Interplay between topology and discrete scaling symmetry : Quasi-crystals

A topological system without magnetic field

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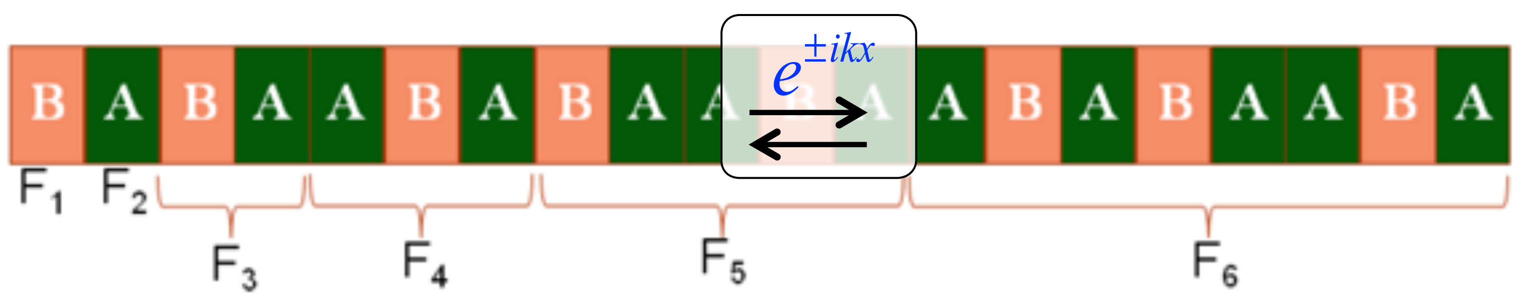
In the previous lecture, we have discussed spectral properties of infinite Fibonacci chains,

and apply them successfully to finite chains.

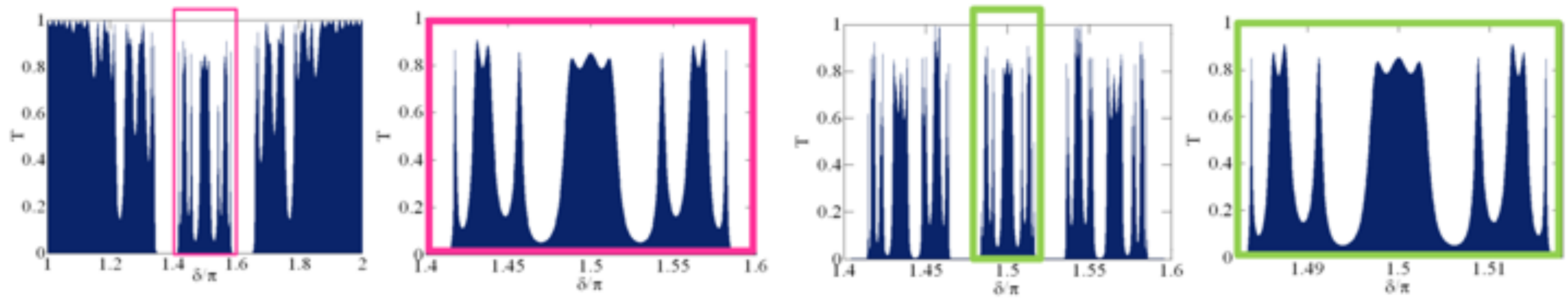
Quasi-periodic stack of dielectric layers of 2 types A, B

Fibonacci sequence : $F_1 = B;\ \ F_2 = A;\ \ F_{j\geq 3} = \left[F_{j-2} F_{j-1} \right]$

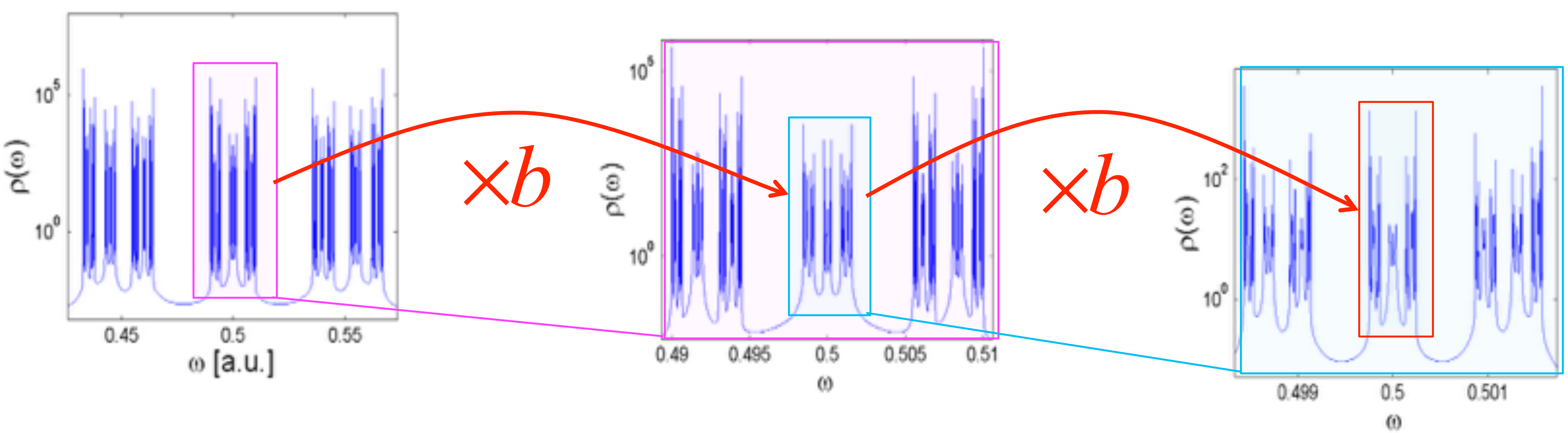


Defines a cavity whose mode spectrum is fractal.

Scaled finite size Fibonacci chains

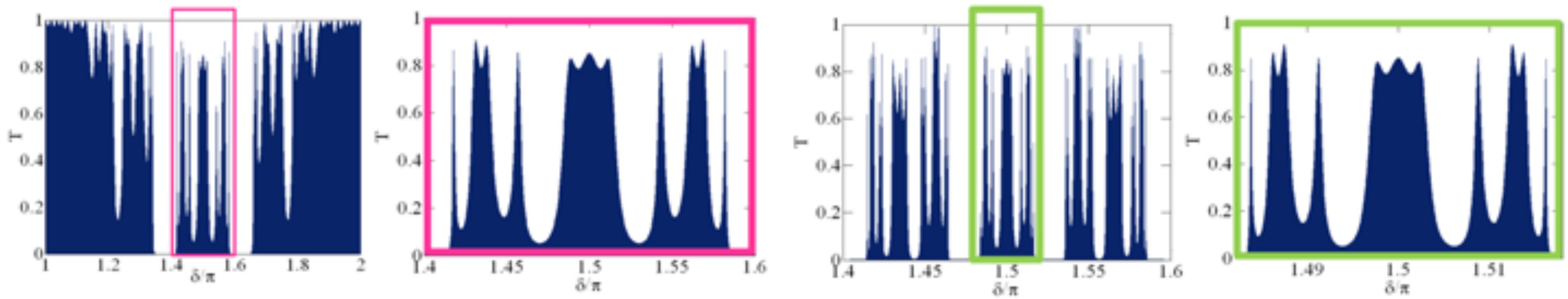


Density of modes

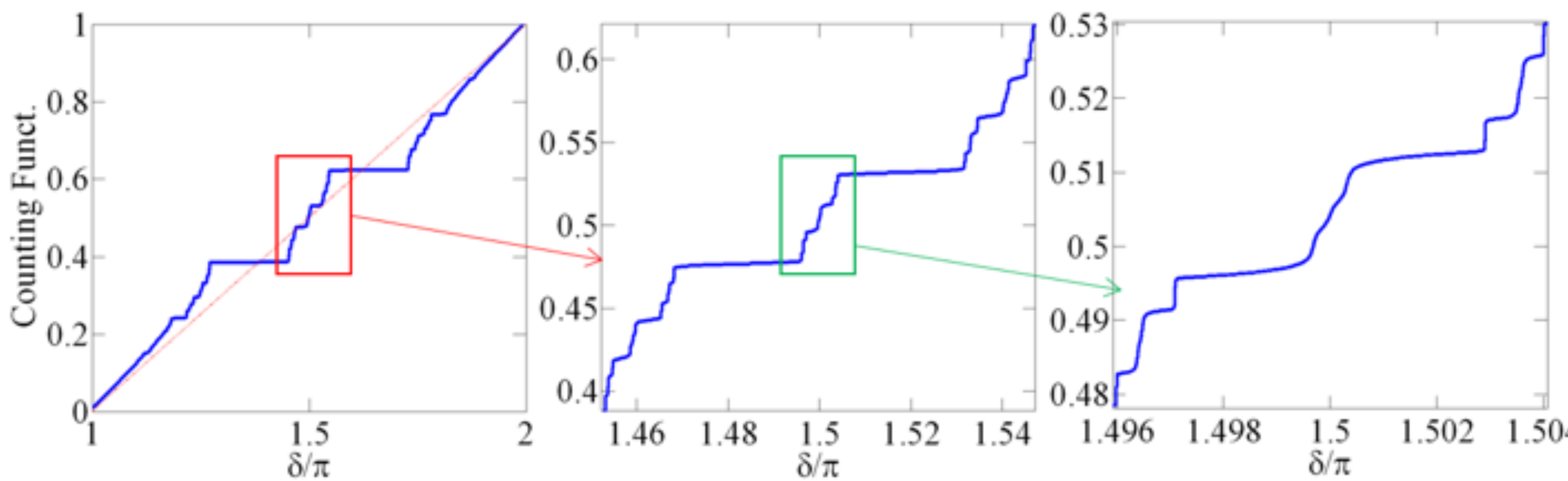


The mode spectrum is self-similar

Scaled finite size Fibonacci chains

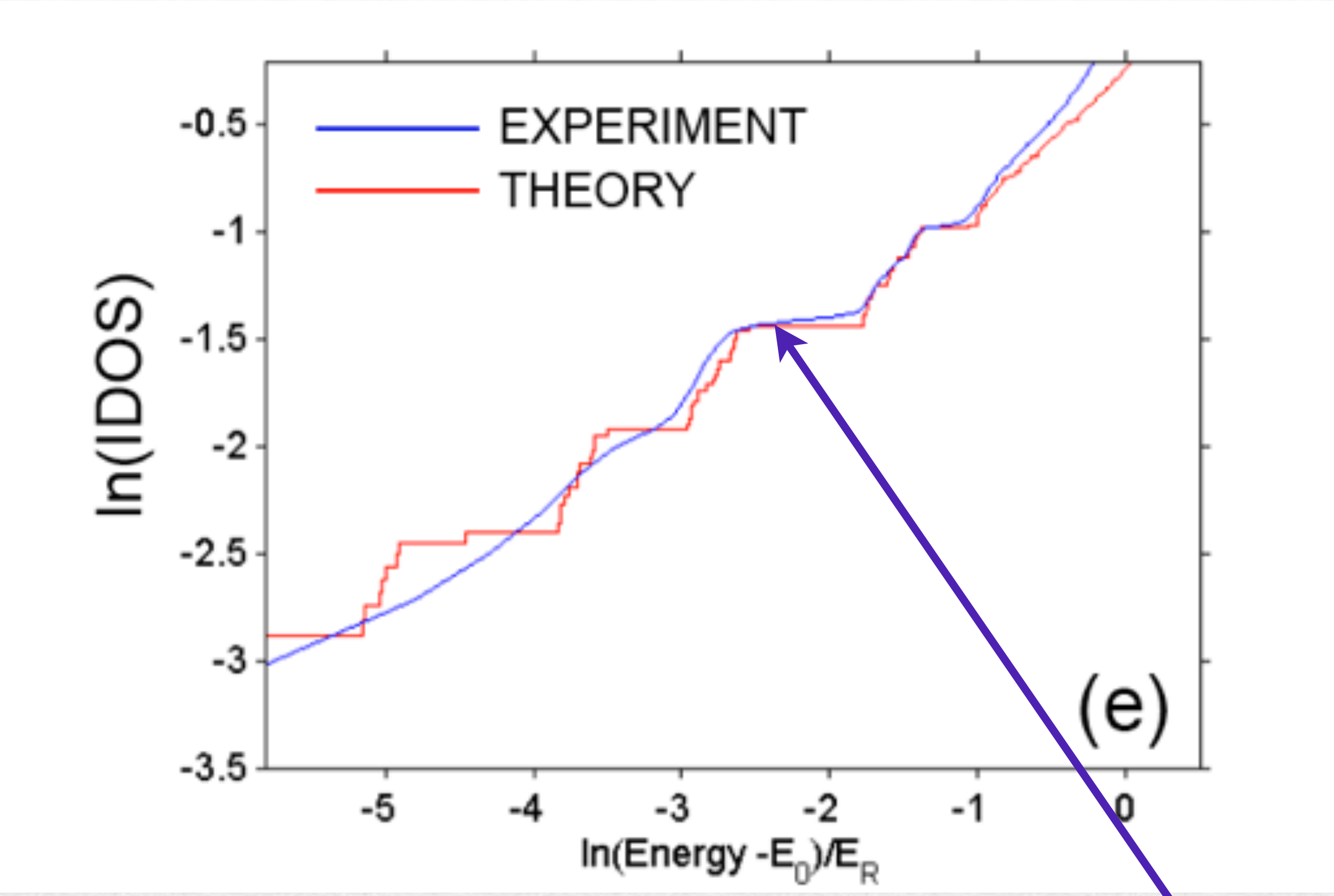


Density of modes



Integrated Density of

Log-periodic oscillating structure is the indisputable fingerprint of the underlying fractal structure of the spectrum.

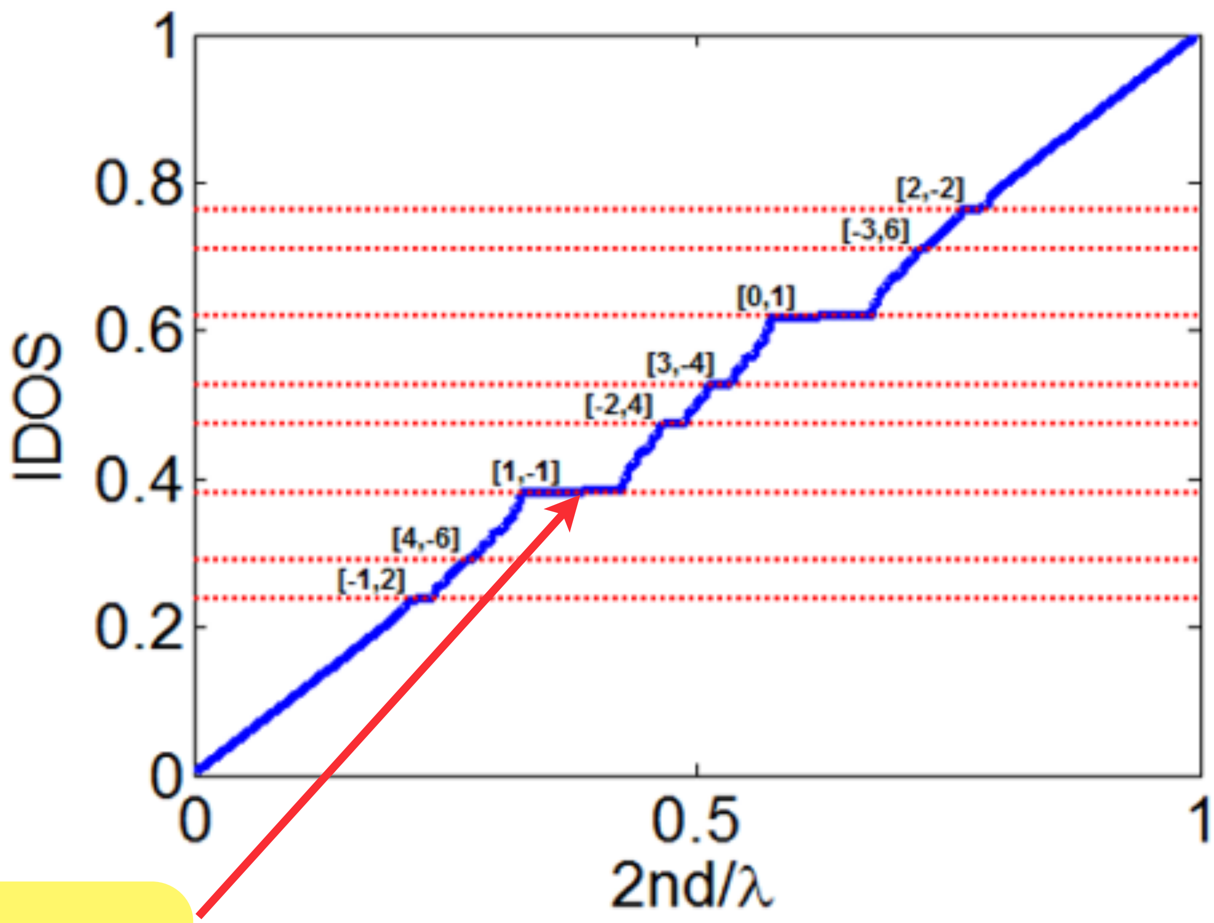


$$N_\omega(\Delta\omega) = (\Delta\omega)^\alpha \times F\left(\frac{\ln|\Delta\omega|}{\ln b}\right), \qquad \alpha = \frac{\ln a}{\ln b}, \quad F(x+1) = F(x)$$

Integrated Density of States-Gap Labeling

$$\tau = \left(1+\sqrt{5}\right)\big/2$$

golden mean



$$N\left(\omega_{gap}\right) = p + q\tau^{-1}$$

within a $\left[p,q\right]$ gap

$\left(p,q\right) \in \mathbb{Z}$ are topological invariants (Chern numbers).
Independent of the potential strength, inhomogeneity, ...

Today's program

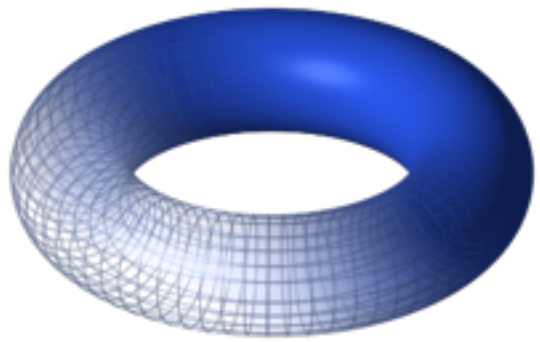
- Investigate topological properties of Fibonacci chains.
- Nature and origin of Chern numbers
- How to obtain Chern numbers from scattering

We mentioned the existence of Chern numbers in the gap labeling theorem.

