An ansatz for eigenstates in quasicrystalline potentials

P Kalugin
Laboratoire de Physique des Solides,
Université Paris-Sud
(joint work with André Katz, Centre de Physique Théorique,
Ecole Polytechnique)

SubTile 2013, CIRM, Jan 16, 2013

Introduction

Consider a single-particle Schrödinger Hamiltonian for a perfect quasicrystalline potential:

$$H = -\Delta + U$$

There are two points of view:

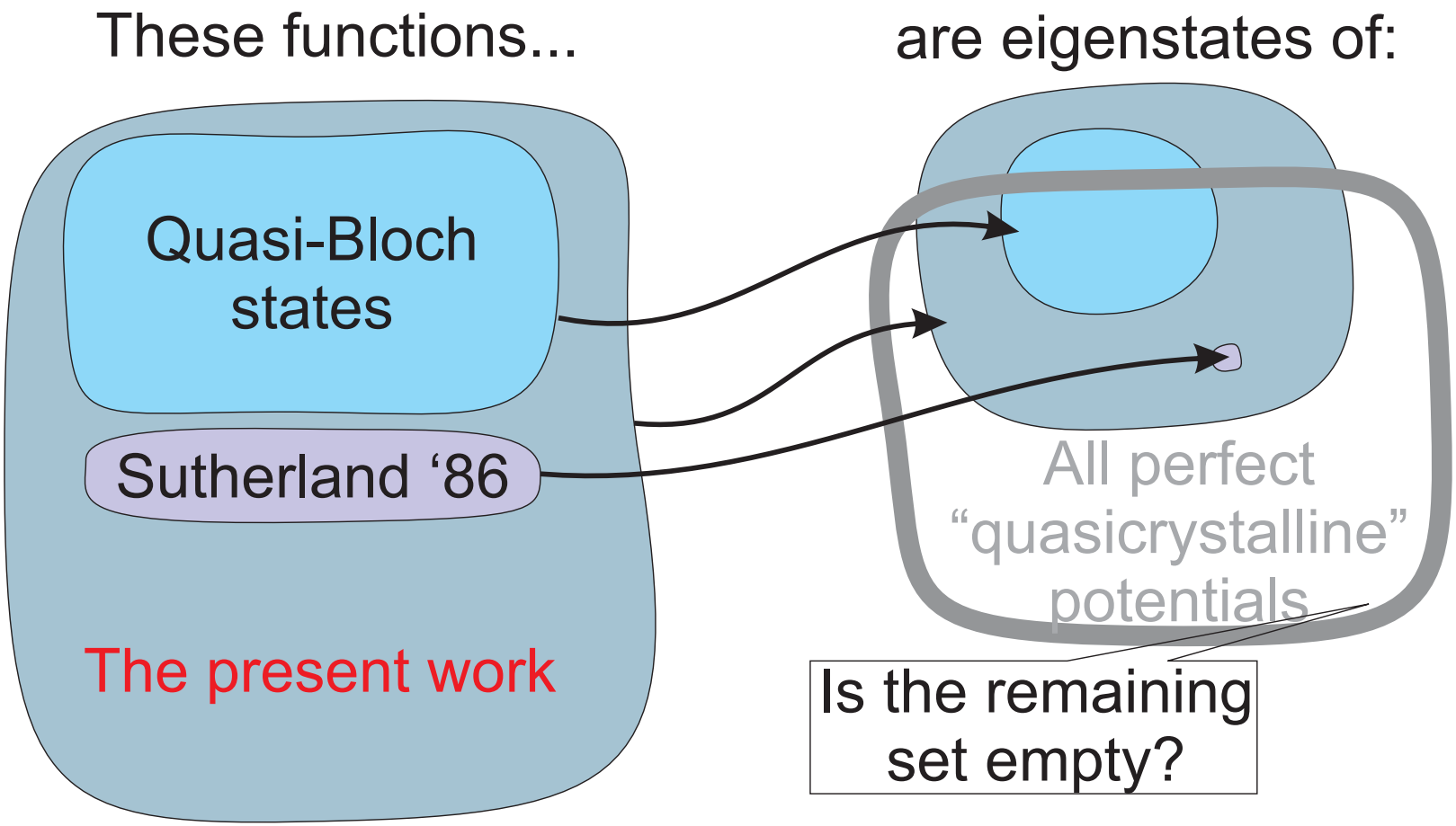
- Global analysis: One has first to define the Hilbert space and the domain. The main results are gap labelling theorems (Bellisard).
- Local analysis: consider a PDE $H\psi = E\psi$, look for the solutions ψ (and fix the boundary conditions later...). The main results are about spectra and (generalized) eigenstates for one dimensional potentials by the technique of trace map (Kohmoto, Sütő).

We adopt the local approach...

Motivation

. . . an ansatz is an educated guess . . . (Wikipedia)

All known *analytical solutions* of the eigenstate problem in perfect quasicrystals in more than one dimension are (educated) guesses:



A perfect QC potenial?

- The naïve cut (-and-project) approach:

$$U(\mathbf{x}) = u(\alpha(\mathbf{x})),$$

where α is an irrational winding

$$\alpha : \mathbb{R}^n \to \mathbb{T}^N$$

and u is a (*discontinuous?!*) function on $\mathbb{T}^N$.

A perfect QC potenial?

- The naïve cut (-and-project) approach:

$$U(\mathbf{x}) = u(\alpha(\mathbf{x})),$$

where α is an irrational winding

$$\alpha : \mathbb{R}^n \to \mathbb{T}^N$$

and u is a (*discontinuous?!*) function on $\mathbb{T}^N$.

