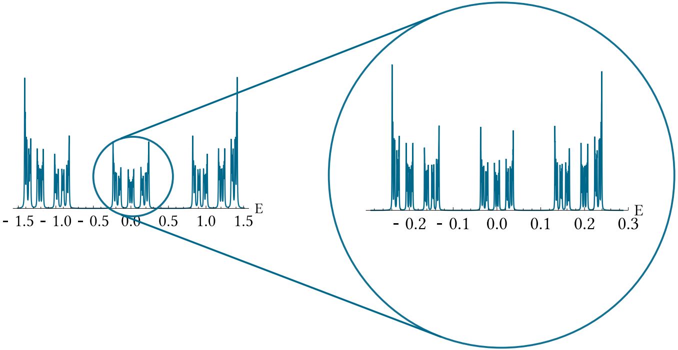
$$t_{m-1,m}\psi_{m-1} + t_{m,m+1}\psi_{m+1} = E\psi_m$$

$$t_{m-1,m} = t_s \text{ or } t_w \text{ we introduce the ratio } \rho = t_w/t_s$$

What can be say about the spectrum/eigenstates of this model?

Spectrum and eigenstates

- The spectrum is scale invariant (or multifractal)



(Spectrum computed for $\rho = 0.5$)

- The eigenstates are all critical (neither localized nor extended)

What is the structure of these critical states?

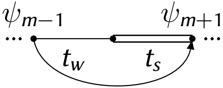
A baby example: the eigenstate at zero energy

- Schrödinger equation for the $E = 0$ state:

$$t_{m-1,m}\psi_{m-1} + t_{m,m+1}\psi_{m+1} = 0$$

- If we know the wavefunction on one site we know it on the next

$$\psi_{m+1} = -\frac{t_{m-1,m}}{t_{m,m+1}}\psi_{m-1}$$



- There are 4 possible cases:

 $\psi_{m+1} = \frac{t_w}{t_s}\psi_{m-1} = \rho^{+1}\psi_{m-1}$

 $\psi_{m+1} = \frac{t_s}{t_w}\psi_{m-1} = \rho^{-1}\psi_{m-1}$

 $\psi_{m+1} = \frac{t_w}{t_w}\psi_{m-1} = \rho^{+0}\psi_{m-1}$

 $\psi_{m+1} = \frac{t_s}{t_s}\psi_{m-1} = \rho^{+0}\psi_{m-1}$

A baby example: the eigenstate at zero energy

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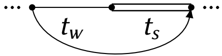


- Introduce $A_{m-1,m+1}$, the **arrow** from $m-1$ to $m+1$:


$A_{m-1,m+1} = +1$ $\quad \psi_{m+1} = \rho^{+1}\psi_{m-1}$


$A_{m-1,m+1} = -1$ $\quad \psi_{m+1} = \rho^{-1}\psi_{m-1}$


$A_{m-1,m+1} = +0$ $\quad \psi_{m+1} = \rho^{+0}\psi_{m-1}$


$A_{m-1,m+1} = +0$ $\quad \psi_{m+1} = \rho^{+0}\psi_{m-1}$

Then, $\boxed{\psi_{m+1} = \rho^{A_{m-1,m+1}}\psi_{m-1}}$

The field of arrows and the field of heights

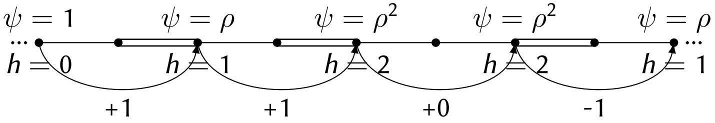
Iterating $\psi_{m+1} = \rho^{A_{m-1,m+1}} \psi_{m-1}$,

$$\psi_m = \psi_0 \rho^{h(m)}$$

Where h is **the field of heights**, the integral of the field of arrows:

$$h(m) = \sum_{n=1}^{m/2} A_{2n-2,2n}$$

Example (piece of the Fibonacci chain):



Back to the special cases, with arrows!

- Periodic chain:

  - Arrows $= 0 \implies h(m) = 0 \implies \psi_m = \psi_0 \rho^0 = \mathrm{cst}$
  - **uniform** probability $\rightarrow$ **extended states**

- Disordered chain:

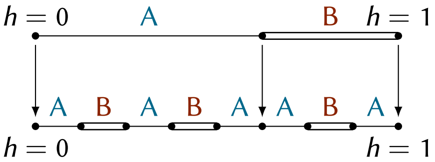
  - Arrows randomly distributed $\implies h(m) \sim \langle A \rangle \times m \implies \psi_m \sim \rho^{\langle A \rangle \times m} \sim e^{-m/\xi}$ with $\xi^{-1} = |\log \rho| \langle A \rangle$
  - **exponentially decreasing** amplitude $\rightarrow$ **localized states**

$\rightarrow$ expected behavior in both cases.
What happens for a quasiperiodic chain?