- Is there a relation with other occurrences of Chern numbers (e.g. in the quantum Hall effect, topological insulators, graphene…) ?

- Not so obvious : in the previous cases, topology and associated Berry connexion result from the existence of underlying magnetic fields, Aharonov-Bohm fluxes, Dirac structure…

Some basic ingredients (more technically),



- Non trivial manifold M (product of manifolds)
- Define over M a structure (fiber bundle) F

Physics: M is the physical space, F is the representation of a continuous symmetry group (field, order parameter,…)

- Define on F a connexion ("vector potential" $\vec{A}$) and a related curvature ("magnetic field" $\vec{B}$).
- Chern classes : define possible topological invariants on F.

Systematic expansion using invariant polynomials (Chern&Weil):

$$\boxed{P(\Omega) = 1 + \underbrace{c_1(\Omega) + c_2(\Omega)}_{\text{Chern classes}} + \cdots}$$

Example : $M=\mathbb{R}^2$ and the order parameter $\psi = |\psi| e^{i\chi}$

Fiber : $F=\mathbb{C}$, Lie group $U(1)$

Connexion 1-form : $\omega = -i\left(A_x dx + A_y dy\right)$

Curvature 2-form : $\Omega = d\omega = -iB$ with $B = \partial_x A_y - \partial_y A_x$

Invariant polynomial : $P(\Omega) = 1 + c_1(\Omega) = 1 + \dfrac{B}{2\pi}$

Chern number : $\dfrac{1}{2\pi}\int_M c_1(\Omega) = n \in \mathbb{Z}$

over a closed manifold M

Flux quantisation condition.

K. Mallick, E.A., “topological aspects of low dimensional systems”, Les Houches, 1998

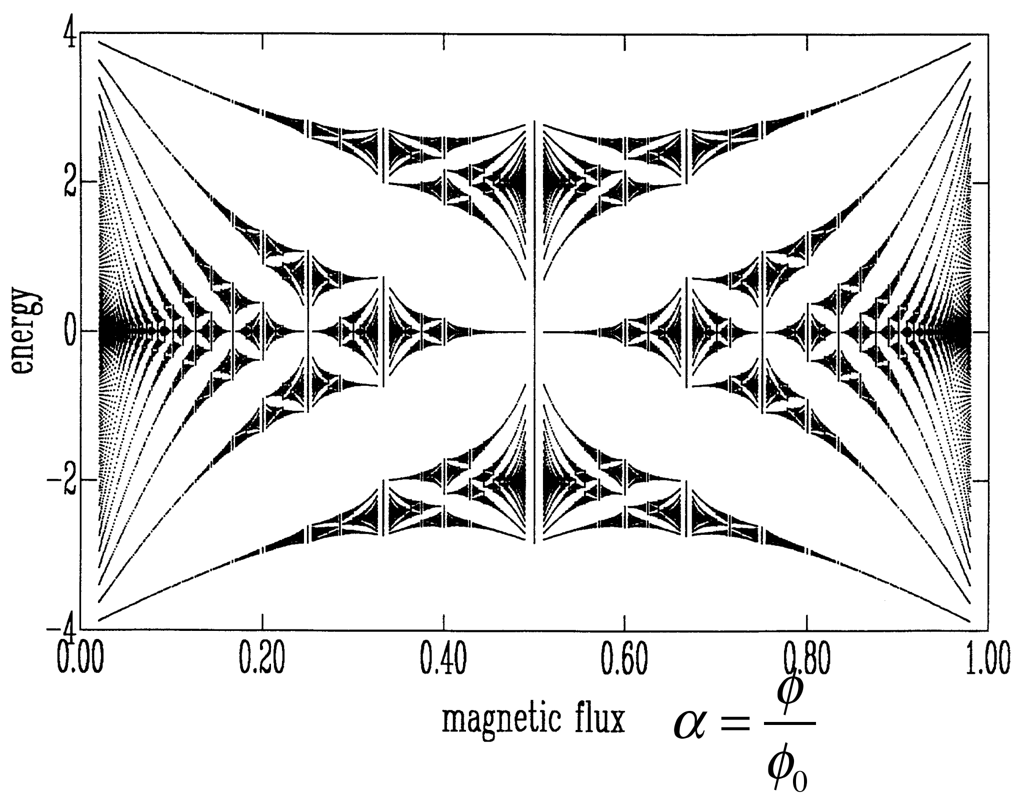
Example : Free electrons in a 2D crystal + magnetic field

(Harper problem)

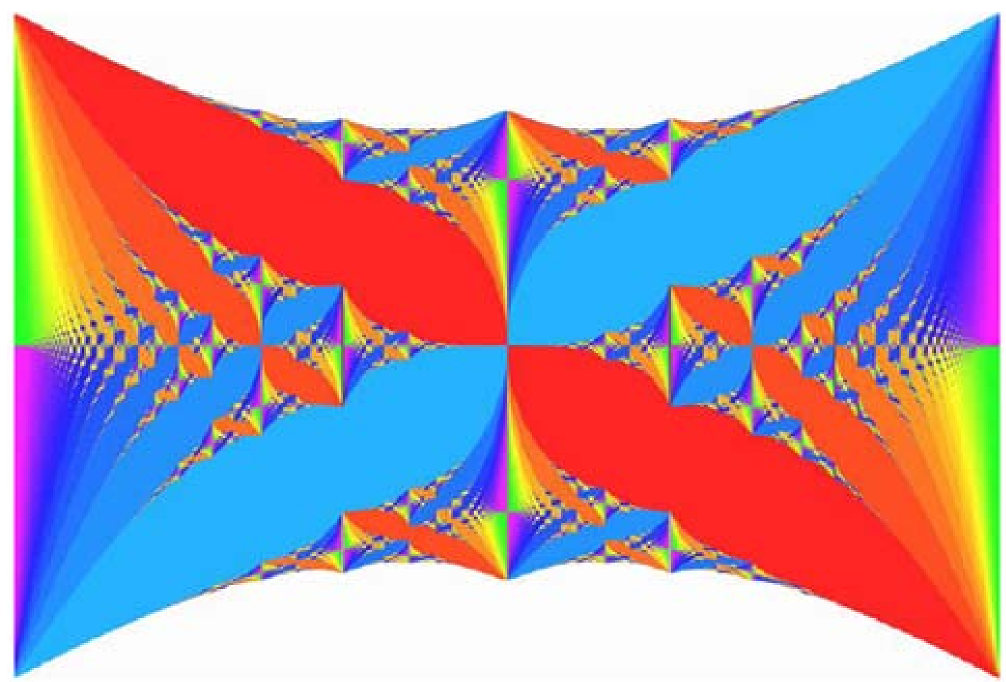
Non trivial group of magnetic translations: $\begin{cases} U_1 = e^{iK_x} \\ U_2 = e^{iK_y} \end{cases}$

$$\boxed{U_1 U_2 = e^{2i\pi\alpha} U_2 U_1}$$

$$\alpha = \frac{\phi}{\phi_0} \qquad \phi_0 = \frac{h}{e}$$



Hofstadter butterfly



Osadchy, Avron, (2001)

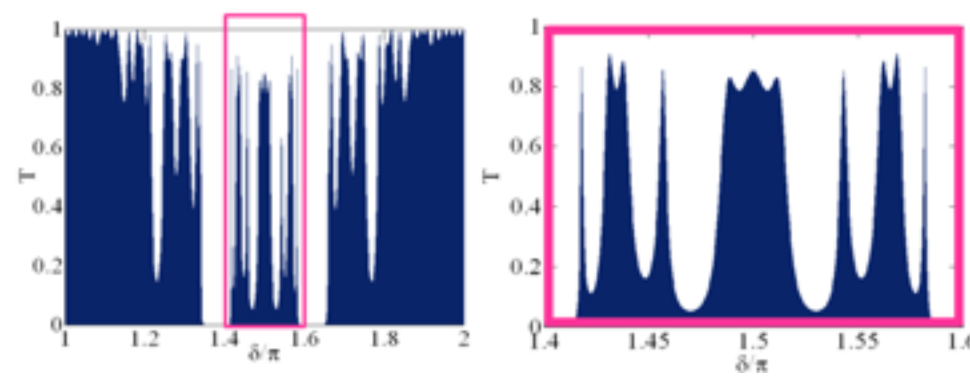
Fibonacci quasi-crystal : Is there a (Berry) connexion and a corresponding curvature whose integral produces corresponding Chern numbers ?

Is it possible to define a non trivial fiber bundle such as the group of magnetic translations in the Harper model ?

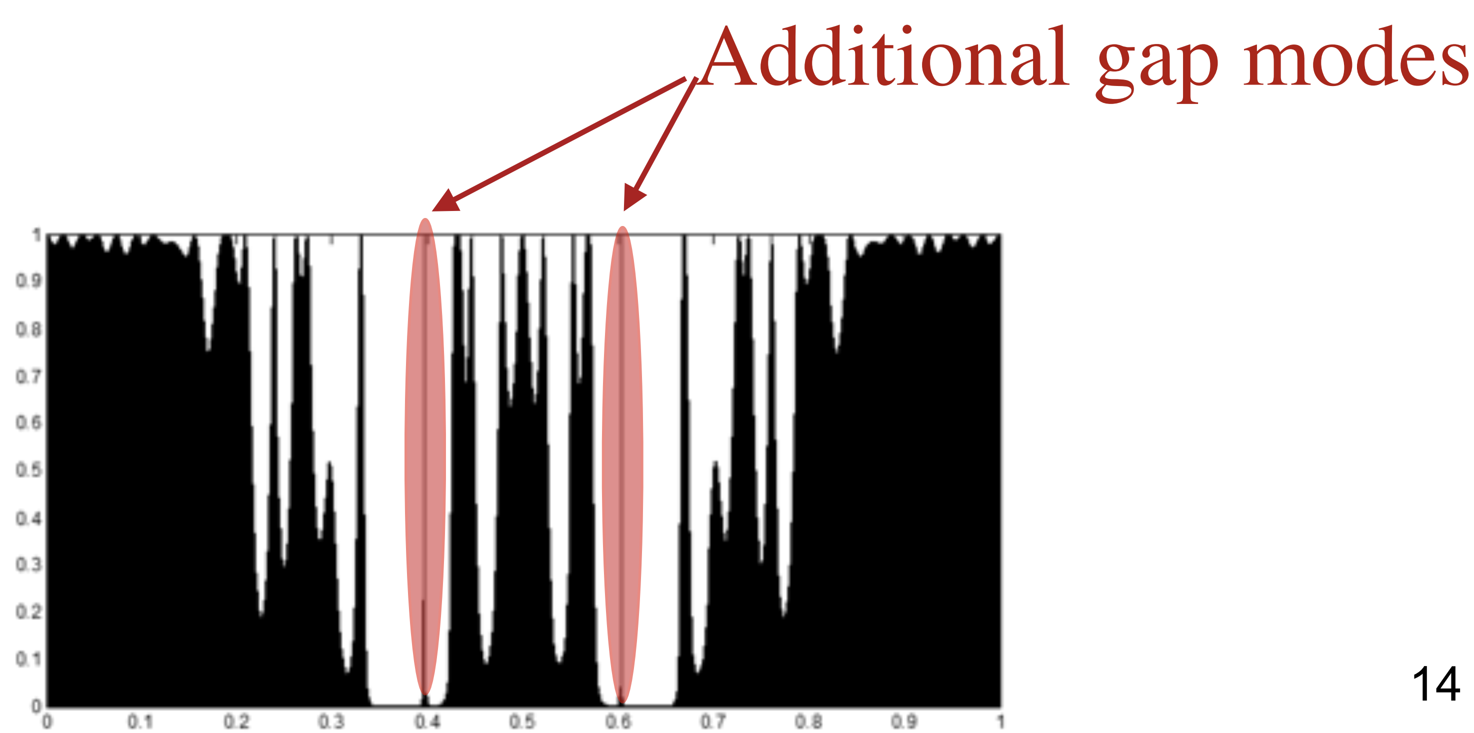
Is there a quantity playing the role of a magnetic field ?

Topological features manifest through specific properties of edge (gap) modes in the presence of boundaries

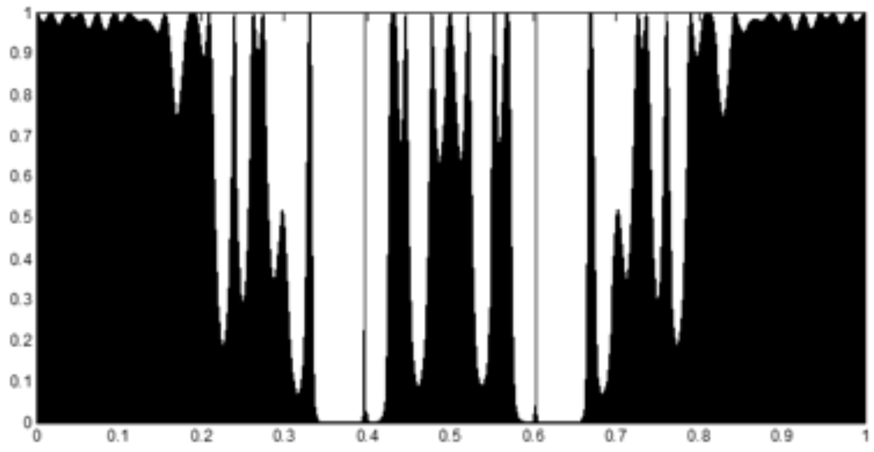
Under certain (boundary) conditions, instead of observing

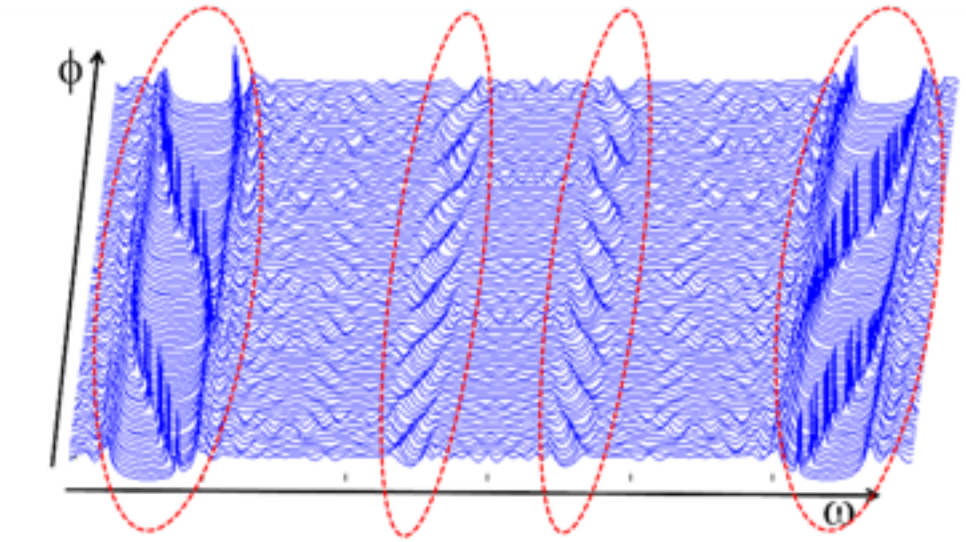


we observe

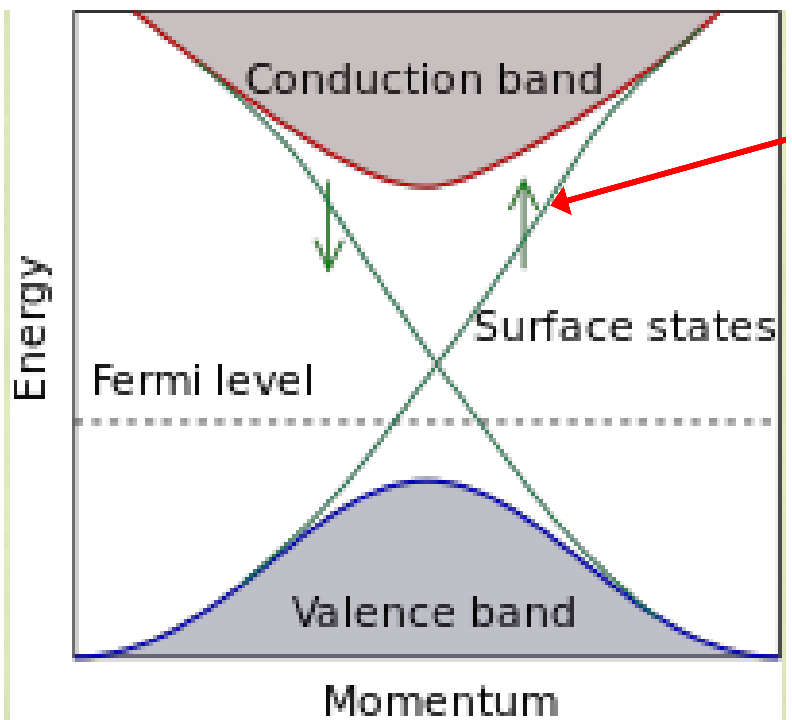


These gap modes "move" through the gaps as a function of a parameter ϕ yet to be determined





analogous to

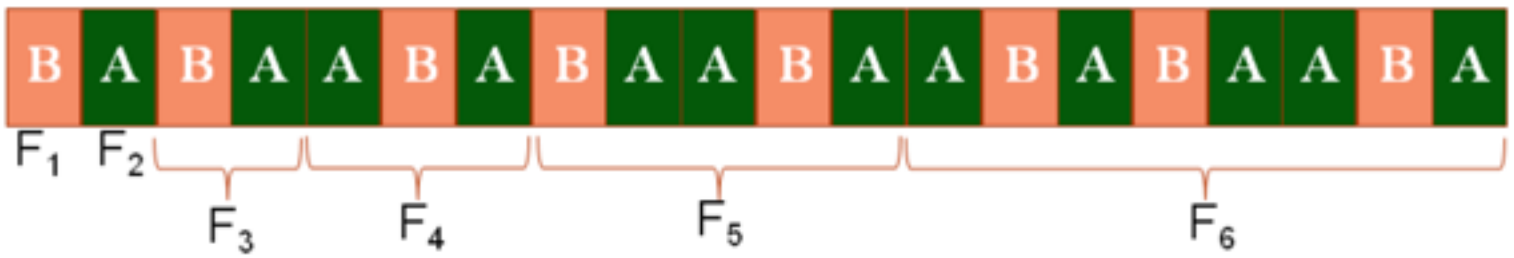


To understand the existence and nature of edge states, we need to discuss the different (equivalent) ways to build a quasi-periodic chain.