- Less naïve way: start with the Hull Ω

$$\mathbb{R}^n \xrightarrow{\mu} \Omega \xrightarrow{\epsilon} \mathbb{T}^N,$$

and define the potential as a pullback:

$$U(\mathbf{x}) = u(\mu(\mathbf{x})),$$

where u is a *continuous* function on Ω. In other words, $U(\mathbf{x})$ is weakly pattern equivariant.

What's wrong with quasi-Bloch states?

- An electron with a momentum $\hbar\mathbf{k}$ can only be scattered by a quasi-lattice momentum $\hbar\mathbf{k}_{\{\mathbf{n}\}}$:

$$\psi(\mathbf{x}, t) = \sum_{\mathbf{n}} c_{\{\mathbf{n}\}}(t) \exp\left(i(\mathbf{k} + \mathbf{k}_{\{\mathbf{n}\}})\mathbf{x}\right)$$

  The quasi-Bloch states are just stationary solutions of the above. They always exist, don't they?

What's wrong with quasi-Bloch states?

- An electron with a momentum $\hbar\mathbf{k}$ can only be scattered by a quasi-lattice momentum $\hbar\mathbf{k}_{\{\mathbf{n}\}}$:

$$\psi(\mathbf{x}, t) = \sum_{\mathbf{n}} c_{\{\mathbf{n}\}}(t) \exp\left(i(\mathbf{k} + \mathbf{k}_{\{\mathbf{n}\}})\mathbf{x}\right)$$

  The quasi-Bloch states are just stationary solutions of the above. They always exist, don't they?

- Not necessarily! If the Fourier harmonics $\tilde{U}(\mathbf{k}_{\{\mathbf{n}\}})$ decay slowly, the electron is delocalized in the momentum space. And this is what happens in the most interesting case of a QC with matching rules (Kitaev '89):

$$\tilde{U}(\mathbf{k}_{\{\mathbf{n}\}}) \sim 1/|\mathbf{k}_{\{\mathbf{n}\}\perp}|$$

(Quasi-)Bloch functions revisited

- Let us look for the solutions in the following form:

$$\psi(\mathbf{x}) = \exp(f)\psi_0\left(\alpha(\mathbf{x})\right),$$

where ψ_0 be a continuous function on Ω. One has

$$\Delta\psi = \exp(f)\left(\Delta\psi_0 + 2\nabla\psi_0\nabla f + \Delta f + (\nabla f)^2\right)$$

If ∇f is weakly PE (and we are lucky enough), ψ is a solution for the stationary Schrödinger equation for some (real!) weakly PE U.

(Quasi-)Bloch functions revisited

- Let us look for the solutions in the following form:

$$\psi(\mathbf{x}) = \exp(f)\psi_0\left(\alpha(\mathbf{x})\right),$$

where ψ_0 be a continuous function on Ω. One has

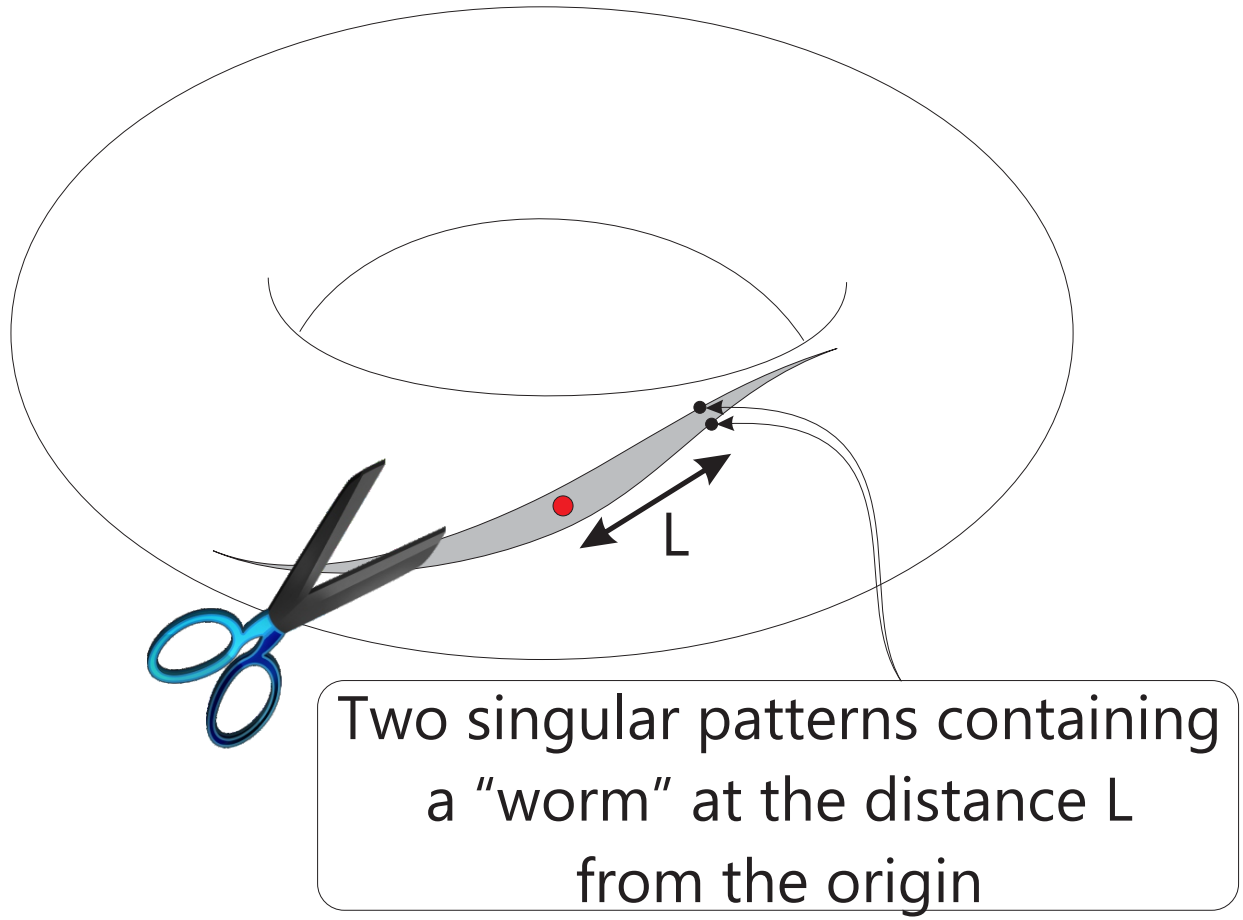
$$\Delta\psi = \exp(f)\left(\Delta\psi_0 + 2\nabla\psi_0\nabla f + \Delta f + (\nabla f)^2\right)$$

