Exact results on electronic wavefunctions of 2D quasicrystals

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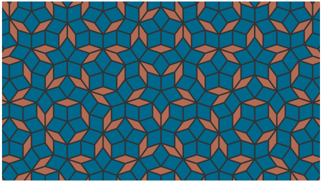
September 20, 2016



Electronic properties of quasicrystals

We can we do to access the electronic properties of quasicrystals?

- Experiments
    - Measure of physical properties: conductivity, ???
- "Realistic" simulations
    - Direct access to the electronic states
- Toy models
    - More managable (sometimes exactly solvable) $\rightarrow$ easier to see the consequences of quasiperiodicity
    - Simple states can be seen as "building block" for more realistic ones (like Bloch's states for periodic materials)

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

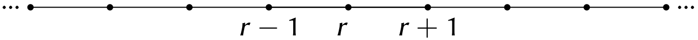
$$H = \sum_{\langle i,j \rangle} t_{i,j} \left| i \right\rangle \left\langle j \right|$$

[Picture of the hoppings on a tiling]
The challenge now is to find a proper description of these eigenstates...

WHAT IS KNOWN: PERIODIC AND DISORDERED MODELS

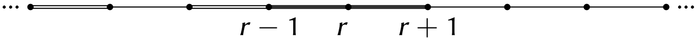
- Eigenstates on periodic materials:
  - Plane waves
  - **constant** amplitude $\rightarrow$ **extended states**

$$\psi(r) = e^{ikr}$$



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

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



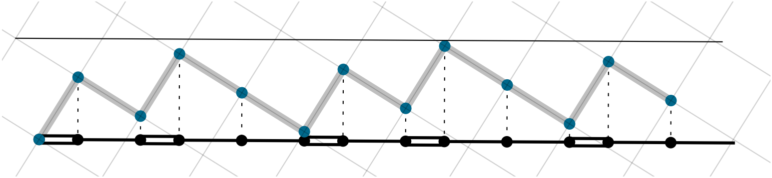
What about quasiperiodic materials?

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

Outline

Cut and project chains: what is known

The geometrical model:



The corresponding chain of atoms:

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

$$t_{=} = 1,\ t_{-} = \rho,\ \rho < 1$$

- spectrum is (multi)fractal
- wavefunctions are generically critical (all of them are for Fibo)

A special case: the eigenstate at the middle of the spectrum

- Even and odd sites are decoupled, and if we know the wf on one site we know it everywhere
- Concept of arrows: wf properties stem from the geometrical properties of the field of arrows

Back to the special cases, with arrows!

- Periodic chain: no arrows $\rightarrow$ extended
- Disordered chain: random arrows $\rightarrow \langle h \rangle = 0$: localized

Fibo and the inflation

- Inflation rule $\phi : A \to AB, \dots$
- Concepts of atoms and molecules, spectrum seen as broadening of atomic ($E = 0$) and molecular ($E = \pm 1$) levels.
- Atomic inflation (ϕ^3) should be relevant since we expect the $E = 0$ wf to have have mainly weight on the atomic sites
- Indeed yes: ϕ^3 is an inflation rule for the arrows: $\phi^3 : R \to \dots, L \to \dots$

The Fibo arrows and the Fibo wf

- On old sites height is constant $\rightarrow$ cannot be localized
- On new sites height increases at most linearly $\rightarrow$ $\log L$ growth, local power law behavior
- Rigorously: *IPR* computed analytically from the arrow statistics $\rightarrow$ critical wf.

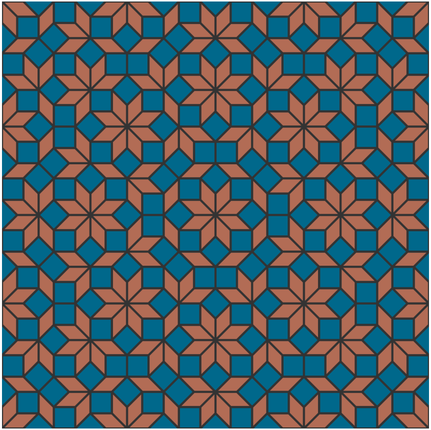
Summing up what happens in 1D

- max height $\sim \log L$, typical height $\sim \sqrt{\log L}$
- Arrow is a quasiperiodic function
- Its integral, the height, is not
- As a result, the wf is critical: it behaves locally as a power law
- We will find again all these features in 2D

Cut and project 1D models are special!

- B3 substitution: a two letters, deterministic chain, that is non-Pisot $\rightarrow$ cannot be built by cut and project.
- Height resembles a random walk, and typical height $\sim \sqrt{L}$
- $\rightarrow$ wf localized

Construction of the model: Ammann-Beenker and Penrose



$$- \sum_{n \in V(m)} \psi_n = E \psi_m$$

No parameters: the quasiperiodic features are encoded in the adjacency of the vertices.

What is known

- Spectrum is more regular: only a few gaps, no apparent fractal structure
- $E = 0$ wfs are localized: too bad!
- The other wf are critical (numerical result)

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

The ground state

- Sutherland's idea: introduce local potentials to make the construction of the grounstate simpler.
- Sutherland's groundstates on Penrose and AB tilings is constructed via the introduction of a field of arrows, exactly like the 1D ones

$\rightarrow$ what are the properties of this field of arrows?

Inflation and the field of arrows

Here we focus on the AB example, but everything works the same for Penrose.

- Arrows $\leftrightarrow$ matching rules for the tiles
- Matching rules are enforced by the inflation rules $\rightarrow$ we should be able to study the properties of the arrows via the inflation (just like in 1D)
- From the inflation rules, we deduce the maximal height $\sim \log L$
- Statistics of the heights $P_{\mu}^{l}(h)$ obeys a diffusion-like equation where l plays the role of time and h the role of space
- $\rightarrow$ typical height is $\sim \sqrt{\log L}$

So we understand everything about Stutherland's wavefunction, but the model has been built for this wavefunction to exist. Can we use this field of arrows to describe wavefunctions on more realistic models? Yes: Pavel.

Characterization of the groundstate wavefunction

- We go back to the model with no local potentials.
- From the plot of the groundstate: we see a complicated local structure (role of the local environment) and the phason line (role of the arrow field)
- Indeed, the wf decomposes into a local part and an arrow part (this was guessed from involved algebraic arguments).
- Computation of the IPR scaling and the multifractal exponents: the local part doesn't play any role $\rightarrow$ exponents only sensitive to the arrow part, ie to the quasiperiodicity!
- Remains valid for a larger class of models $H = \sum_{\langle i,j \rangle} |i\rangle \langle j| + V_i |i\rangle \langle i|$

Conclusion

- Non-interacting eigenstates on quasicrystals are generically critical: here we were able to understand it for some specific states, both in 1D and 2D.
- On our examples, wavefunction construction involves a geometrical quasiperiodic function, the field of arrows.
- Its integral, the height function, has logarithmic growth,
- As a result, the wavefunction is critical: it has a local power law behavior.

Perspectives:

- What happens for the grounstate of other quasicrystals, like the dodecagonal ones?
- For Penrose and AB, the arrow field cannot be used to describe other states. What extra ingredients are required?

More perpsectives!

- A plot of the state just below the gap, with its quasiperiodic array of lines of zeros, that remain to be understood!