- Concatenation
- Substitution matrix
- Characteristic function
- Cut & Project

Concatenation

Fibonacci sequence : $F_1 = B;\ \ F_2 = A;\ \ F_{j\geq 3} = \left[F_{j-2} F_{j-1} \right]$



The length of the chain is necessarily a Fibonacci number :

1,2,3,5,8,13,21…

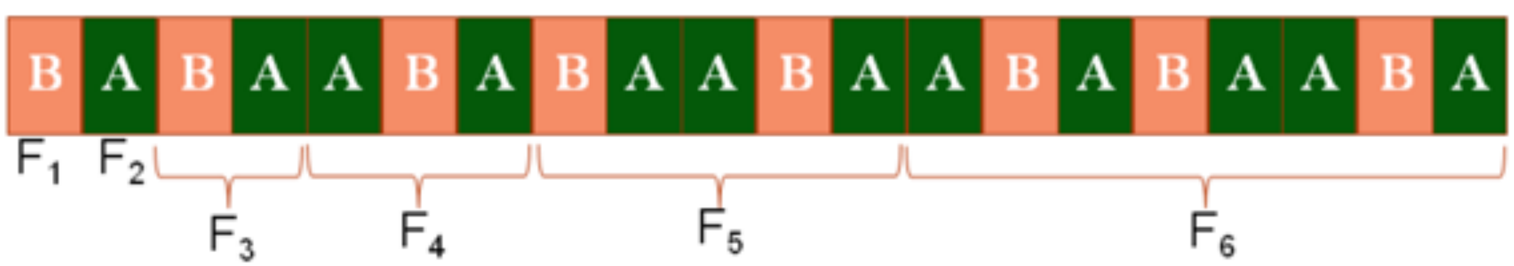
It is thus not possible to generate a chain of arbitrary length.

Substitution matrix

Consider a substitution σ acting on an alphabet of two letters A and B :

$$\sigma : \begin{cases} A \rightarrow BA \\ B \rightarrow A \end{cases} \qquad M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$

To this substitution, we associate a matrix M, whose columns give the number of letters A and B which occurs in the transforms.



By successive applications of σ we generate a word $F_{N+1} = \sigma^N(B)$ of length F_N (a Fibonacci number). The words $\sigma^N(B)$ converge to an infinite sequence $\sigma^\infty(A)$ left invariant by σ (fixed point).

Characteristic function

(B. Simon, J.M. Luck, Krauss & Zilberberg, PRL, 2012.

$$\chi_n = sign\left[\cos\left(2\pi n\tau^{-1}+\phi\right)-\cos\left(\pi\tau^{-1}\right)\right]$$

$-1 =$ B
$+1 =$ A

$$F_N = \left[\chi_1\,\chi_2\cdots\chi_n\cdots\chi_N\right] \quad \Leftrightarrow$$

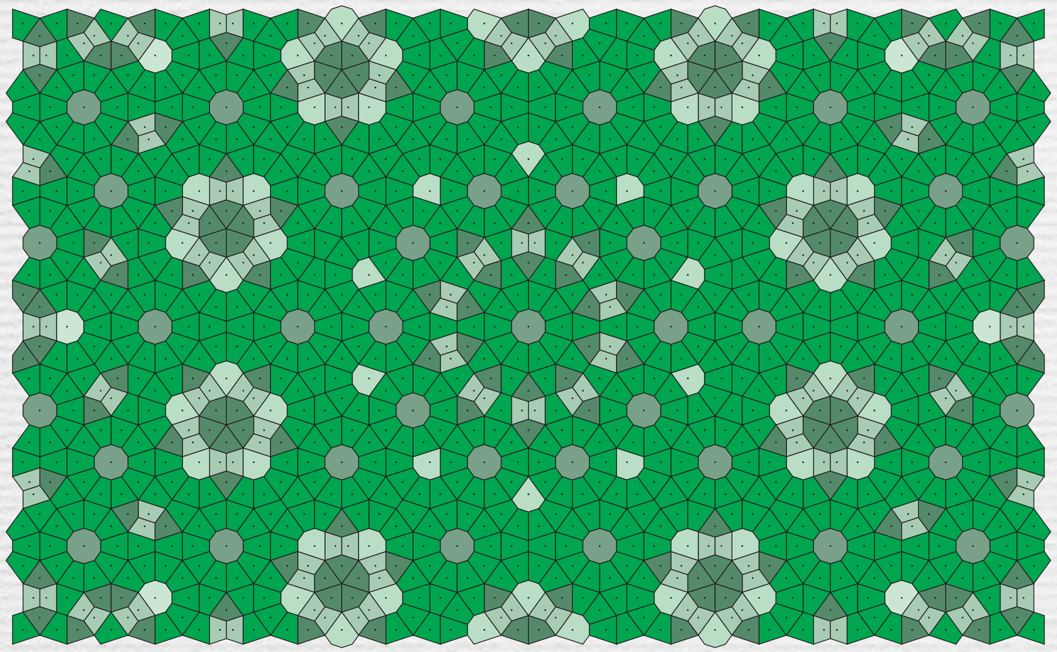
A B A A B A B A A B A A B ...

The angle ϕ appears as a new and legitimate degree of freedom. It is usually ignored.

when ϕ is not ignored it is considered a nuisance,
not here!

Cut & Project method (maps)

Very active branch in maths of tiling, dynamical systems, (classical) information theory,….

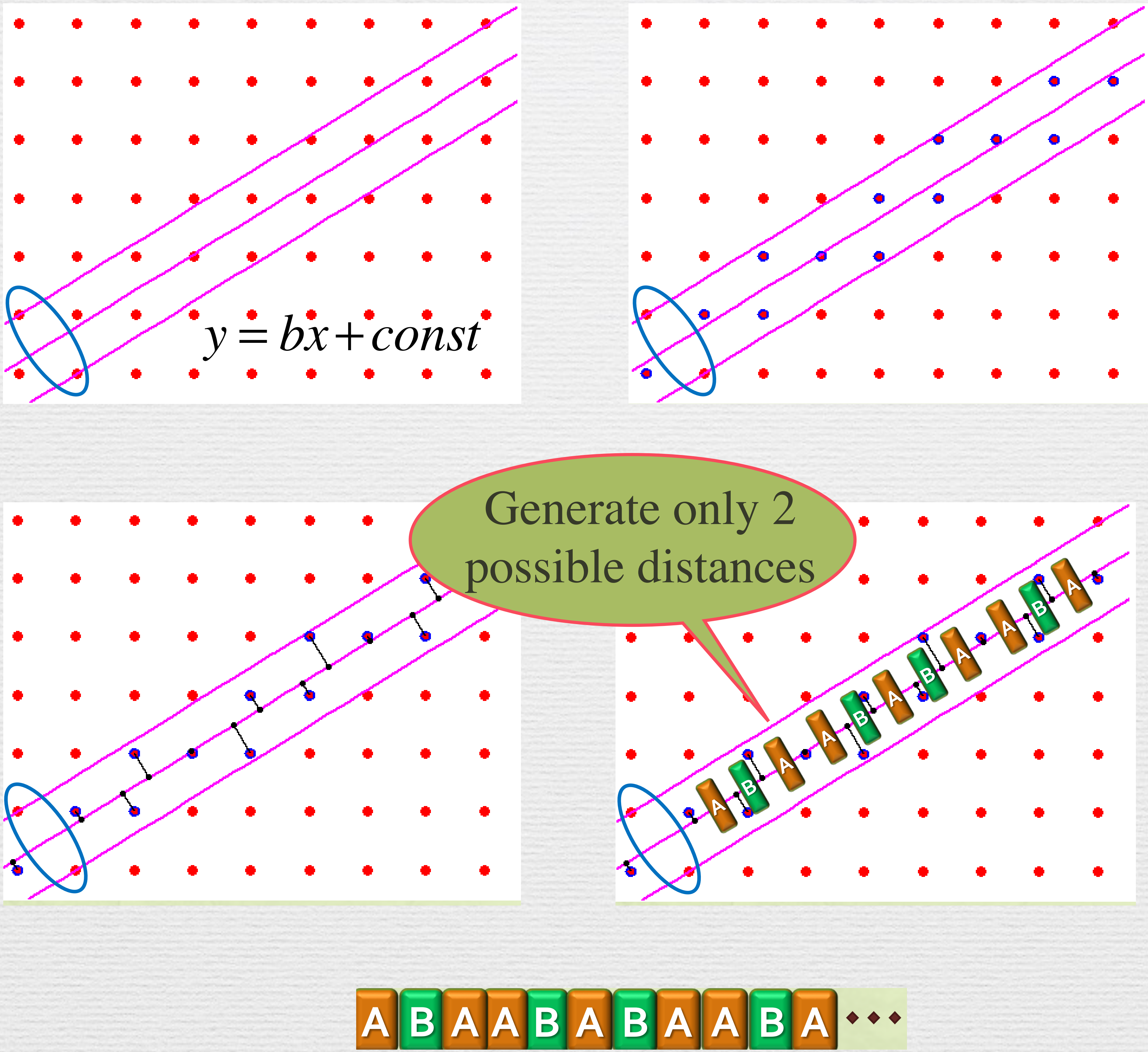


Duneau & Katz
Moody, Meyer
Pinsner, Voiculescu
Mendes-France, Allouche
Bombieri, Taylor,
Kellendonk, Grimm,
Queffelec, Bellissard, ……

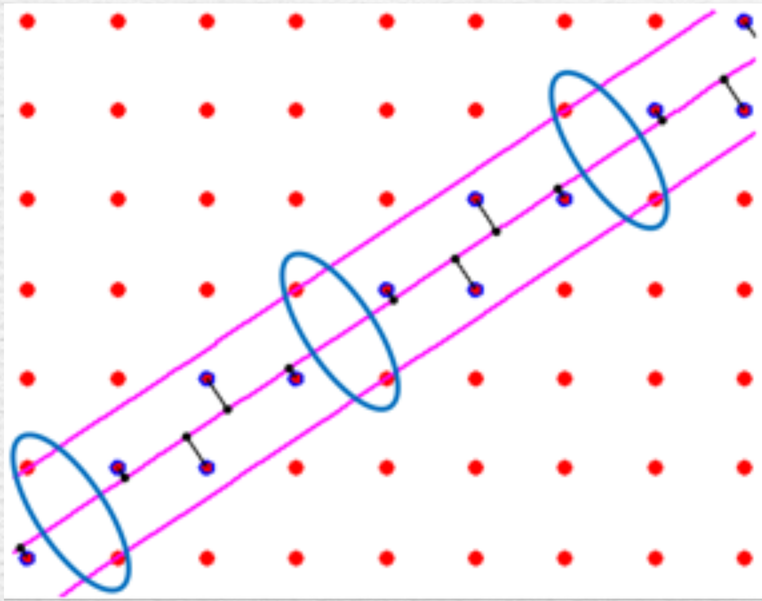
Generate both periodic and quasi-periodic (quasicrystals) structures.

A brief tutorial for practical implementation in 1D.

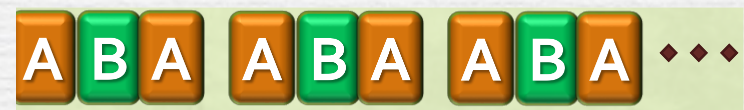
Start from a 2D periodic lattice $L = \mathbb{Z}^2$



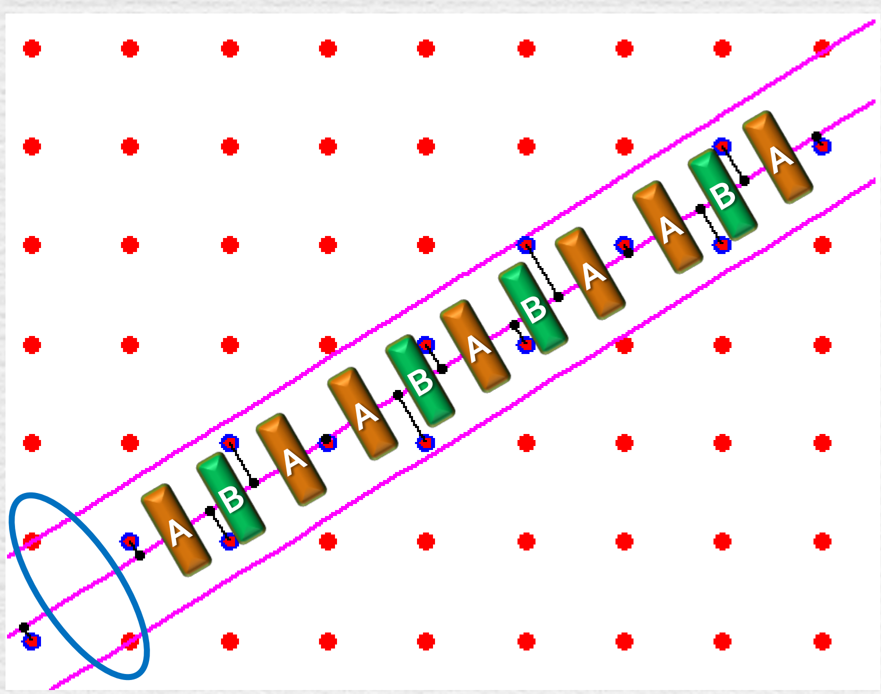
For a rational slope : periodic superlattice



$$y=\tfrac{2}{3}x+const$$



For an irrational slope : quasi-periodic structure



$$y=\tau^{-1}x+const$$

$$\tau = \left(1+\sqrt{5}\right)\big/2$$

golden mean

All the four previous methods are **equivalent** and allow to generate infinite quasi-periodic Fibonacci chains.

But they involve important and interesting differences :

- Substitution and concatenation generate fixed structures : chains of length given by a Fibonacci number.

- C&P and characteristic functions do not involve constraint on the length.

More importantly, they allow for an additional degree of freedom, the phase ϕ which appears in the characteristic function approach.

Meaning of this elusive phase ϕ in the C&P approach ?

Characteristic function

$$\chi_n = sign\left[\cos\left(2\pi n\,\tau^{-1}+\phi\right)-\cos\left(\pi\,\tau^{-1}\right)\right]$$

ϕ is usually an innocuous and thus ignored modulation phase.

For an infinite (Fibonacci) structure :

$$\phi_\infty = 3\pi\sigma = 3\pi\,\tau^{-1}$$

Define instead

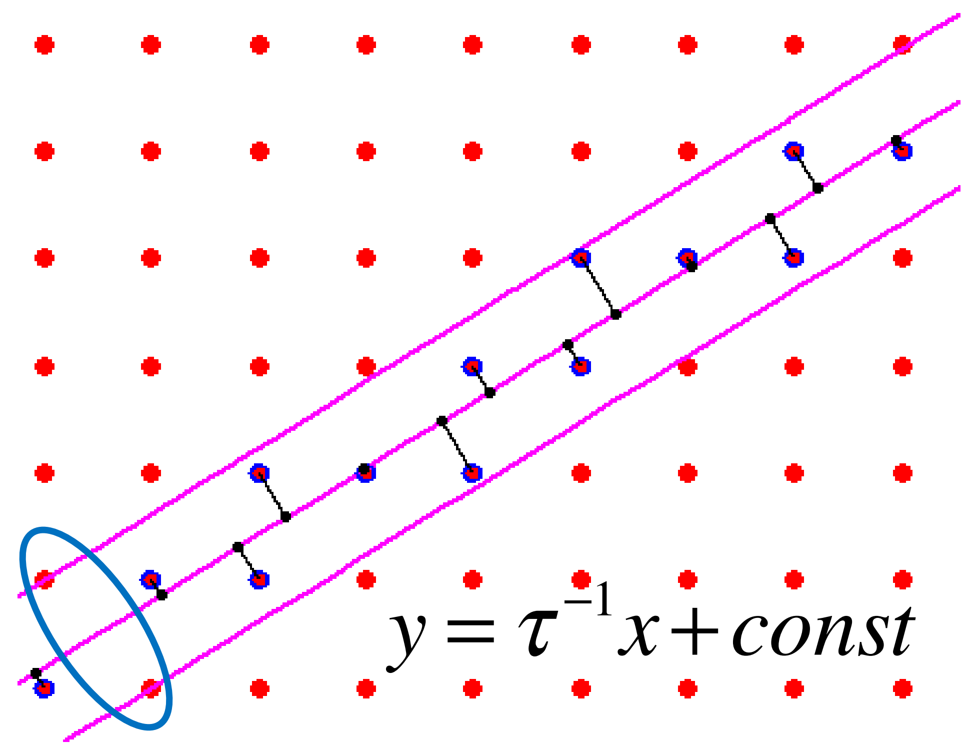
$$\chi_n = sign\left[\cos\left(2\pi n\tau^{-1}+\phi_\infty+\Delta\phi\right)-\cos\left(\pi\tau^{-1}\right)\right]$$

$$\tau = \left(1+\sqrt{5}\right)\big/2$$

golden mean

C&P method

Is it possible to give a meaning to the phase $\Delta\phi$ within the C&P method ?