The $E = 0$ state is not localized

Apply the substitution three times:

$$M^3 : \begin{cases} A \rightarrow & ABABA \\ B \rightarrow & ABA \end{cases}$$

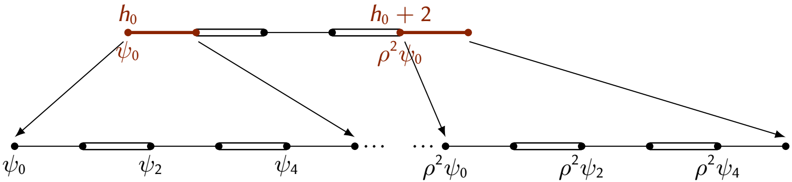


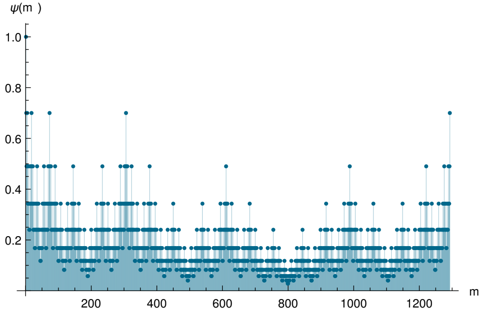
$\rightarrow$ the height is invariant under the substitution M^3: it doesn't change on the preexisting sites

- the wavefunction doesn't change on the preexisting sites
- these preexisting sites get arbitrarily far apart as we iterate the substitution

$\rightarrow$ we can find the electron with high probability arbitrarily far from the origin: **the wavefunction is not localized.**

The $E = 0$ state is not extended





Local scale invariance:

$$\psi_{a\times m} = b \times \psi_m$$

$\rightarrow$ local **power law decay**

$$\psi_{r_n} \sim r_n^{\alpha}, \; (\alpha = \log b / \log a)$$

$\rightarrow$ **wavefunction is not extended**

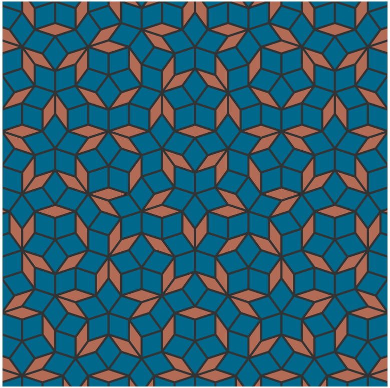
Cut and project chains: a summary

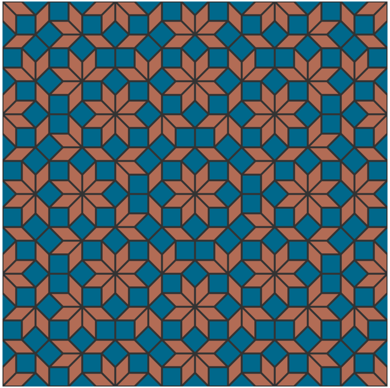
- The $E = 0$ wavefunction of cut and project chains is described by a **height field**
- The height field is the integral of an **arrow field**, which is quasiperiodic
- Geometry of the tiling $\implies$ structure of the wavefunction
- $\rightarrow$ **the wavefunction is critical**: neither localized nor extended, behaves locally as a power law

We will find again all these features in 2D!

2D TILINGS

We consider the Penrose and the Ammann-Beenker tilings.





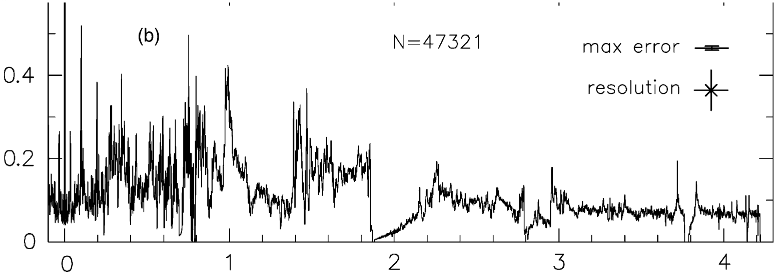
Model for the electron:

$$E\psi_m = V_m\psi_m + \sum_{n\ \mathrm{NN}\ m} t\psi_n$$

Quasiperiodicity encoded in the adjacency of the vertices

What is known

Local density of states [taken from Zijlstra 2014]:

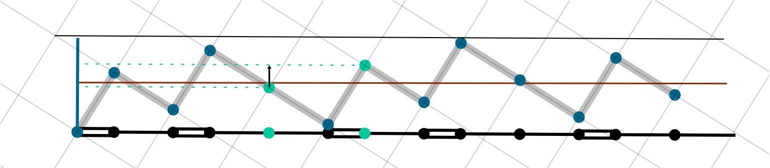


- Spectrum: no apparent fractal structure
- States are critical (numerical result, eg [Rieth, Schreiber 1998])

$\rightarrow$ can we introduce a field of arrows to describe some of these critical wavefunctions?

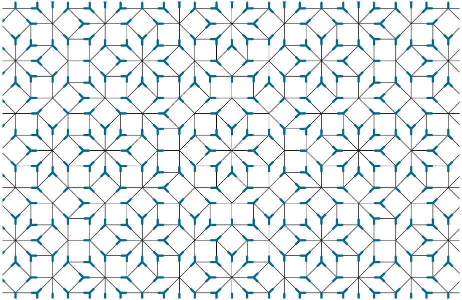
A natural field of arrows

In superspace, arrows go from the center to the border of the slice:



- Define arrows in the same way for 2D tilings (they coincide with the *matching rules*)
- Consider again the height: $h(m) = \sum A$

Can we describe states with this arrow field? $\psi_m = \rho^{h(m)}$ (with ρ a constant)



The groundstate wavefunction

Can we find an "arrowed state" $\psi_m = \rho^{h(m)}$? (with ρ a constant)

- Idea [Sutherland 1986]: tune the potential

$$E\psi_m = V_m\psi_m + t \sum_{n \text{ NN } m} \psi_n \Longleftrightarrow V_m = E - t \sum_n \rho^{A_{m,n}}$$

  Obtain a groundstate which is an arrowed state.
  Not very physical! Generically, potential is not finely tuned.

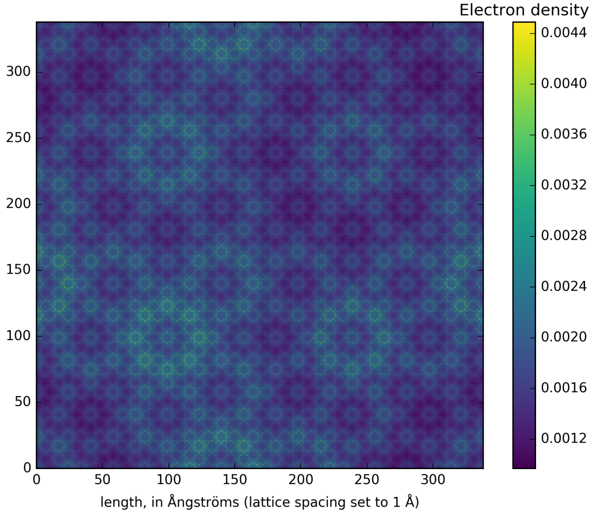
- Guess [Kalugin, Katz 2014] : state still arrowed, but with a local modulation:

$$\psi_m = C_m \rho^{h(m)}$$

  where C_m is local:

$$C_m \simeq C_n \text{ if the tiling looks the same around } m \text{ and } n$$

Robustness of the structure



- The groundstate is **very robust**: For any model of the form

$$E\psi_m = V_m\psi_m + t\sum_n \psi_n$$

the groundstate is an "arrowed state"

$$\psi_m = C_m\rho^{h(m)}$$

- Same arguments as in 1D: the state has power law decay, and is critical.

$\rightarrow$ what can we do now?

Scaling of the groundstate

- Participation ratio over a region $\mathcal{R}$:

$$\mathrm{PR}(\psi, \mathcal{R}) = \frac{\left(\sum_{m\in\mathcal{R}} |\psi_m|^2\right)^2}{\left(\sum_{m\in\mathcal{R}} |\psi_m|^4\right)^4}$$

- Scaling with the region volume $\mathrm{Vol}(\mathcal{R})$:

$$\mathrm{PR}(\psi, \mathcal{R}) \sim \mathrm{Vol}(\mathcal{R})^{D(\psi)}$$

  - $D(\psi) = 0 \implies \psi$ localized
  - $D(\psi) = 1 \implies \psi$ extended
  - $0 < D(\psi) < 1 \implies \psi$ critical

We can compute the scaling analytically for the groundstate:

$$\boxed{D(\psi) = \log\left(\frac{\omega(\rho^2)^2}{\omega(\rho^4)}\right) / \log \omega(1)}$$

with (for Ammann-Beenker)

$$\omega(z) = \frac{a(z) + \sqrt{a(z)^2 - z^2}}{z}$$
$$a(z) = 4z^2 + 9z + 4$$

Scaling only depends on the arrow distribution, only on the **geometry** of the tiling.