If ∇f is weakly PE (and we are lucky enough), ψ is a solution for the stationary Schrödinger equation for some (real!) weakly PE U.

- Note that $\exp(f)$ is actually defined up to a weekly PE factor, which can always be absorbed by ψ_0. The non-trivial solutions should be classified by cohomologies of Ω! But by which ones?...

Approximating the Hull by a finite CW complex

Krafting the Hull out of $\mathbb{T}^N$ with scissors:



The figure depicts the space $\mathbb{X}_D = \overline{\mathbb{T}^N \setminus Y_D}$ obtained by the removing the D-neighborhood Y_D of the "worms' from $\mathbb{T}^N$ (and completion w.r.t. the inner metric).

Approximating the Hull by a finite CW complex

Let us consider the inverse limit of the sequence of natural inclusions

$$\mathbb{X} \to \cdots \to \mathbb{X}_{D_{m+1}} \to \mathbb{X}_{D_m} \to \mathbb{X}_{D_{m-1}} \cdots$$

Theorem (PK 2004): for the almost canonical tilings, the Hull Ω is homeomorphic to $\mathbb{X}$.
In the most important cases (e.g. patterns with strong matching rules) the sequence stabilizes (in the sens of homotopy equivalence) at some term, which can be considered as an approximation of the Hull:

$$\Omega \xrightarrow{\epsilon_D} \mathbb{X}_D$$

Since $\mathbb{X}_D$ is a smooth manifold with boundary, one can work with de Rham cohomology...

The Ansatz

Let ω be a closed $\mathbb{C}$-valued 1-form on $\mathbb{X}_D$. Its pullback by the (differentiable) map $\mu_D = \epsilon_D \mu$ is exact:

$$\mu_D^* \omega = df$$

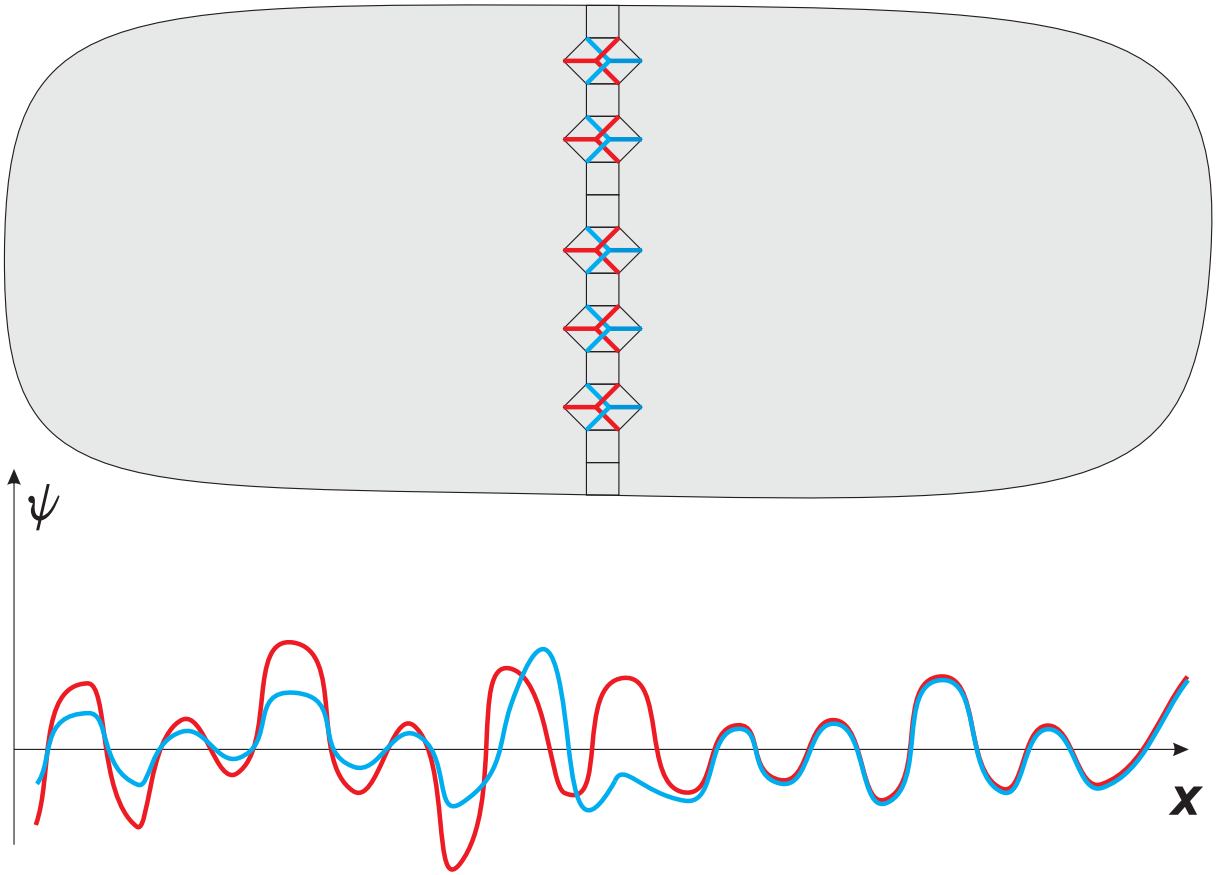
Lel ψ_0 be a (smooth enough) function $\Omega \to \mathbb{C}$. Then the ansatz for the eigenstate has the following form:

$$\psi(\mathbf{x}) = \exp(f)\psi_0\left(\mu(\mathbf{x})\right)$$

This expression is actually parametrized by the class of ω in $H^1(\mathbb{X}_D, \mathbb{C})$ only. The latter plays therefore the role of Bloch quasimomentum.

How does it look in the real space?

Switching of the "worm":



The wavefunction at the left side is multiplied by $\exp\left(\oint_\Gamma \omega\right)$ for some contour Γ encircling Y_D.

Relation to Sutherland's wavefunction

Sutherland observed that the standard arrows of Penrose tiling form an irrotational (co)vector field. The similar construction exists for Ammann tiling — and one can see that Sutherland's field has a non-trivial cohomology class in $H^1(\overline{\mathbb{T}^N \setminus Y_D})$.

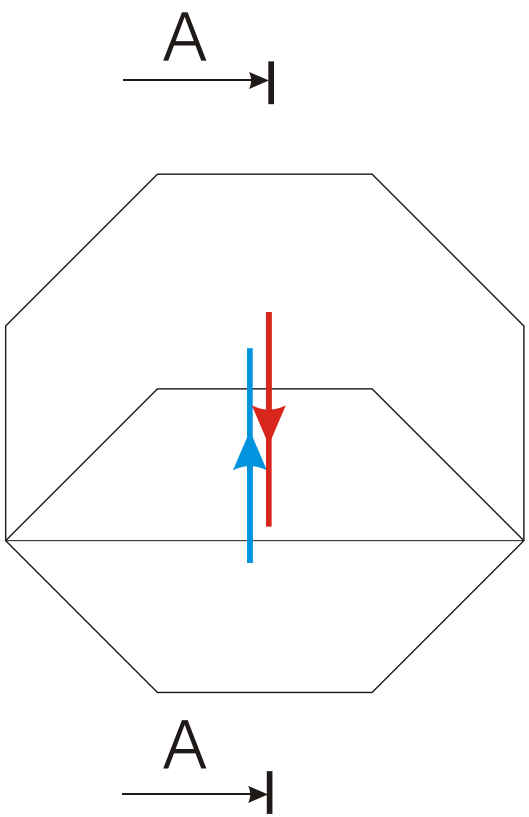
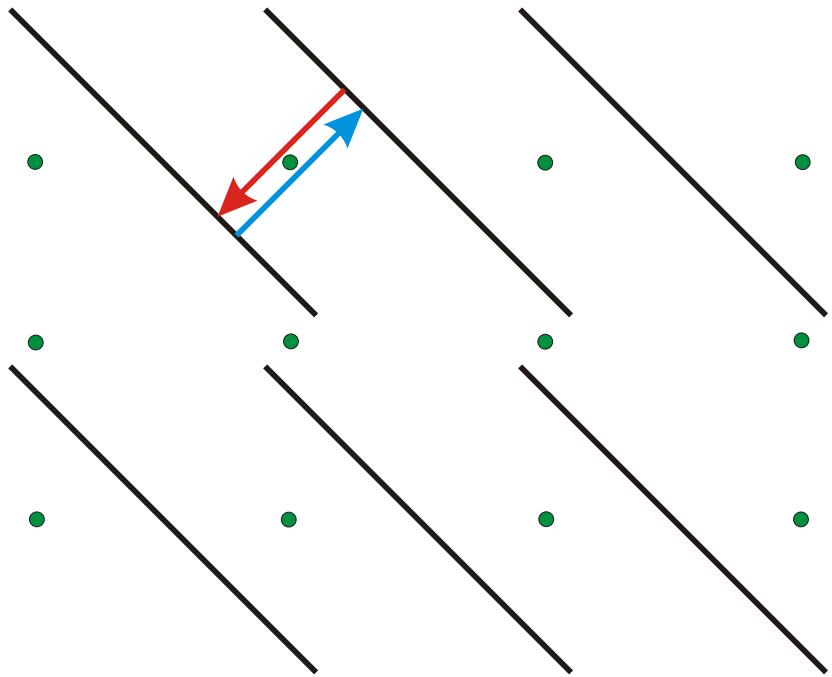


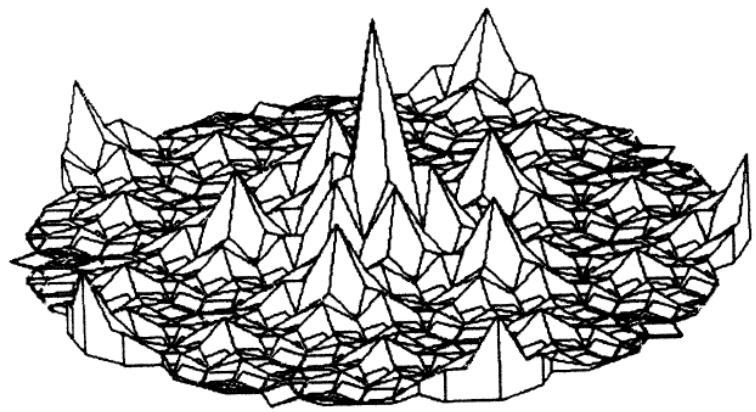
Exhibit Ammann tiling / Section A-A



Global behavior of the wavefunction

Consider a quasicrystalline patch of radius R. How much does the scaling function f fluctuate inside the patch? More precisely, what's the difference of the value $f(0)$ at the center of the patch and the average value $\bar{f}$? One can answer this question if the Hull possesses an inflation symmetry M:

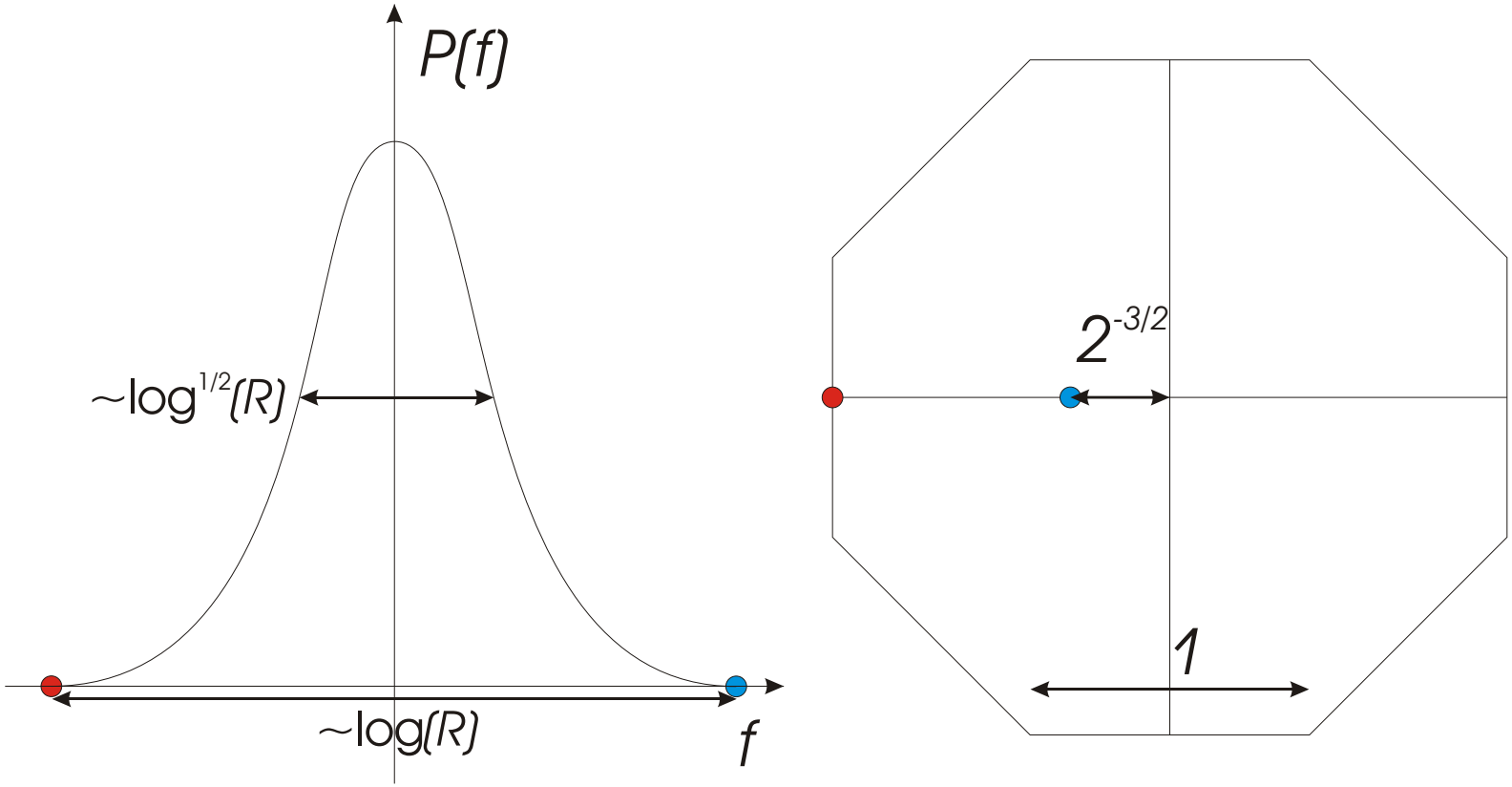
- If the center of the patch is a fixpoint of M^p for some finite p, then $f(0) - \bar{f} \sim \log |R|$.
- Otherwise, $f(0) - \bar{f} \sim \sqrt{\log |R|}$



This figure from Sutherland's paper depicts the typical behavior of $\exp(f)$

The blind spots

None of the wavefunctions of the ansatz can be big simultaneously at the blue and at the red spots — hence the corresponding zones are effectively electrically isolated from each other.



The figure shows the distribution of the values of f and the positions of the extremal spots on the atomic surface for the octogonal Ammann tiling.

Generalizing the ansatz

Do we really need the closeness of the form ω? Actually, it suffices that $\mu_D^*(d\omega) = 0$. One should therefore consider the cohomologies $H^\bullet(\mathbb{X}_D)$ of the quotient complex on $\Omega^\bullet_{\|}(\mathbb{X}_D)$:

$$0 \to \Omega^\bullet_\perp(\mathbb{X}_D) \to \Omega^\bullet(\mathbb{X}_D) \to \Omega^\bullet_{\|}(\mathbb{X}_D) \to 0$$

where $\Omega^\bullet_\perp(\mathbb{X}_D)$ consists of the forms vanishing under μ_D^*.
Bad news: even in the case $N = 2$ and $n = 1$, the group $H^1_{\|}(\mathbb{X}_D)$ is infinetely generated (hint: the derivative map $H^1_{\|}(\mathbb{X}_D) \to H^2_\perp(\mathbb{X}_D)$ is epi and has a non-zero kernel; in the same time $\omega \mapsto \epsilon_\perp \wedge \omega$ establishes an isomorphism between the two groups).
But we can always pick a reasonably looking cocycle and try!
What about guessing the eigenstates for the Fibonacci chain?