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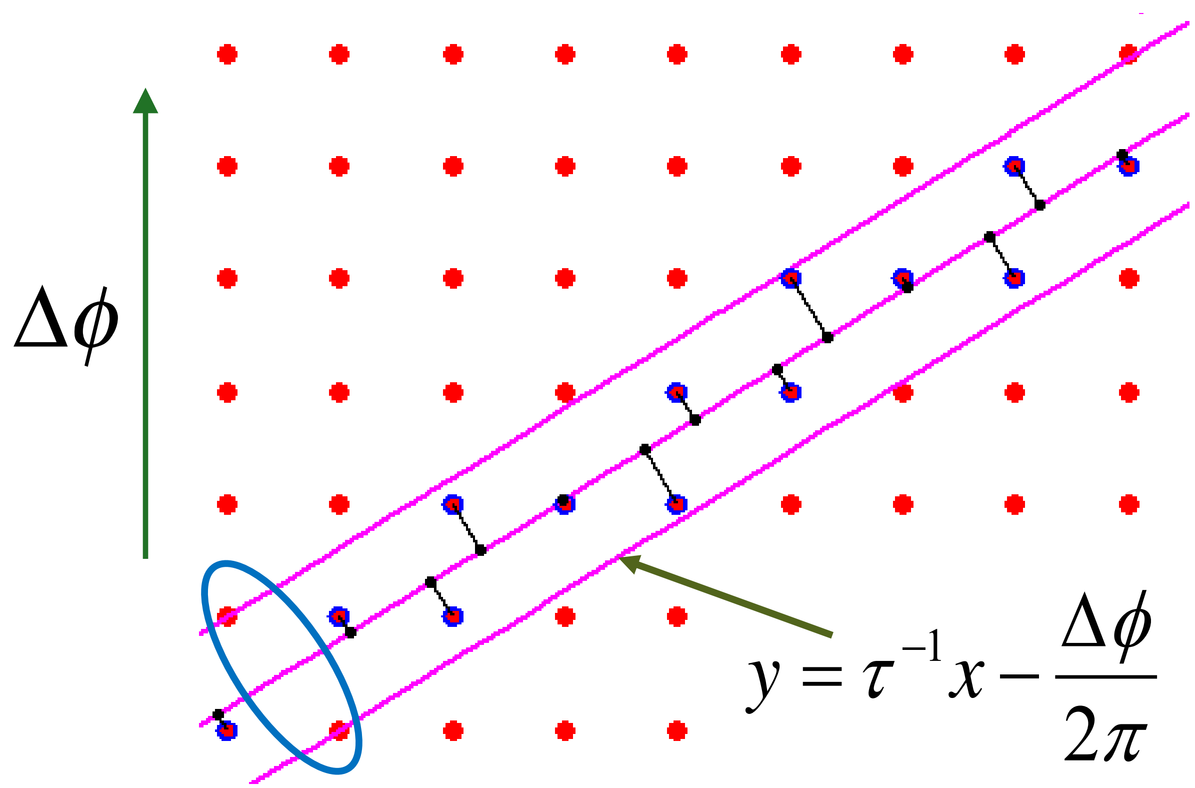
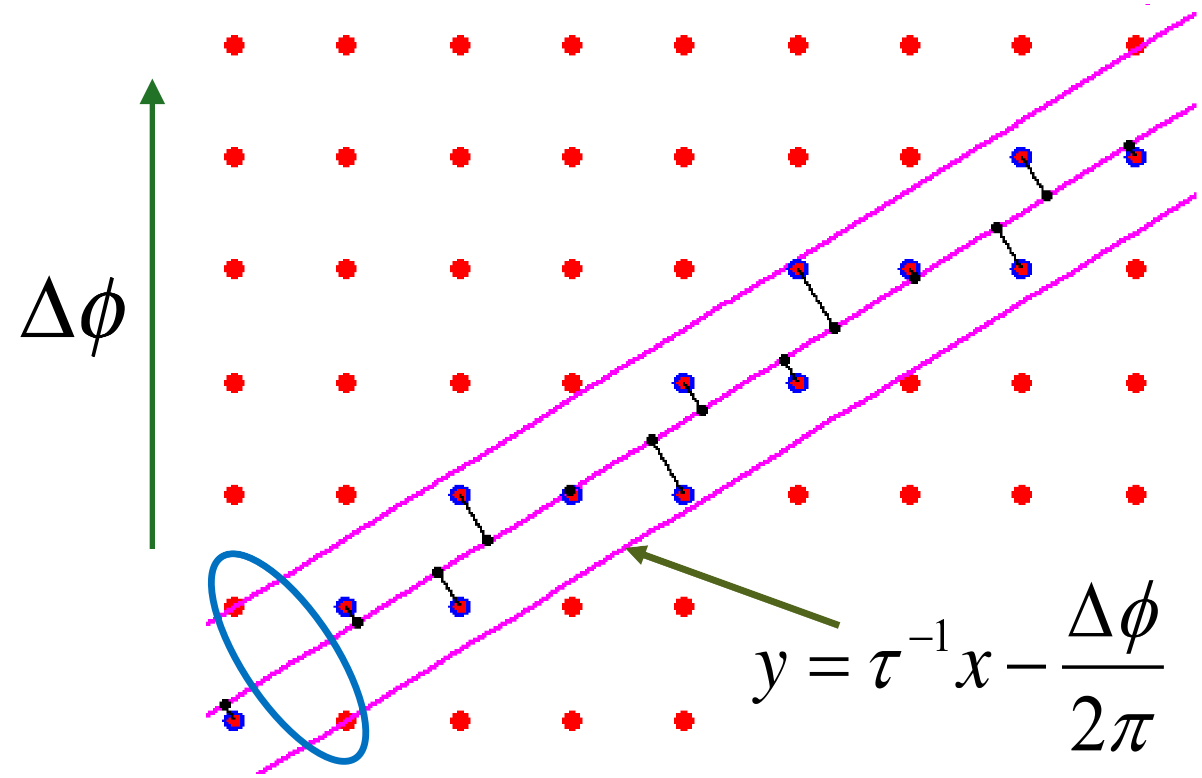


We better understand the meaning of $\Delta\phi$

C&P method - Properties

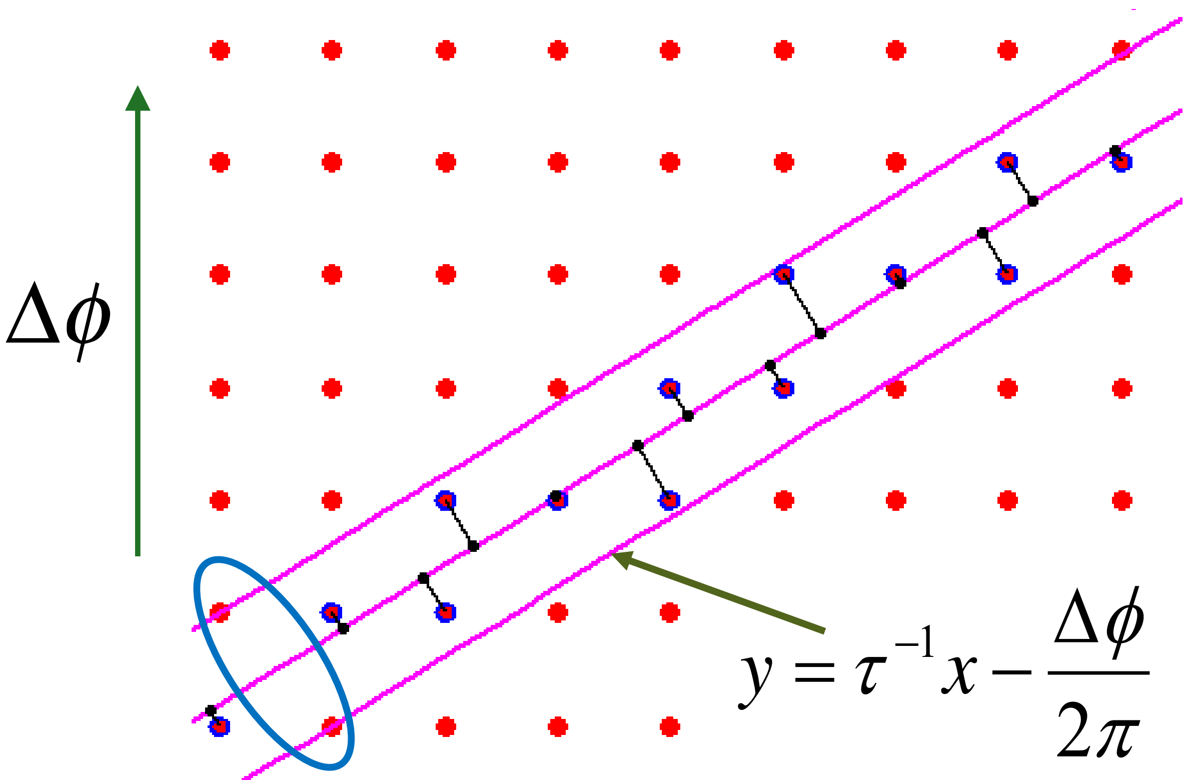


- Each value of the phase $\Delta\phi$ accounts for an existing segment of the infinite Fibonacci chain.

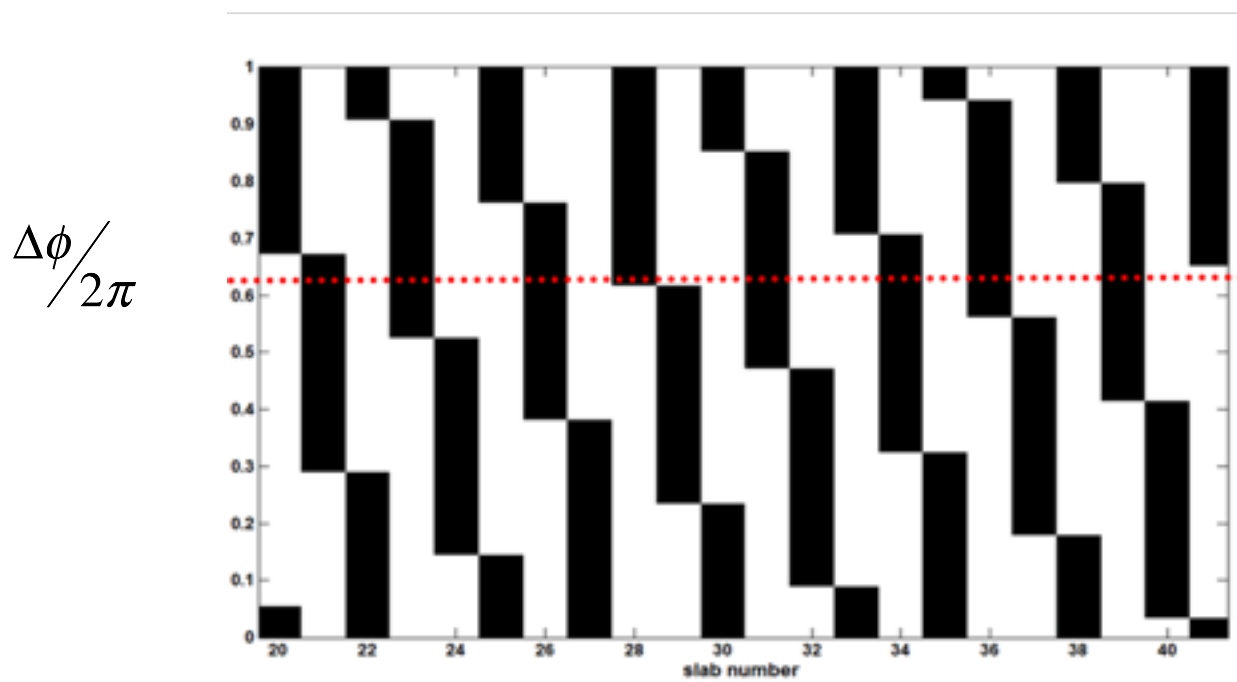
- $\Delta\phi$ is 2π-periodic.

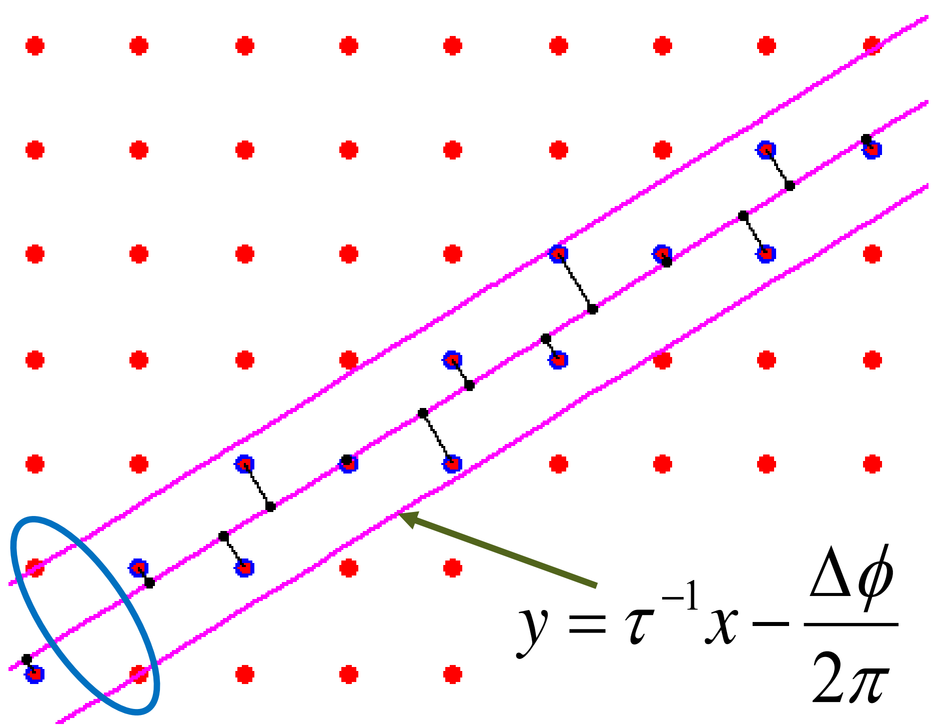
- $\Delta\phi$ corresponds to a translation (along the chain) cycle

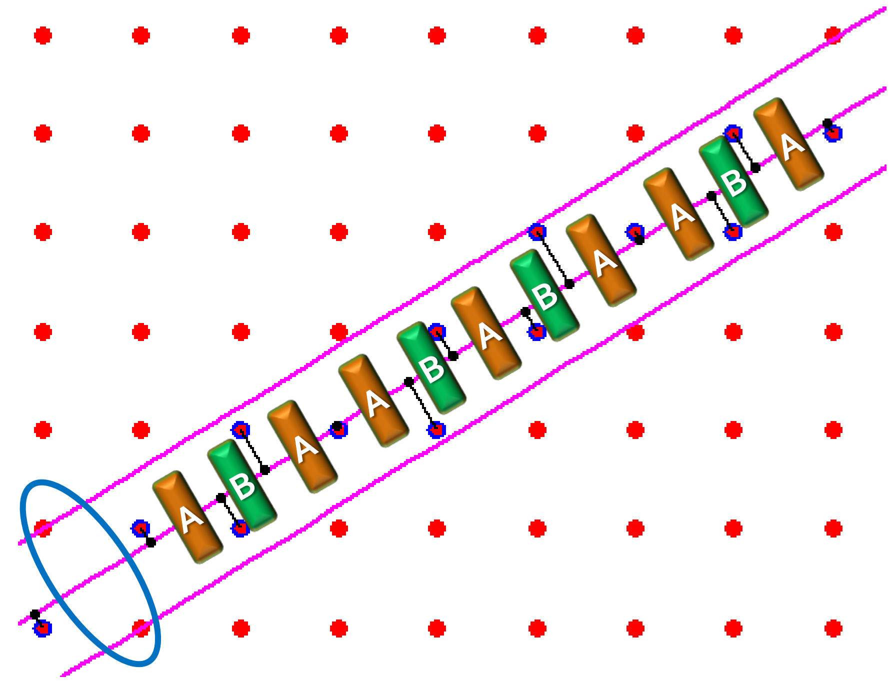
$$\Delta\phi = 2\pi\tau^{-1}\,\Delta n$$



How a change of phase is implemented along the chain ?







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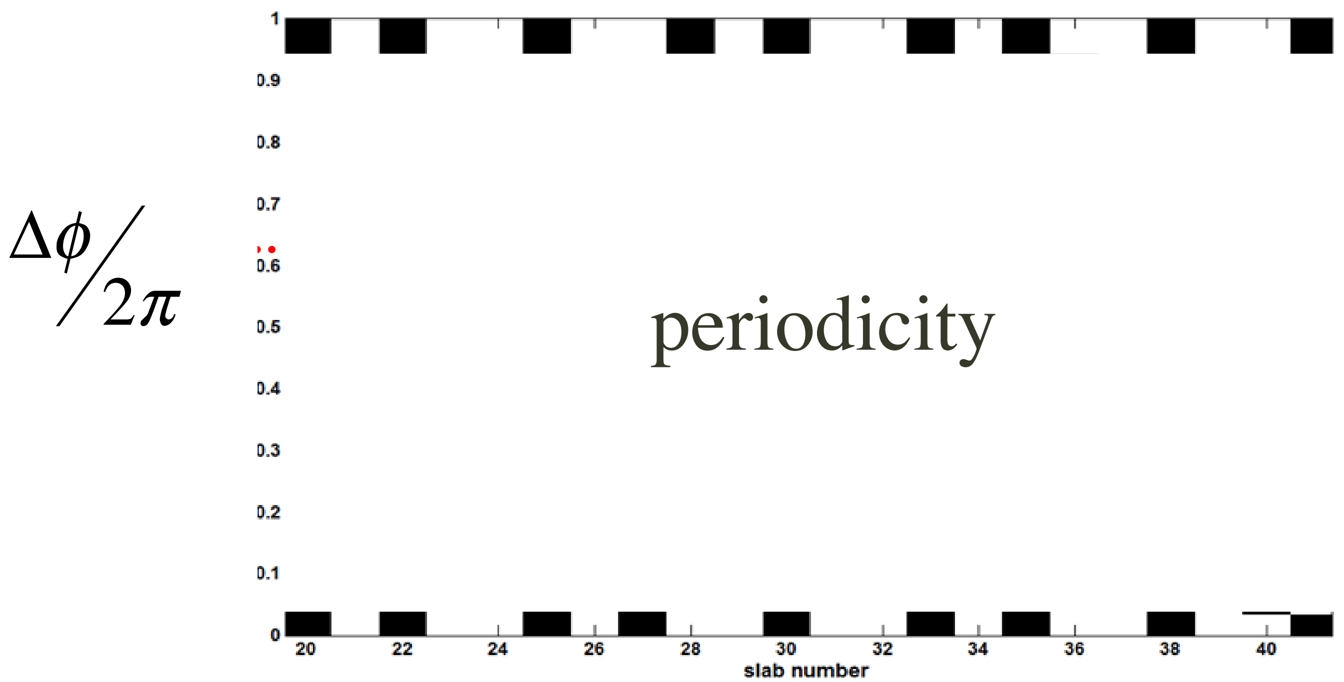

