Exact results on electronic wavefunctions of 2D quasicrystals

Nicolas Macé, Anuradha Jagannathan, Frédéric Piéchon

Laboratoire de Physique des Solides Université Paris-Saclay

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Motivation du talk : relier les propriétés électroniques (et plus précisément la structure des fonctions d'onde) à la géométrie de quasicrystaux.

A TOY MODEL OF QUASICRYSTALS

We want to model:

- 1 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 interactions

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

Benefit compared to more realistic models:

- More managable model \rightarrow easier to see the consequences of quasiperiodicity
- Non-interacting eigenstates as "building block" for more realistic states (like Bloch's states for periodic materials)

The challenge now is to find a proper description of these eigenstates...

PERIODIC AND DISORDERED MODELS

Properties of the eigenstates:

- Periodic: plane waves \rightarrow extended, constant amplitude.
- Disordered: evanescent waves → localized, exponentially decaying amplitude.

Purpose of this talk: show on examples that electrons on quasicrytals are somewhat in between: their wavefunctions have local powerlaw decay, they are critical.

OUTLINE

- 1 1D quasiperiodic models
- 2 2D case

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1D CUT AND PROJECT CHAINS: WHAT IS KNOWN

- 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

- lacksquare 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 → 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

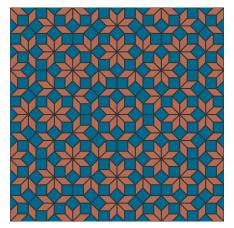
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CUT AND PROJECT 1D MODELS ARE SPECIAL!

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

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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
- \blacksquare F = 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?

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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?

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INFLATION AND THE FIELD OF ARROWS

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

- Arrows ↔ matching rules for the tiles
- Matching rules are enforced by the inflation rules → 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
- \blacksquare \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 → exponents only sensitive to the arrow part, ie to the quasiperiodicity!
- Remains valid for a larger class of models $H = \sum_{\langle i,i \rangle} |i\rangle \langle j| + V_i |i\rangle \langle i|$

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?

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More perpsectives!

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

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