Conclusion

- Examples of generic **critical** eigenstates.
  - 1D (Fibonacci): the $E = 0$ state
  - 2D (Penrose and Ammann-Beenker): the groundstate.
- Geometry $\rightarrow$ quasiperiodic **arrow function** $\rightarrow$ structure of the state.
- In 2D, structure **robust to changes in the model** (varying potential, hopping)
- Using this description, we can easily compute physical observables.

Perspectives:

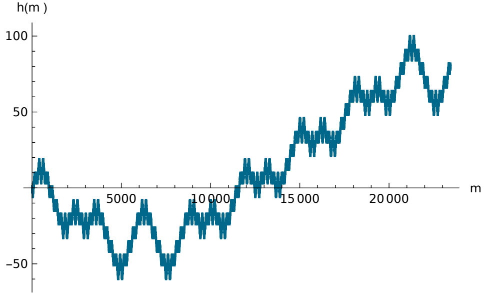
- For Penrose and Ammann-Beenker, the arrow field is not enough to describe excited states. Extra ingredients?
- Other 2D quasicrystals: generalized Penrose, dodecagonal …

Cut and project chains are special!

Consider the chain constructed by the substitution

$$A \to ABBB$$
$$B \to A$$

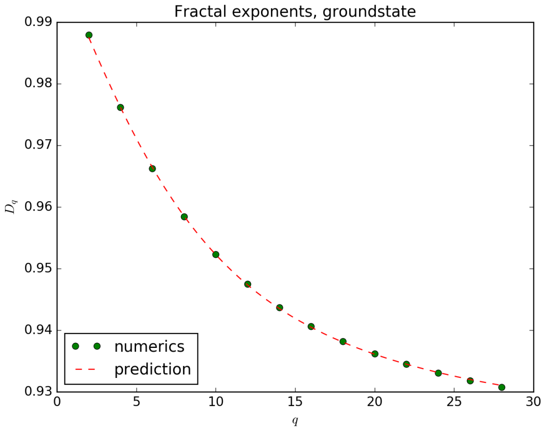
- This substitution cannot be built by cut and project (because it is non-Pisot).
- Height resembles a random walk, and typical height $\sim \sqrt{L}$
- As a result, the wavefunction is localized!

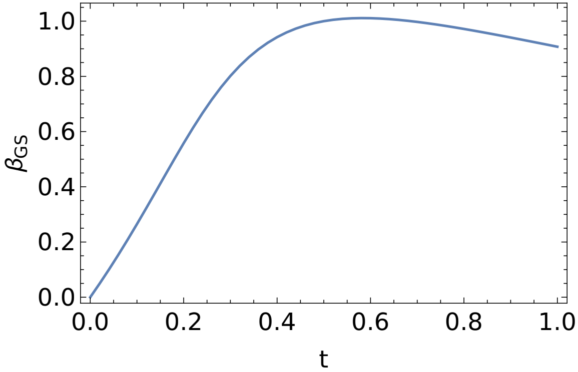


$\to$ criticality is sensitive to the **complexity** of the tiling

Theory/numerics on the 2D groundstate

$$t \sum_{n \text{ NN } m} \psi_n + (t-1) z_m \psi_m = E\psi_m$$





$$\psi_m = C_m \beta^{h(m)}$$

Computation of a local observable

Compute the local observable $\hat{O}$, in the ψ state: $\langle\psi|\hat{O}|\psi\rangle$
Assumptions:

- The observable only depends on the local configuration of the atoms.
- The state is described by an arrow field and a local variation: $\psi_m = C_m \rho^{h(m)}$

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{m,n} \psi_m^* \hat{O}_{m,n} \psi_n$$

$$\boxed{\langle\psi|\hat{O}|\psi\rangle = \sum_{\mu,\nu} C_\mu^* \hat{O}_{\mu,\nu} C_\nu \sum_{h,h'} f(\mu, h; \nu, h') \rho^{h+h'}}$$