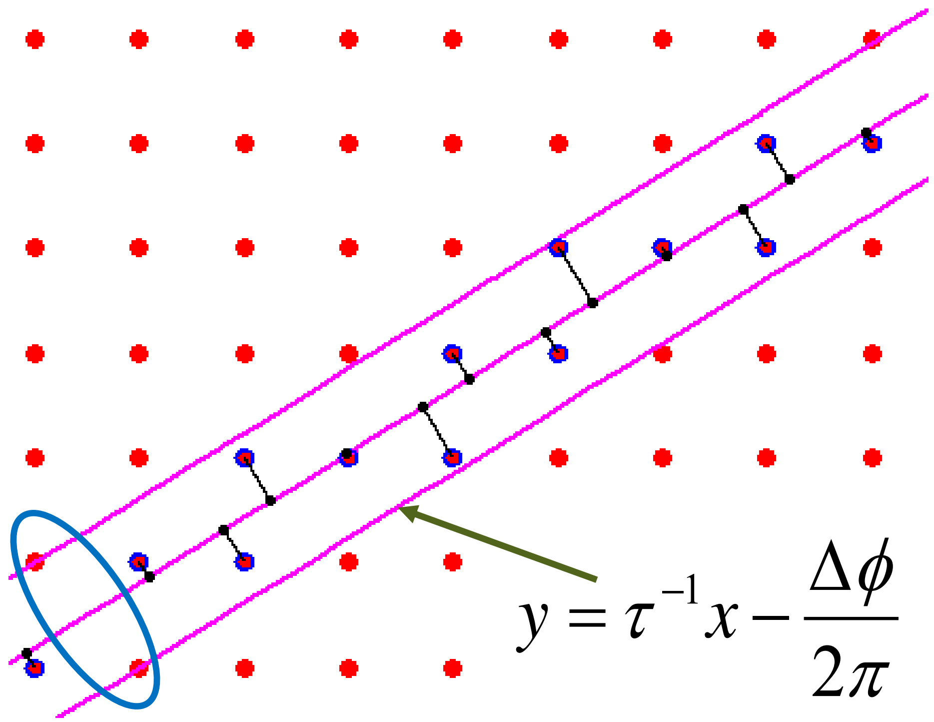

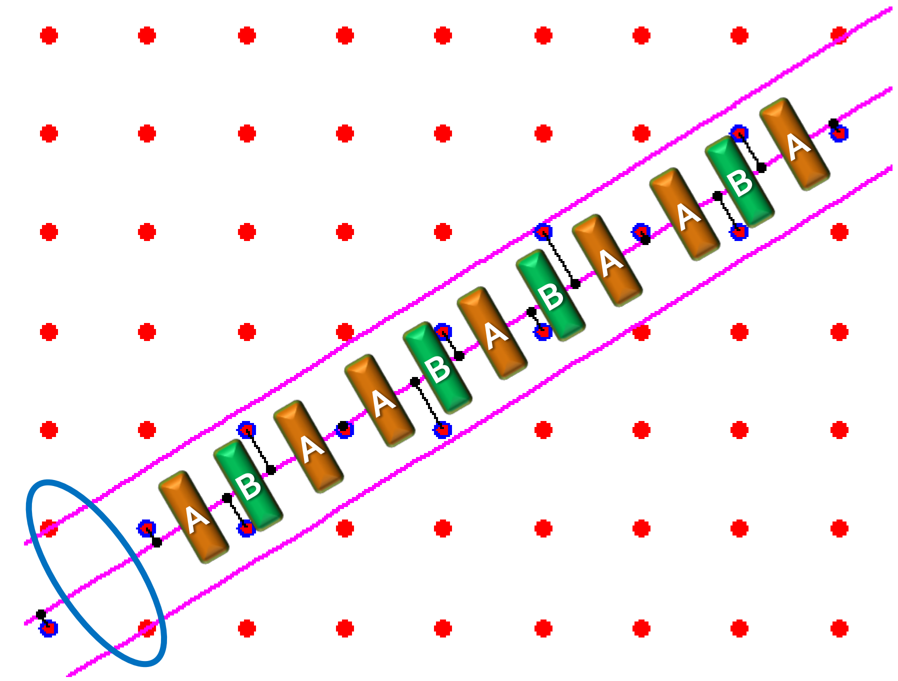

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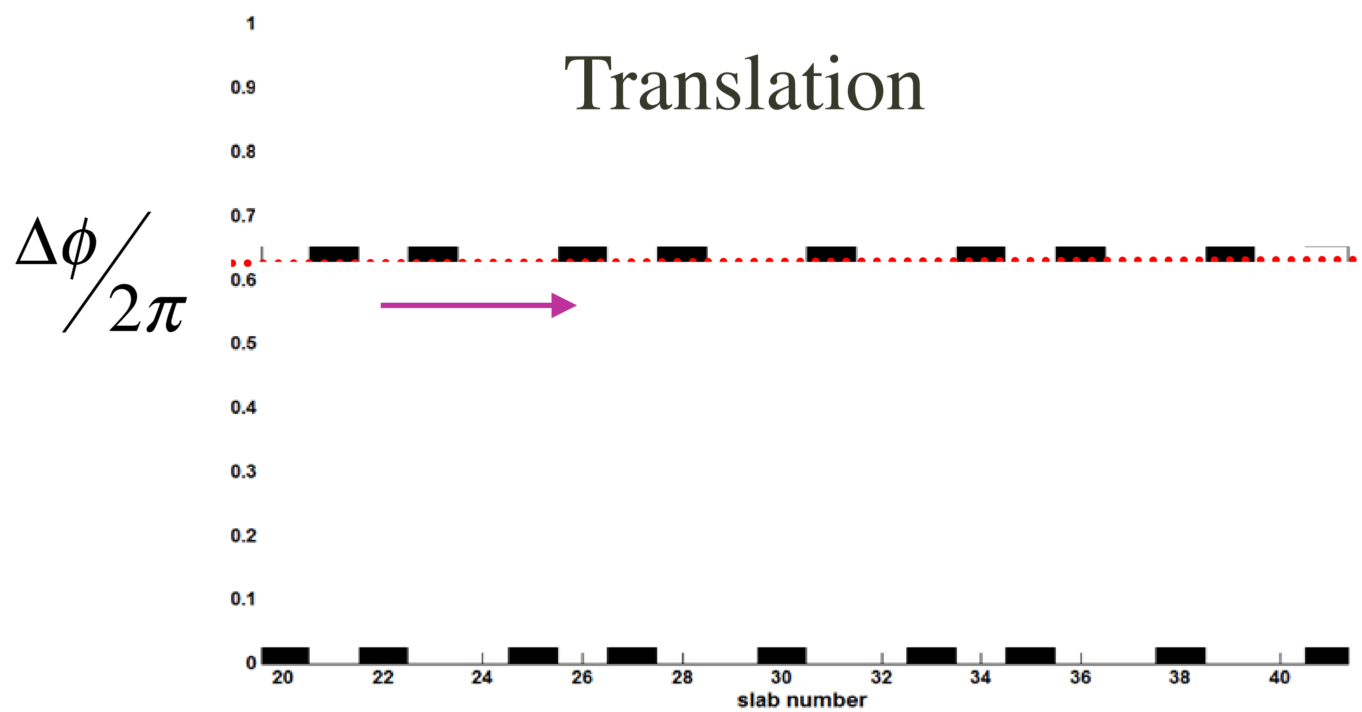
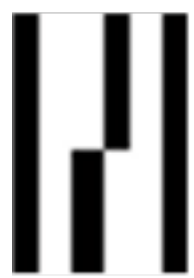
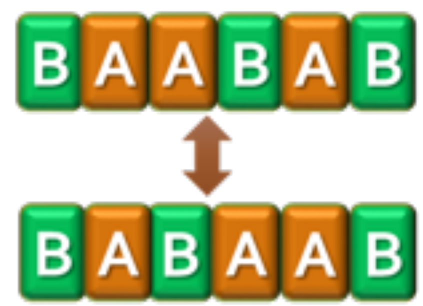


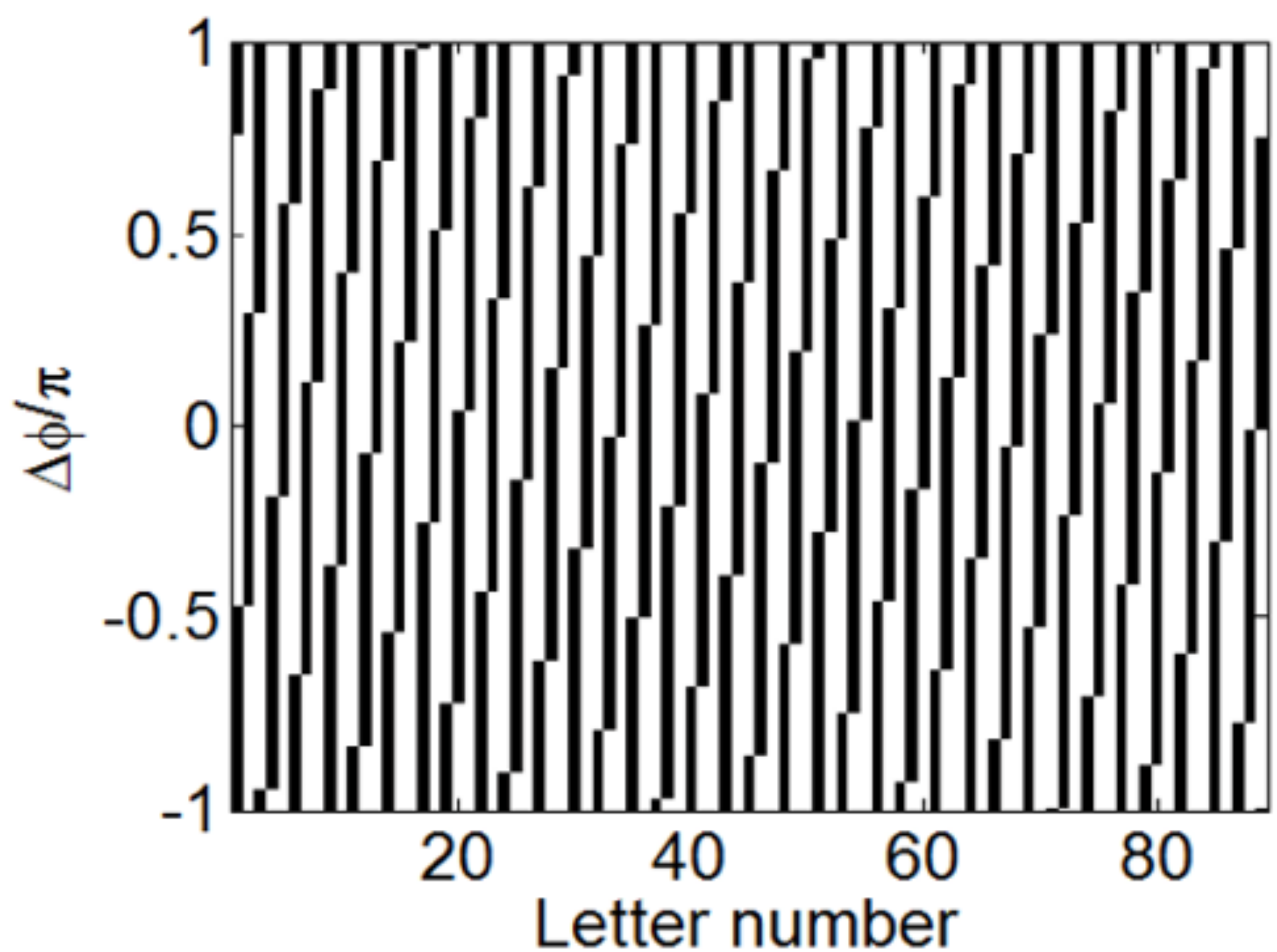
A structural degree of freedom

Scanning $\Delta\phi$ generates **local** structural changes.

These changes have a meaning only for a finite length chain







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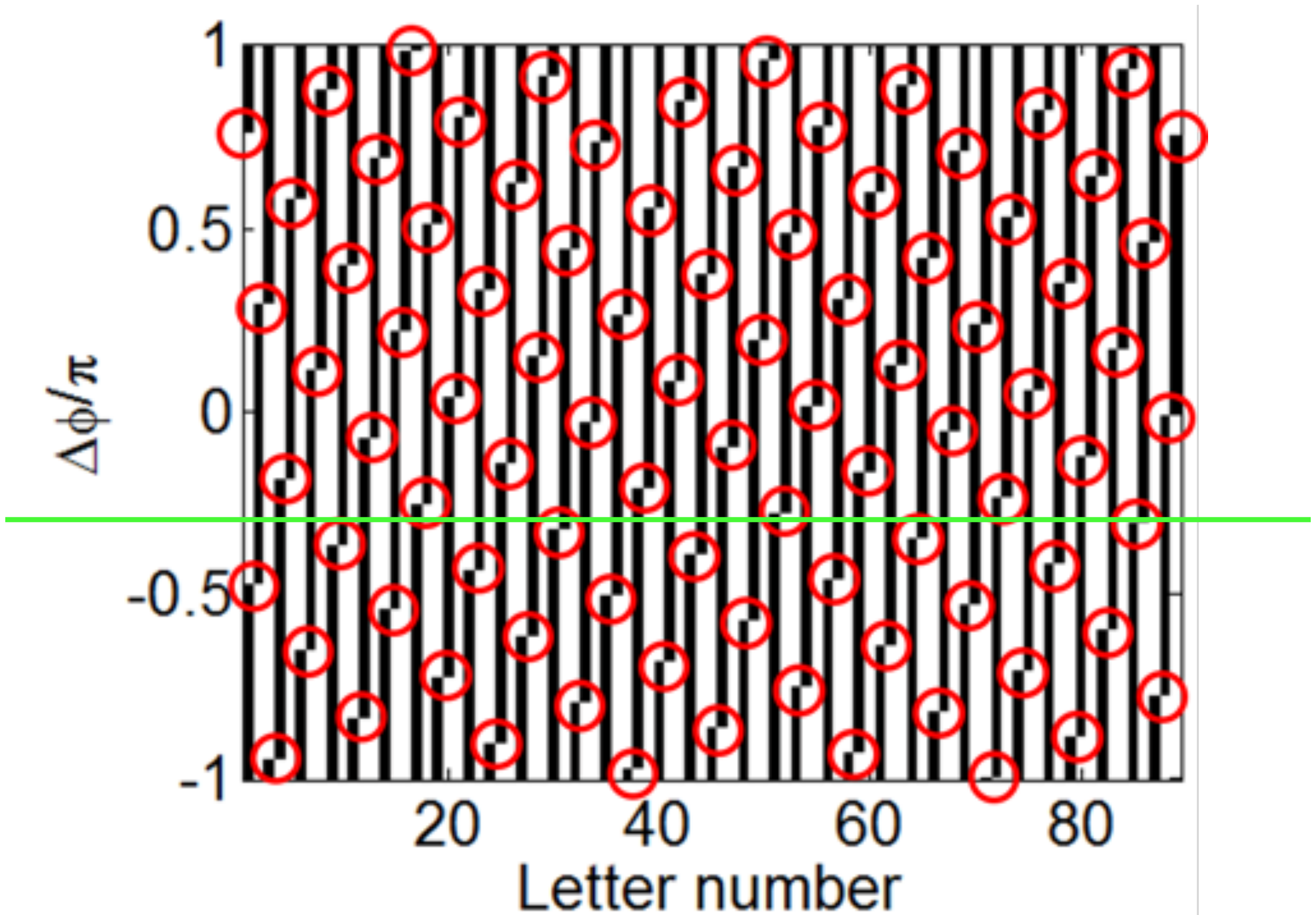
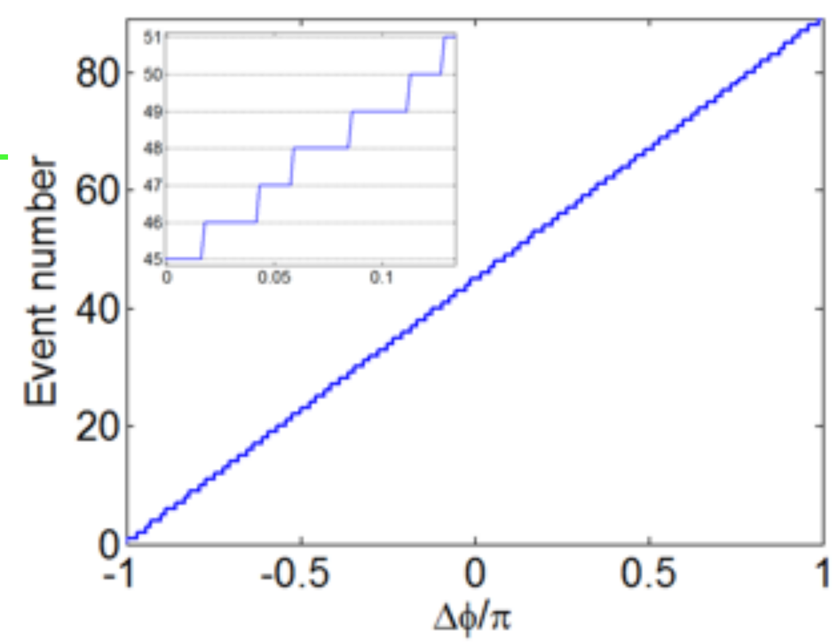


A single structural change for each value of $\Delta\phi$

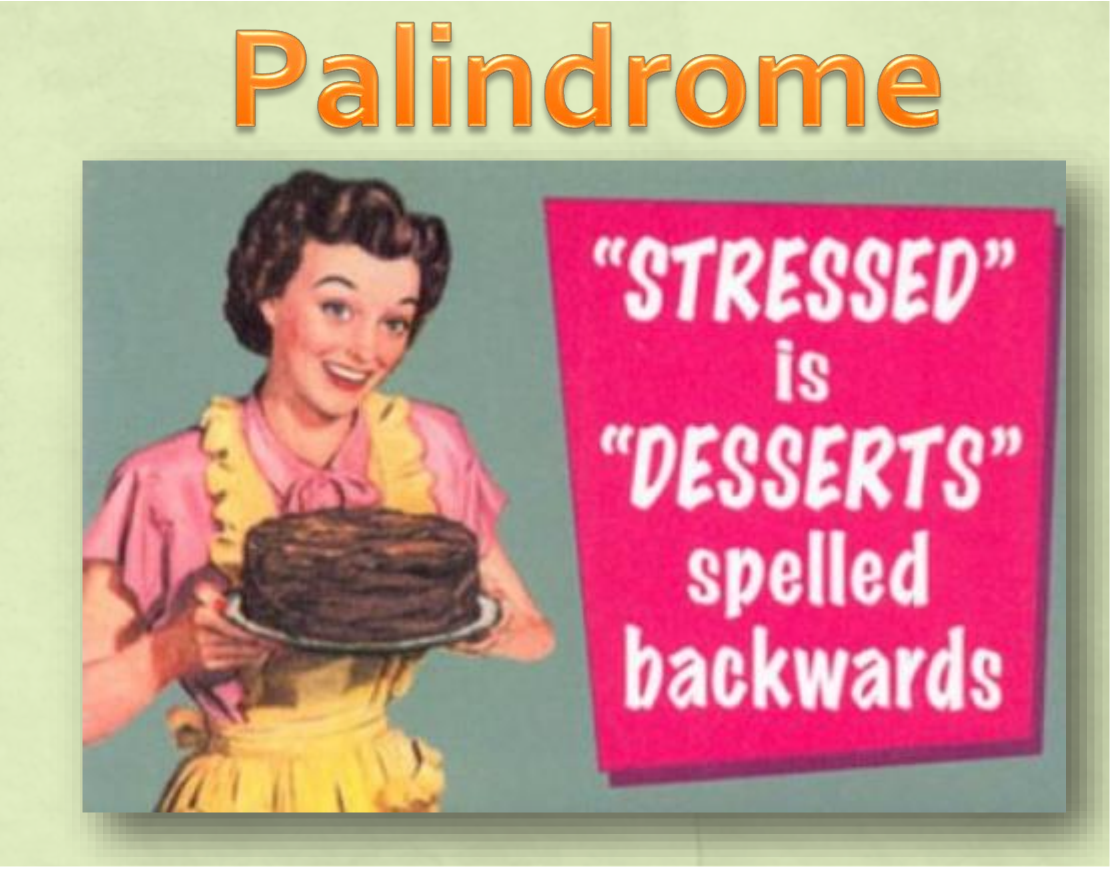


Is there a symmetry of the Fibonacci chain probed when scanning the phase over a period ?