Fibonacci sequence

The transfer matrix recursion:

$$T_{n+1} = T_n T_{n-1}$$

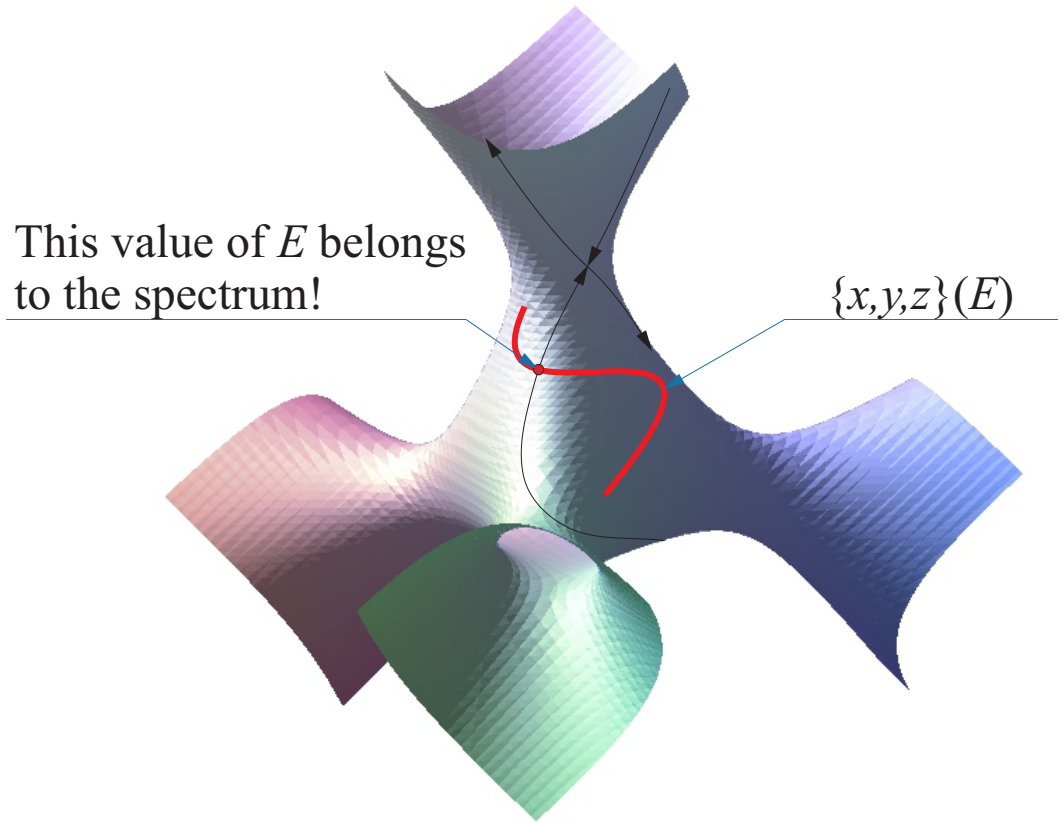
yields the following tracemap M:

$$x \mapsto y$$
$$y \mapsto z$$
$$z \mapsto 2zy - x$$

with the invariant

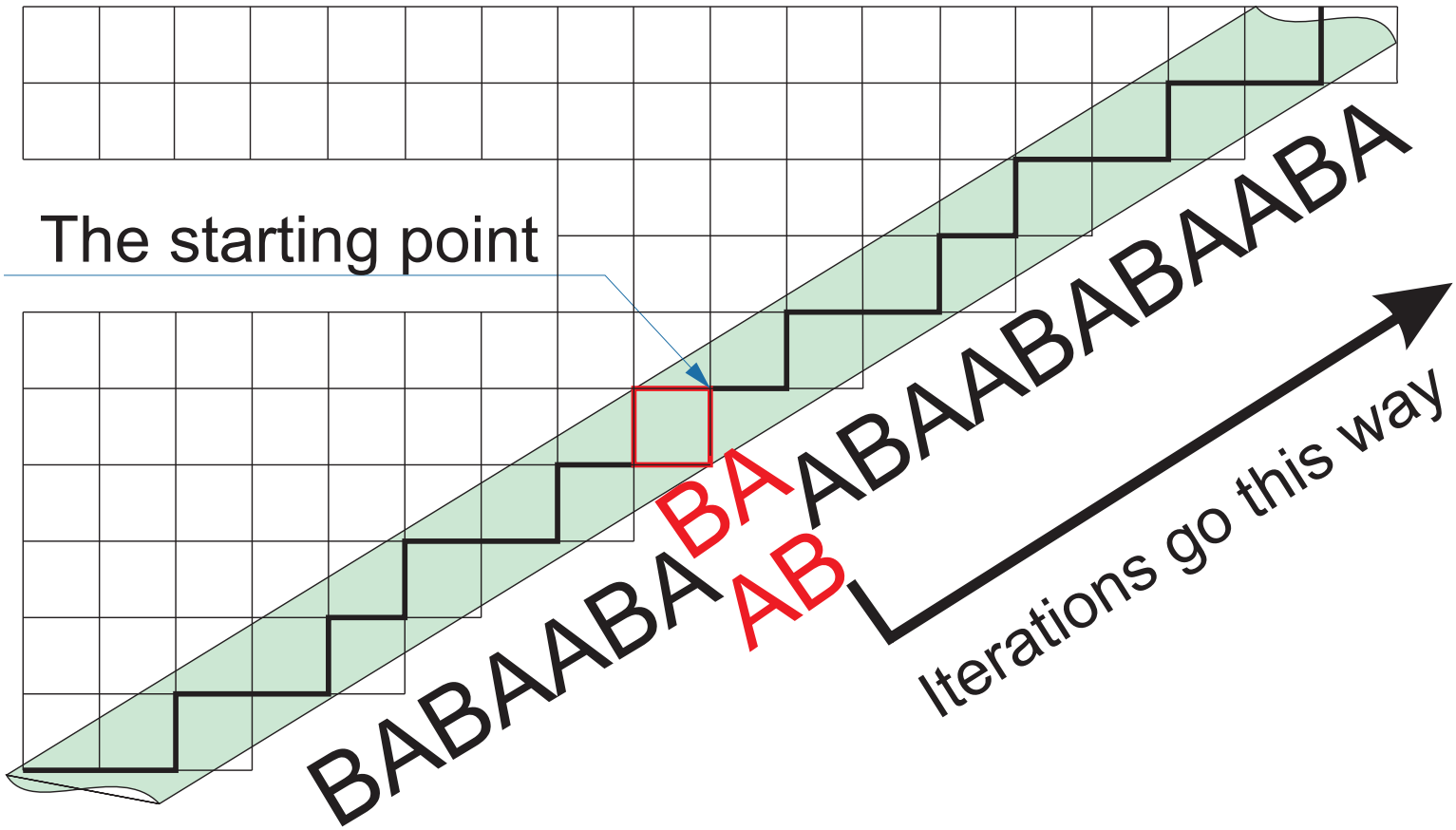
$$J = x^2+y^2+z^2-2xyz$$

Fixpoints of M^n correspond to a dense subset of the spectrum of H



Fibonacci sequence

The sequence obtained by iterations is singular!
It corresponds to two distinct points in the hull.
Q: What happens with the "eigenstate" to the left of the origin?



Fibonacci sequence

Consider the commutator

$$K = T_n T_{n-1} T_n^{-1} T_{n-1}^{-1}$$

The iteration $T_{n+1} = T_n T_{n-1}$ transforms K to K^{-1}. Consider a fixpoint of the order $2p$ of the tracemap

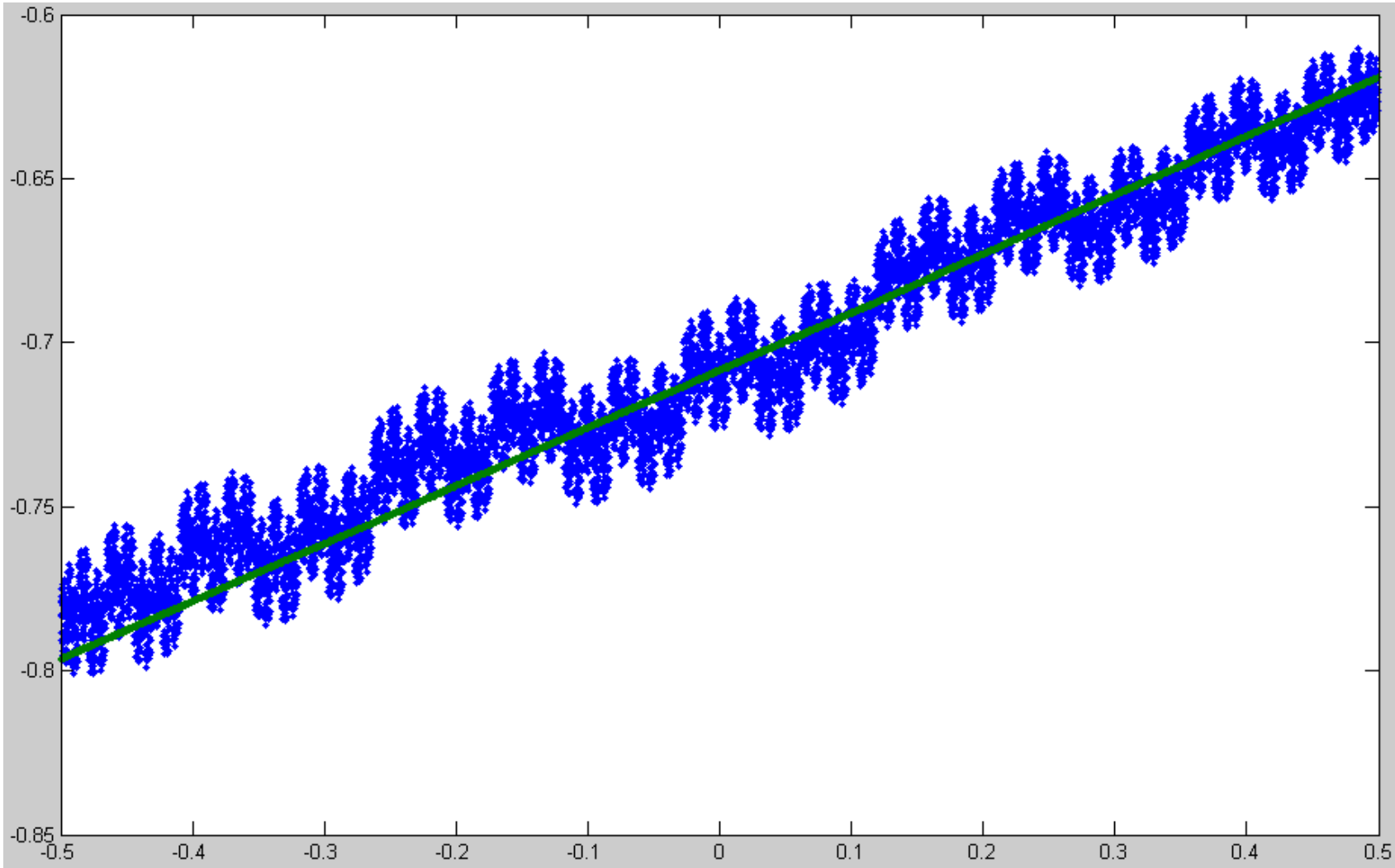
$$\mathrm{T}r(T_{n+2p}) = \mathrm{T}r(T_n)$$