Palindromicity

Scanning the phase $\Delta\phi$ drives the chain through a palindromic cycle.

Palindrome ?



Palindromicity

Scanning the phase $\Delta\phi$ drives the chain through a palindromic cycle.

Fibonacci chains generated using substitution or concatenation are “almost” palindromic.

They correspond to $\Delta\phi = 0 \Leftrightarrow \phi = \phi_\infty = 3\pi\tau^{-1}$

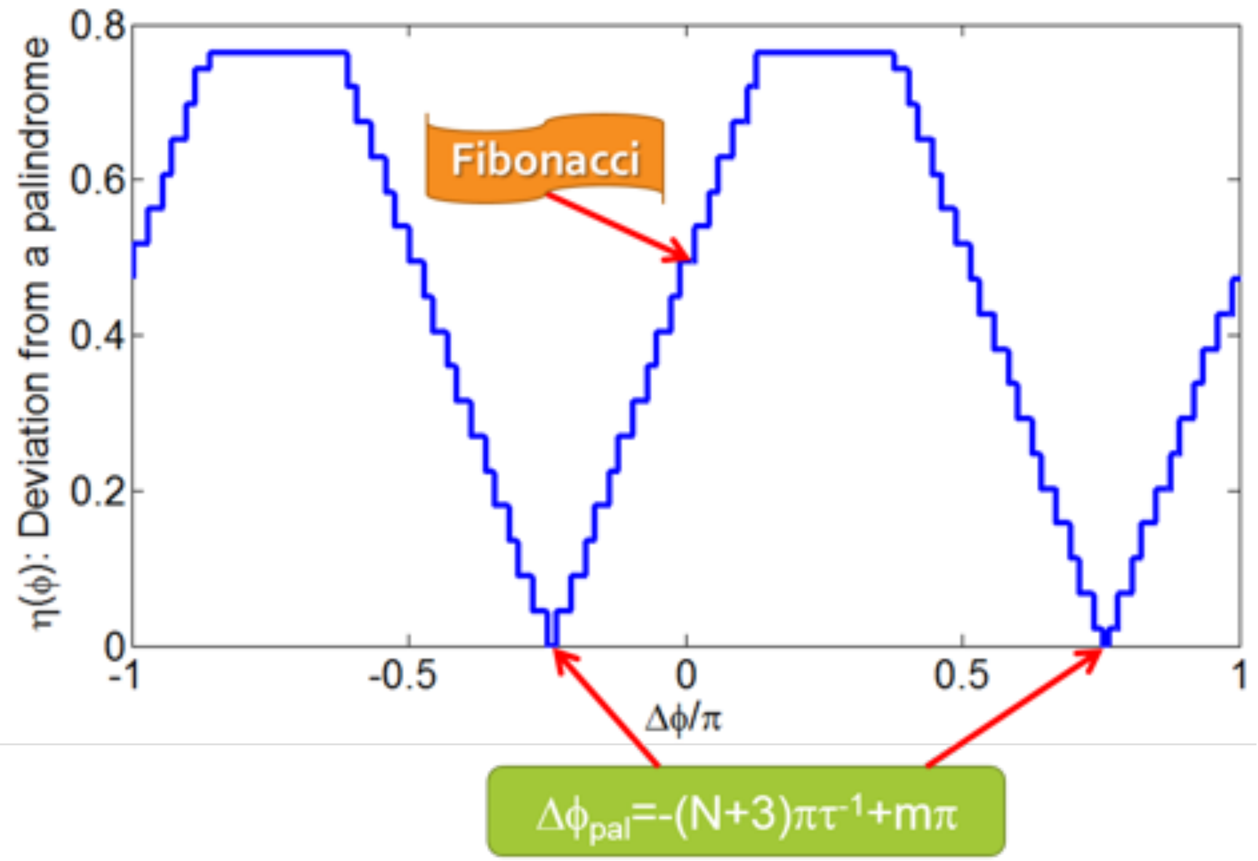
and a length equal to a Fibonacci number N_F

An infinite chain contains arbitrary long palindromic substructures

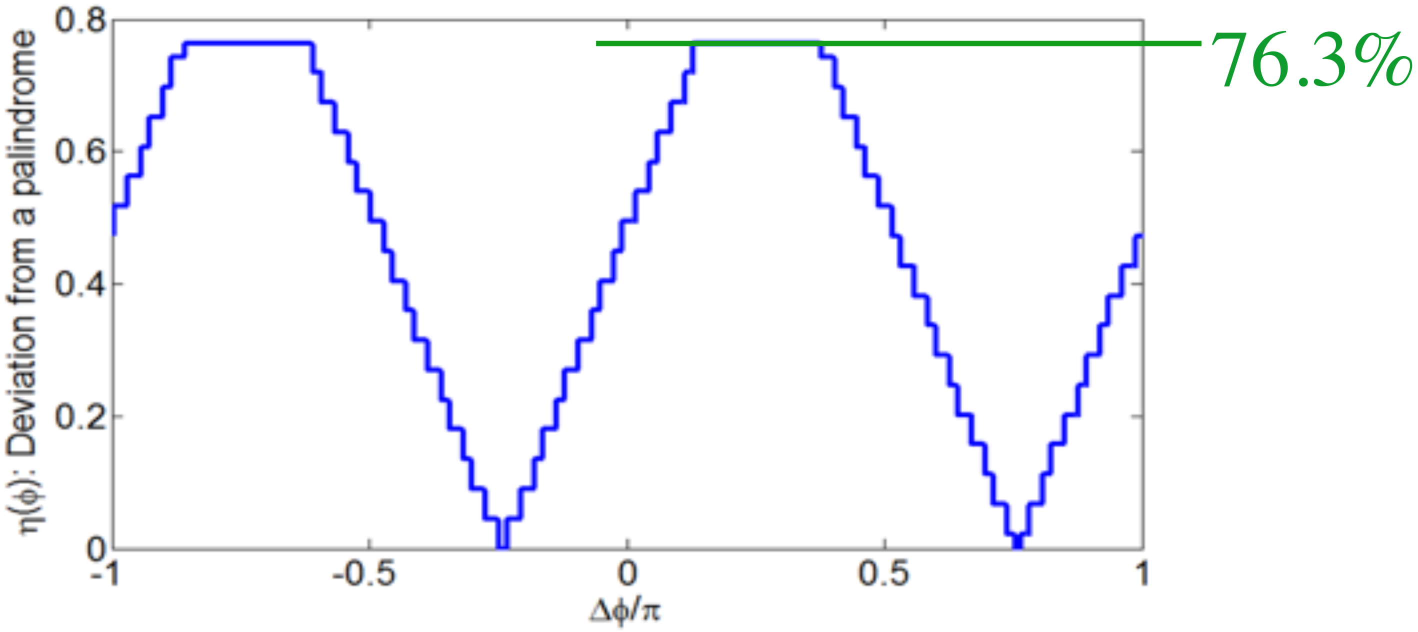
Alternatively, using characteristic function or C&P to generate chains, allows to monitor $\Delta\phi$ and to consider arbitrary lengths.

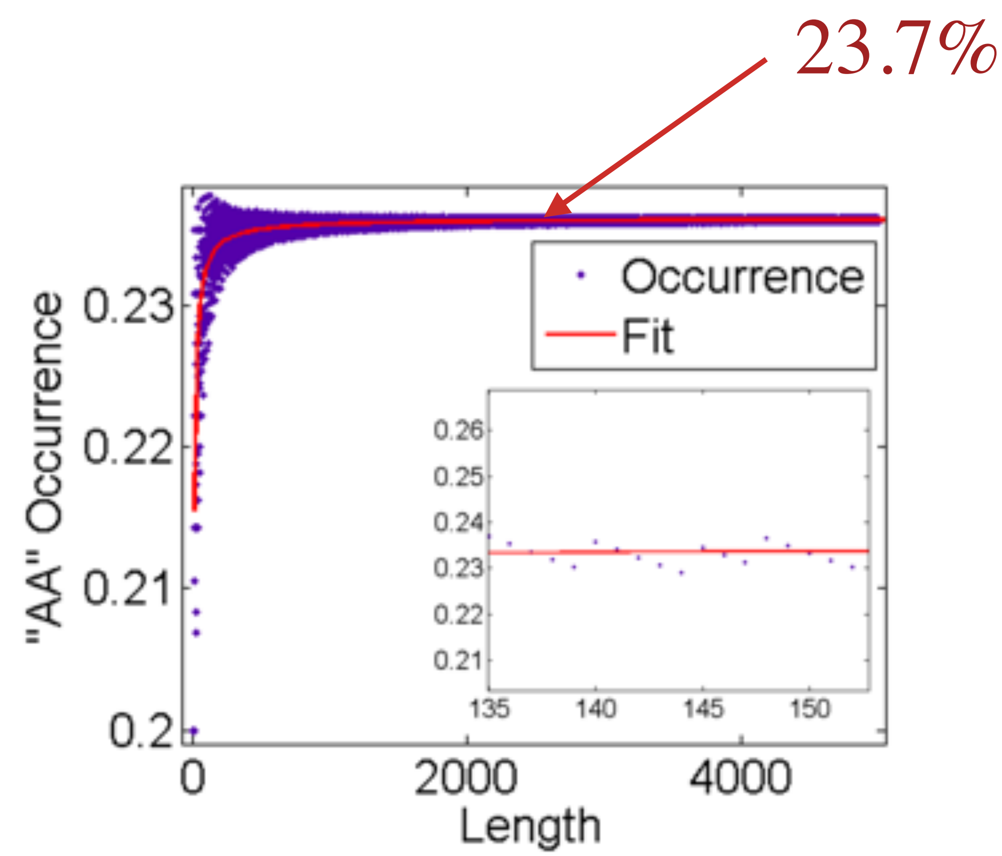
Define a function to account for deviation from structural palindromicity

$$\eta(\Delta\phi) \equiv \frac{1}{N} \sum_{j=0}^{\left[\frac{N-1}{2}\right]} \left|\chi_j(\Delta\phi) - \chi_{N-j}(\Delta\phi)\right|$$



The deviation from palindromicity saturates.





The saturation value depends on the C&P slope, i.e.,
on type of quasi-periodic potential.

For the Fibonacci chain, the saturation corresponds to the occurrence
of [AA] doublets, knowing that [BB] doublets are forbidden.

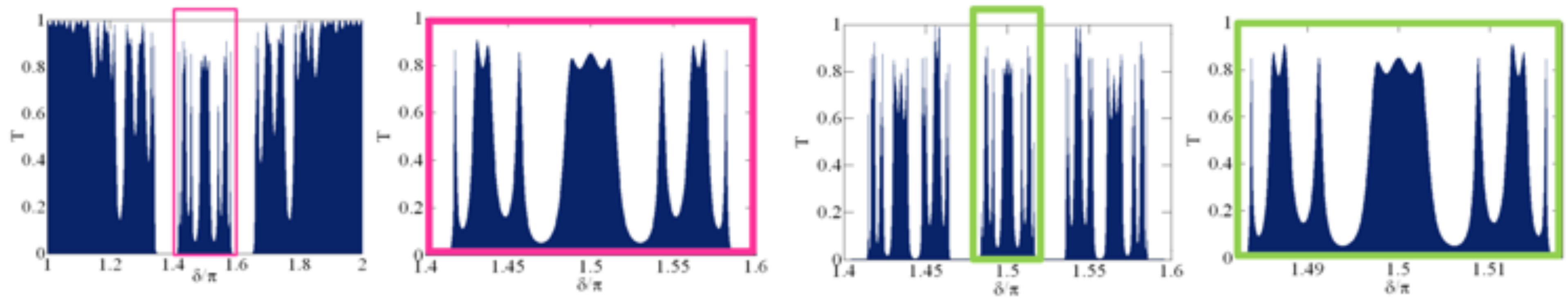
Are there spectral consequences
of these structural properties ?

No !

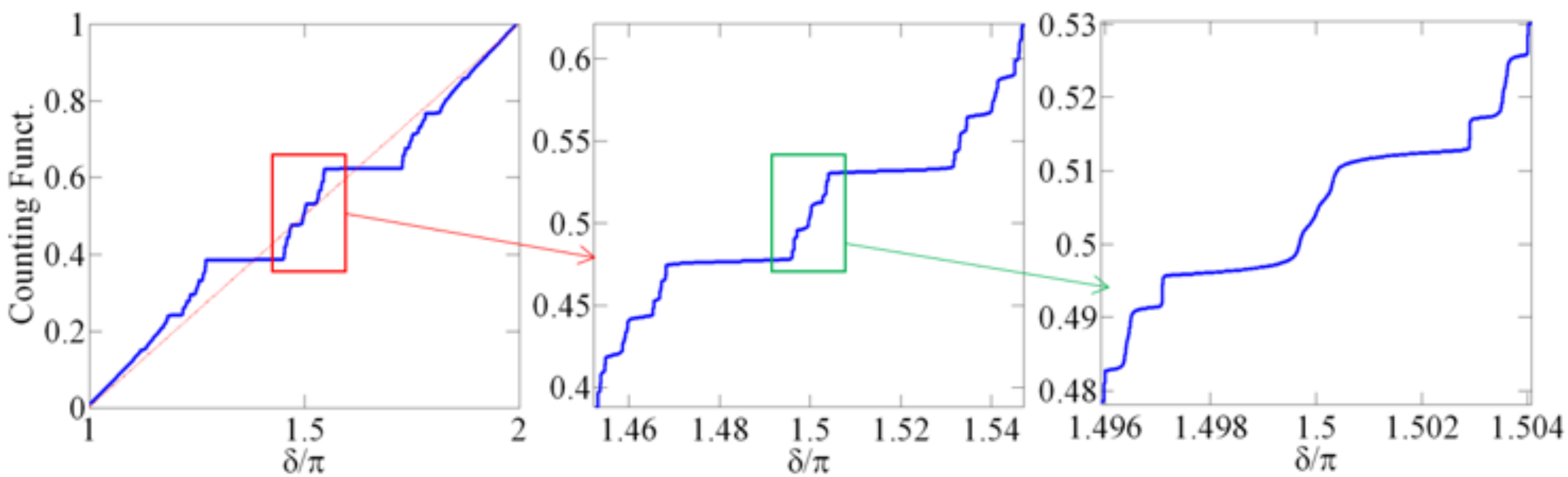
Almost No…

We have already calculated and measure the spectrum in details

Scaled finite size Fibonacci chains



Density of modes



Integrated Density of

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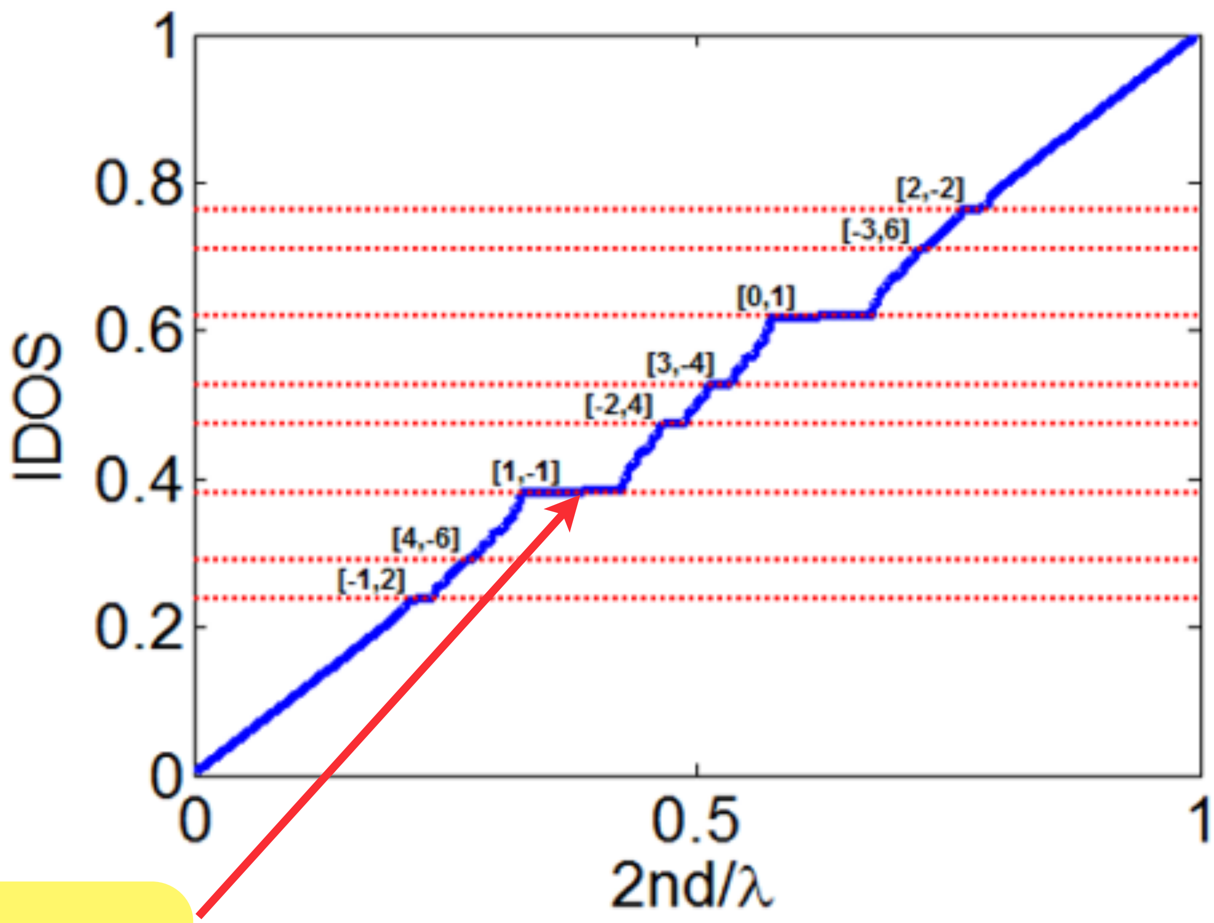


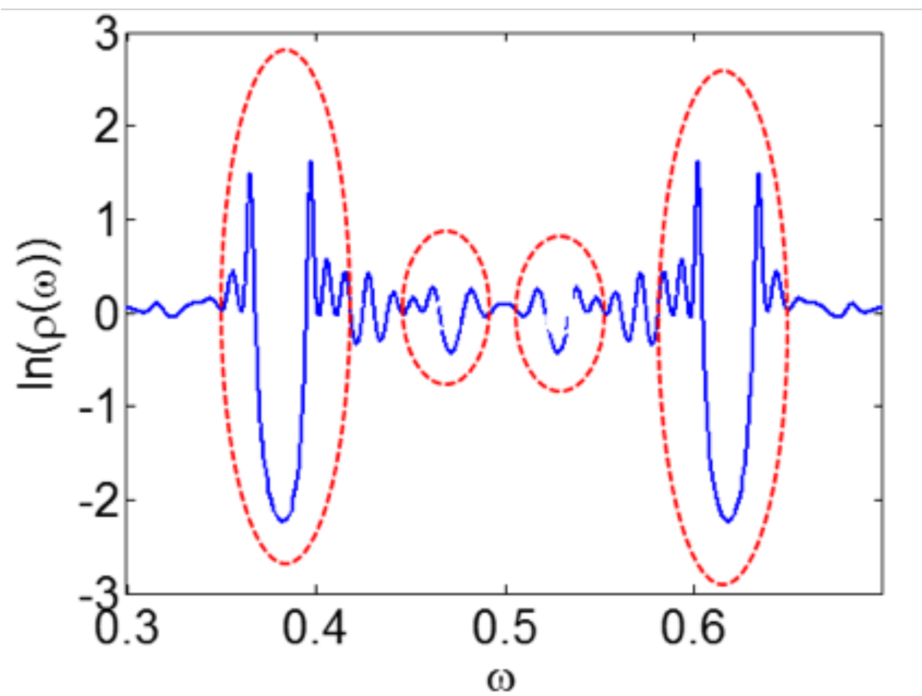
$$N\left(\omega_{gap}\right) = p + q\tau^{-1}$$

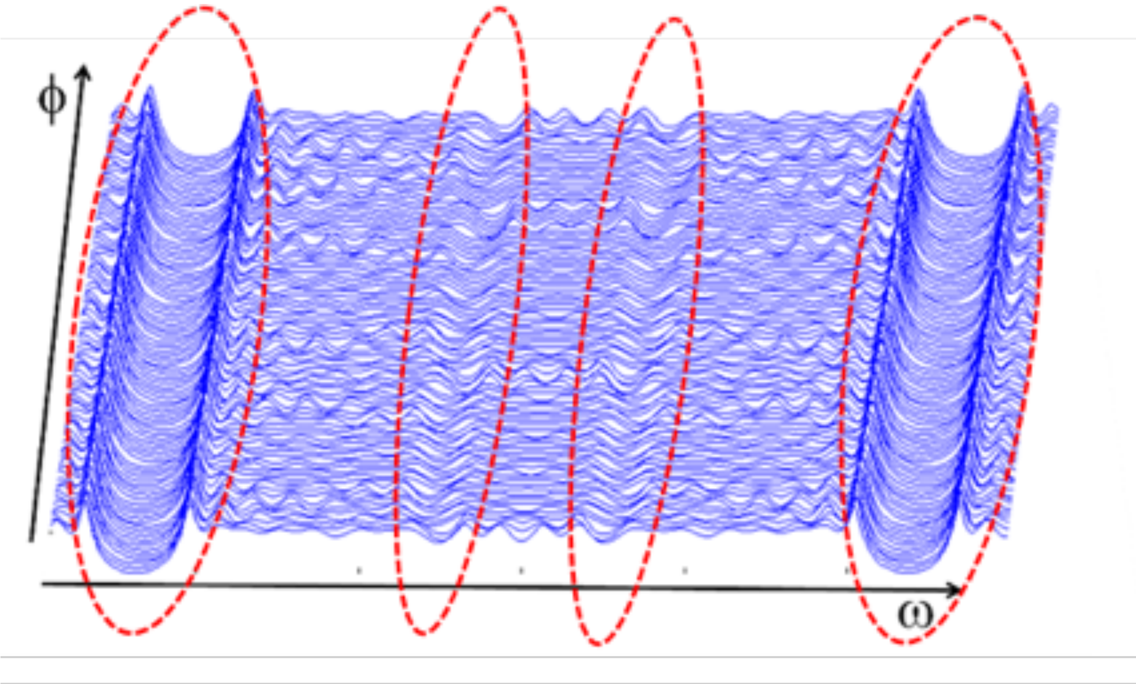
within a $[p,q]$ gap

$(p,q) \in \mathbb{Z}$ are topological invariants (Chern numbers).

Independent of the potential strength, inhomogeneity, ...

All these characteristics are independent of the phase $\Delta\phi$





How do we obtain the gap labeling theorem ?

Using the substitution matrix approach

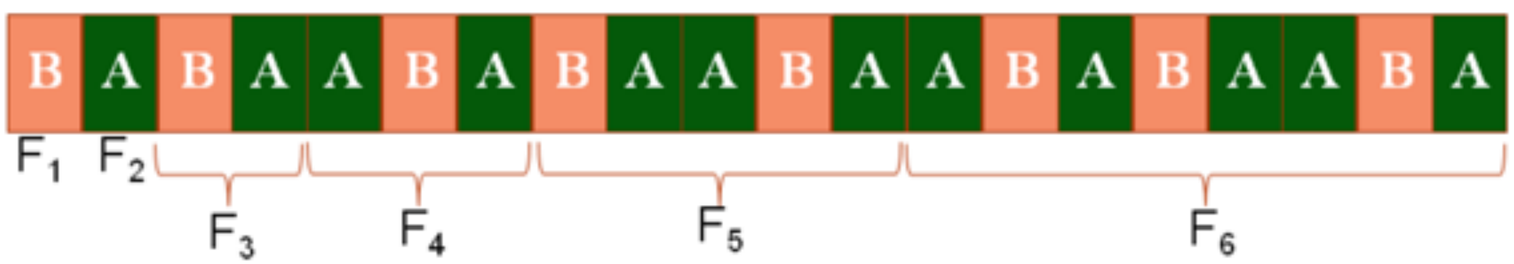
The gap labelling theorem

Substitution matrix

Consider a substitution σ acting on an alphabet of two letters A and B :

$$\sigma : \begin{cases} A \to BA \\ B \to A \end{cases} \qquad M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$

To this substitution, we associate a matrix M, whose columns give the number of letters A and B which occurs in the transforms.



By successive applications of σ we generate a word $F_{N+1} = \sigma^N(B)$ of length F_N (a Fibonacci number). The words $\sigma^N(B)$ converge to an infinite sequence $\sigma^\infty(A)$ left invariant by σ (fixed point).

Densities (d_A, d_B) of letters in the fixed point **infinite** Fibonacci chain $\sigma^{\infty}(A)$ are given by the components of the positive eigenvector:

$$v_1 = \begin{pmatrix} d_A \\ d_B \end{pmatrix}$$

of the matrix M with highest eigenvalue normalised so that $d_A + d_B = 1$

For the Fibonacci chain, eigenvalues of M are solutions of $x^2 - x - 1 = 0$

namely, (τ, τ^{-1}) and $v_1 = \begin{pmatrix} d_A = \tau - 1 \\ d_B = 2 - \tau \end{pmatrix}$

$$\tau = {(1+\sqrt{5})}/{2}$$

golden mean

In order to state the gap labeling theorem, we need also the substitution matrix for two letters. The possible words with 2 letters are:

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

$$\sigma(AA) = ABAB$$
$$\sigma(AB) = ABA$$
$$\sigma(BA) = AAB$$
$$\sigma(BB) = AA$$

$$M_2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix}$$

Substitution matrix

For the Fibonacci chain, eigenvalues of M_2 are solutions of

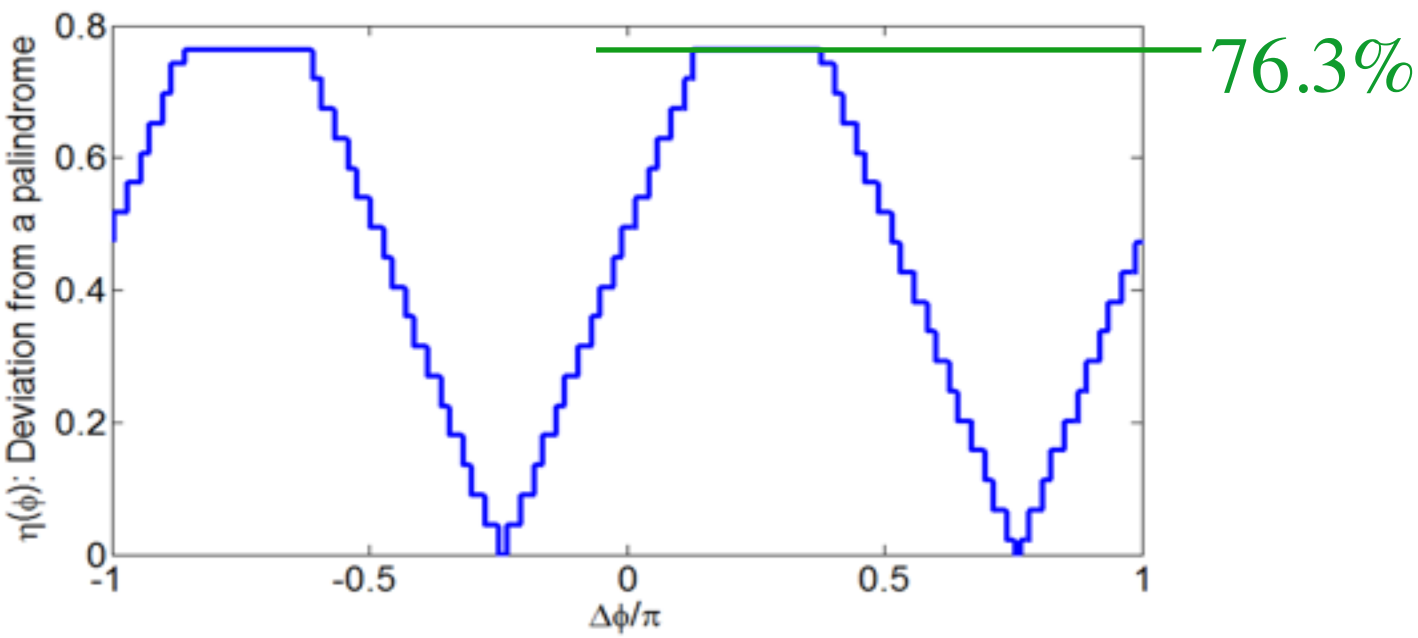
$$x(x^2 - x - 1) = 0$$

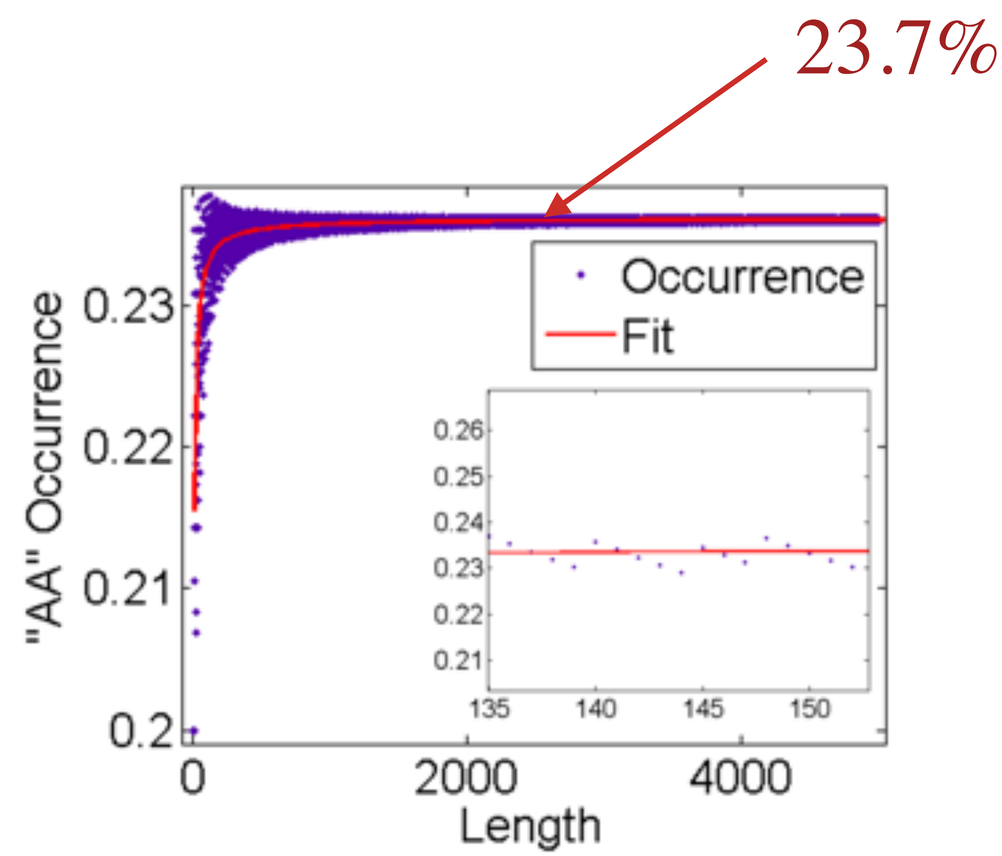
i.e., with the same highest eigenvalue τ and the corresponding normalised eigenvector

$$v_2 = \begin{pmatrix} d_{AA} = 2\tau - 3 \\ d_{AB} = 2 - \tau \\ d_{BA} = 2 - \tau \end{pmatrix}$$

Note: frequency of AA in the infinite chain : $d_{AA} = 2\tau - 3 \approx 23.7\%$

The deviation from palindromicity saturates.





The saturation value depends on the C&P slope, i.e., on type of quasi-periodic potential.

For the Fibonacci chain, the saturation corresponds to the occurrence of [AA] doublets, knowing that [BB] doublets are forbidden.

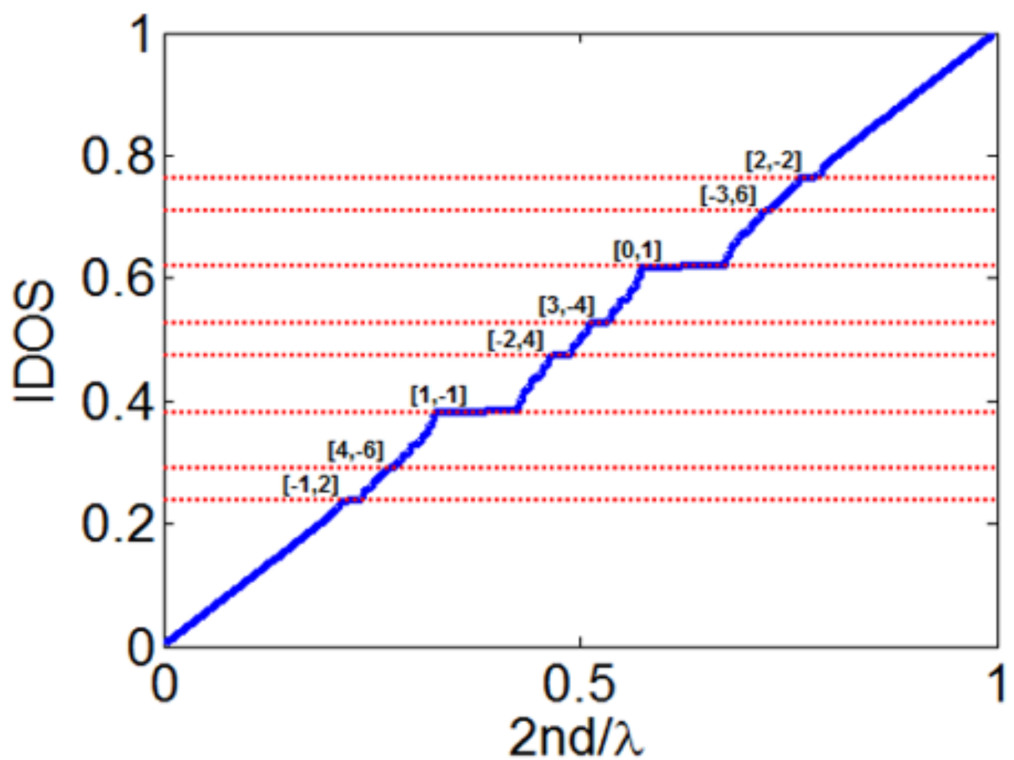
Gap labeling theorem (poor man's version) : for a Hamiltonian determined by a substitution on a finite alphabet, the values of the integrated density of states (counting function) on the spectral gaps in [0,1] belong to $\mathbb{Z}\left[\tau^{-1}\right]$ generated by the components of the normalised eigenvectors (v_1, v_2) with maximal eigenvalue τ of M and M_2.

For the Fibonacci chain, it gives directly,

$$\boxed{N\left(\varepsilon_{gap}\right) = \left(\mathbb{Z} + \tau^{-1}\mathbb{Z}\right) \cap [0,1]}$$

$$\Leftrightarrow \quad N\left(\varepsilon_{gap}\right) = p + q\tau^{-1}$$

$$\tau^{-1} = \tau - 1$$



The 2 integers [p,q] in the gap counting function are Chern numbers.

The substitution matrix approach does not involve the structural modulation phase $\Delta\phi$ which (as we saw) is *irrelevant* for the infinite chain.

Important consequence : the counting function in the spectral gaps is independent of the structural modulation phase $\Delta\phi$

More generally, the counting function (and the density of states) over the whole spectrum is *independent* of the structural phase $\Delta\phi$

How to see it : scattering formalism and the Krein-Schwinger formula

Intermezzo : Scattering formalism - Krein-Schwinger formula

Scattering formalism

It offers a general and elegant framework in order to investigate spectral properties and transport (Landauer approach)

Here, we consider 1D systems only.

A (quantum,wave) system with a potential (defined w.r.t. a free part) is enclosed in a “black box”. We probe it using scattering waves.