For 2×2 matrices this implies

$$T_{n+2p} = K^{\alpha} T_n K^{-\alpha}$$

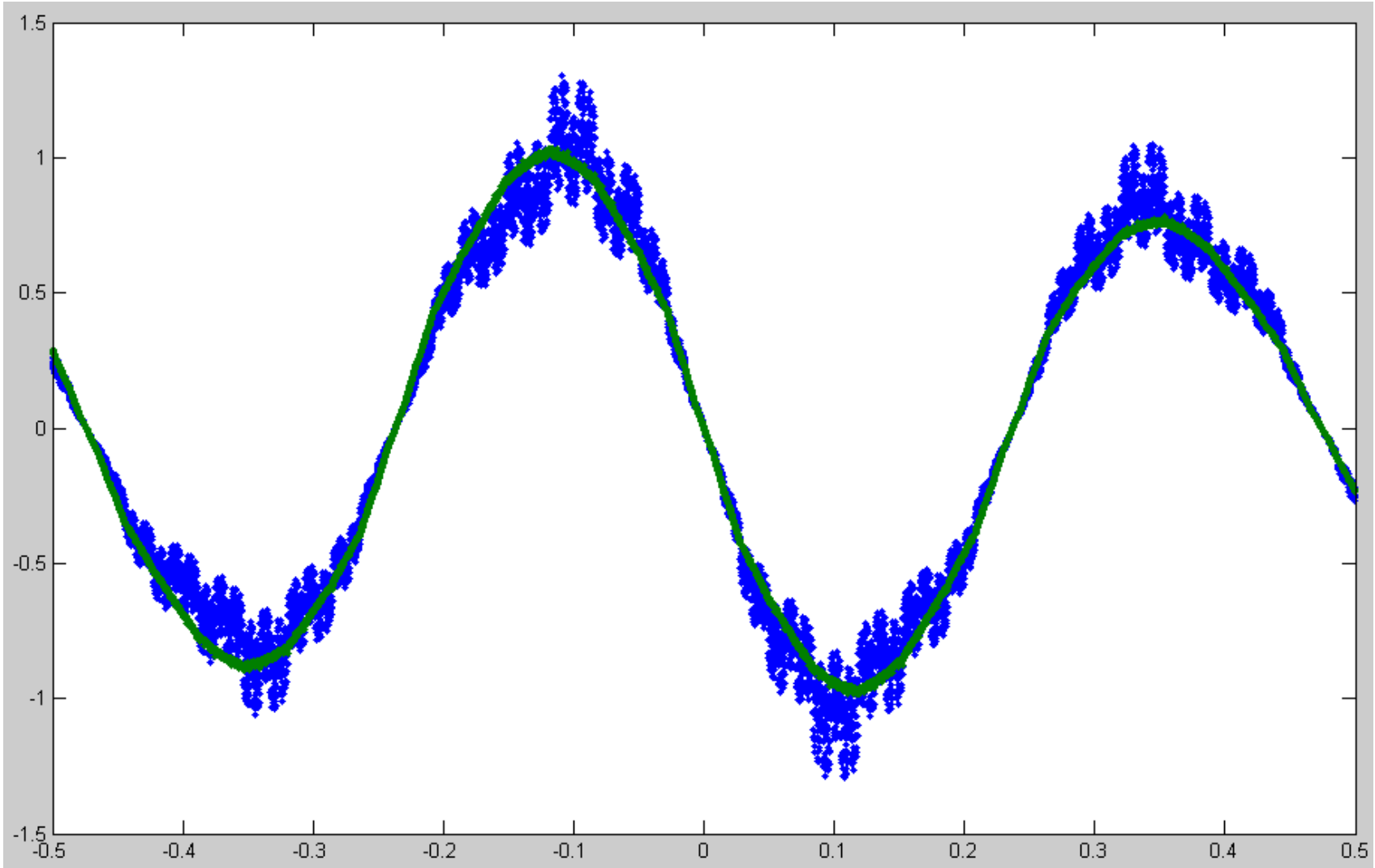
for some real α. Therefore, the wavefunction started with the eigenvector of K with the eigenvalue $\lambda > 1$ grows slower than all others.
Thus, the effect of switching between two singular sequences is that the eigenstate to the left of the origin is multiplied by λ — this is exactly the way the ansatz should behave!

Fibonacci sequence — the ground state



Blue line corresponds to the ground state wave function ψ on the canonical transverse. Green line represents ψ_0.

Fibonacci sequence — some other state



The values of ψ and ψ_0 on the canonical transverse for a state in the middle of the spectrum (on the edge of a gap).

Conclusions

- The proposed ansatz provides the eigenstates for a subset of perfect quasicrystalline potentials. It englobes both quasi-Bloch and hierarchical solutions.
- The eigenstates are parametrized by Floquet multipliers associated with the "worms" (lines or planes of "atoms ready to jump") in the singular patterns.
- If the set of eigenstates given by the proposed ansatz is complete (and there are strong indications in favor of this hypothesis), one of the consequences would be the presence of the "blind spots" - small regions which are weakly electrically connected to the bulk of the quasicrystal.