With obvious notations, the (unitary) scattering matrix is :

$$\begin{pmatrix} o_L \\ o_R \end{pmatrix} = \begin{pmatrix} r & t \\ t & r' \end{pmatrix} \begin{pmatrix} i_L \\ i_R \end{pmatrix} \equiv S \begin{pmatrix} i_L \\ i_R \end{pmatrix}$$

It can be diagonalised as $\begin{pmatrix} e^{i\phi_1} & 0 \\ 0 & e^{i\phi_2} \end{pmatrix}$

Defining the total phase shift : $\delta(k) \equiv (\phi_1(k) + \phi_2(k))/2$

Assume that the scattering potential decreases fast enough and enclose the system in a large “blackbox” of size L (much larger than the system size). Apply periodic boundary conditions to this box, namely,

$$\begin{aligned} \psi(0) = \psi(L) \quad &\Rightarrow \quad i_L + o_L = o_R e^{ikL} + i_R e^{-ikL} \\ \psi'(0) = \psi'(L) \quad &\Rightarrow \quad ik(i_L - o_L) = ik(o_R e^{ikL} - i_R e^{-ikL}) \end{aligned}$$

These algebraic equations can be written as a spectral condition:

$$\det\left(1 - e^{ikL}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} S(k)\right) = 0\,.$$

Spectral condition:

$$\det\left(1 - e^{ikL}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} S(k)\right) = 0\,.$$

leads to a relation between the total phase shift
and the possible wave vectors :

$$k_n(L) = \frac{\pi n}{L} - \frac{\delta(k_n)}{L}$$

From this relation we obtain the change of density of states :

$$\rho(k) - \rho_0(k) = \frac{1}{\pi}\frac{d\delta(k)}{dk} = \frac{1}{2\pi}\,\mathrm{Im}\,\frac{\partial}{\partial k}\ln\det S(k)$$

since

$$\det S(k) = e^{2i\delta(k)} = -\frac{t}{t^*}$$

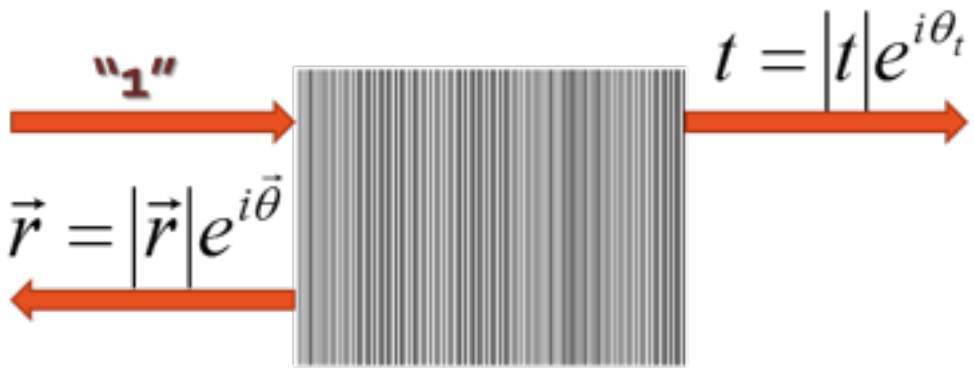
An exemple of the general Krein-Birman-Schwinger relation :

$$\mathrm{Tr}\left[\Phi(H) - \Phi(H_0)\right] = \int_{-\infty}^{+\infty} dE\,\frac{d\Phi}{dE}\,\frac{i}{2\pi}\,\ln\det S(E)$$

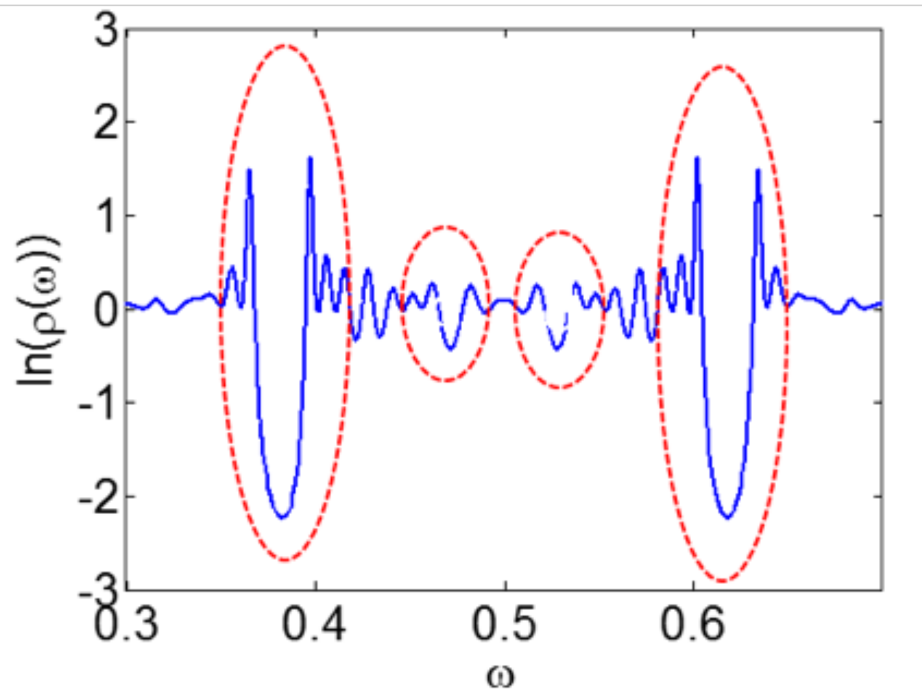
where $\Phi(H)$ is a regular function of the Hamiltonian.

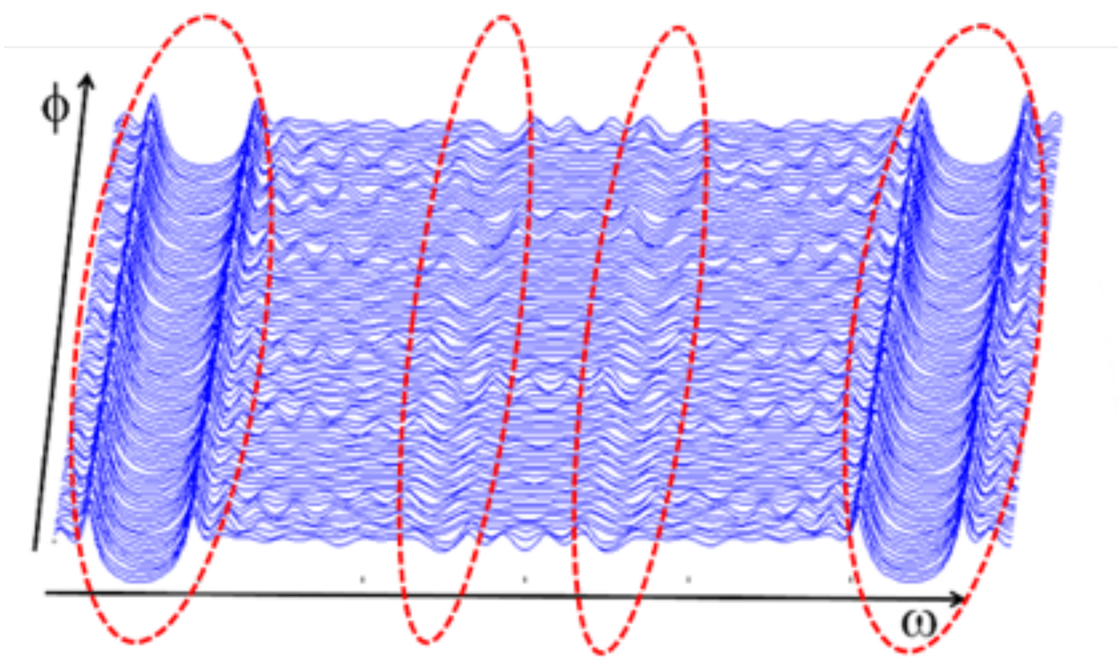
End of the intermezzo

Fibonacci chain embedded between free spaces:



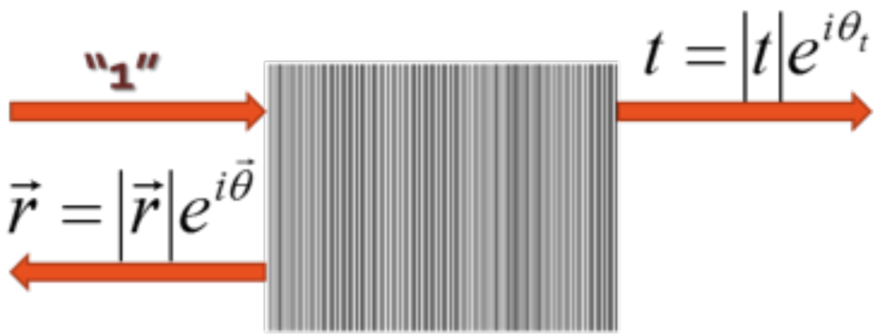
$$\rho(k) - \rho_0(k) = \frac{1}{\pi}\frac{d\delta(k)}{dk}$$
$$= \frac{1}{2\pi}\,\mathrm{Im}\,\frac{\partial}{\partial k}\ln\det S(k)$$





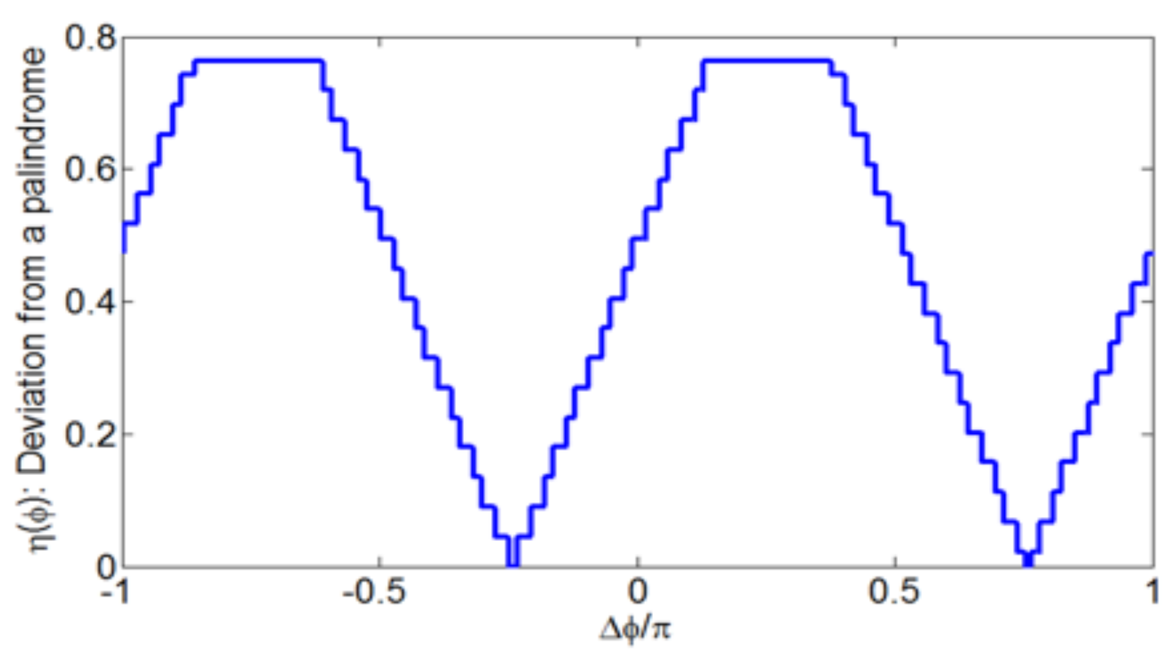
$\delta(k) = \theta_t(k) + \frac{\pi}{2}$ is independent of the modulation phase $\Delta\phi$

But…since the phase $\Delta\phi$ measures the deviation from palindromicity,
it should show up in the difference between the 2 scattering configurations,



$$\overleftarrow{r} = \overrightarrow{r}\, e^{i\alpha}$$

α should depend on the structural phase $\Delta\phi$



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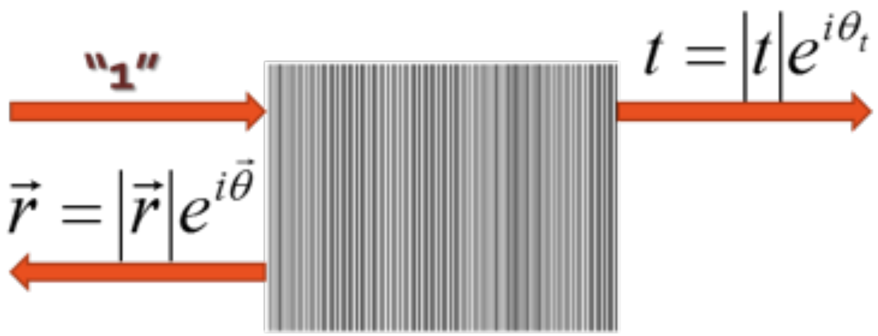

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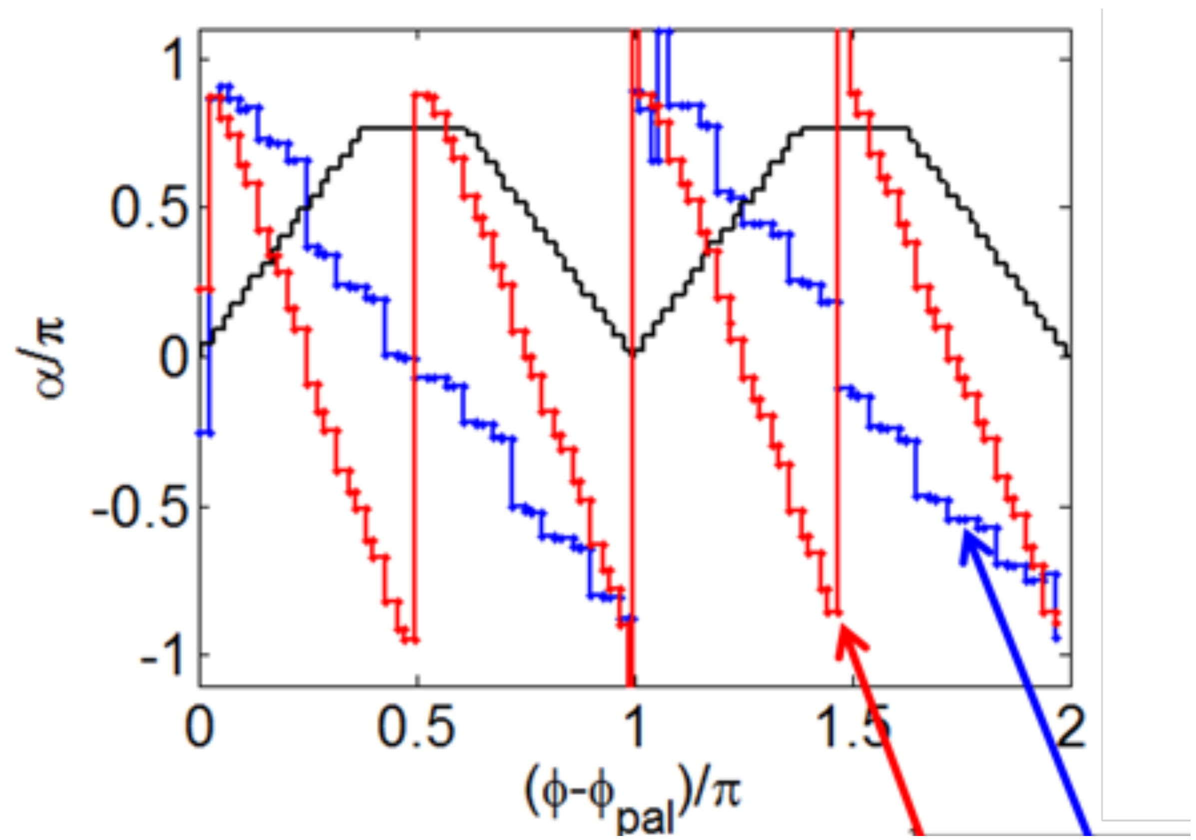


Two different wave vectors

On which physical quantity do we see a $\Delta\phi$ dependence ?

On boundary (edge) states…since scattering states are independent of the structural phase $\Delta\phi$

How to relate boundary (edge) states to the scattering formalism ?

Creating edge modes

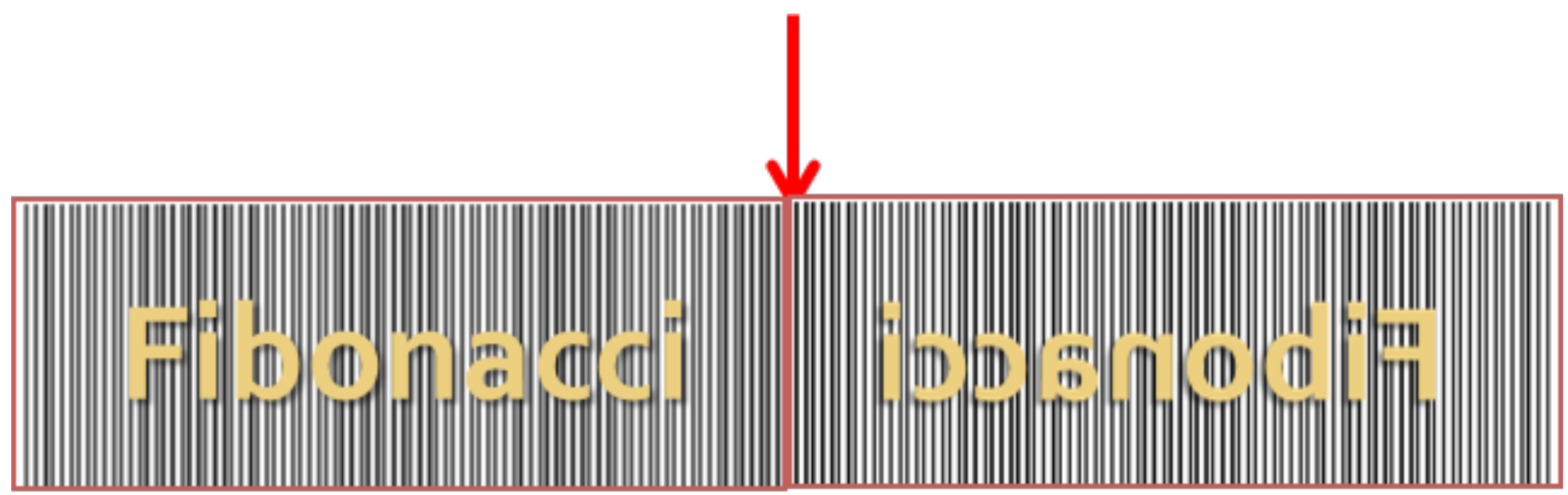
- Edge modes show up in most finite superlattices at gap frequencies which depend on boundary conditions:

  A. Boundary states due to a "closed" boundary condition (*e.g.*, mirror)
  B. Interface modes
  C. Defect modes

- Edge modes have the same origin and are of topological nature.

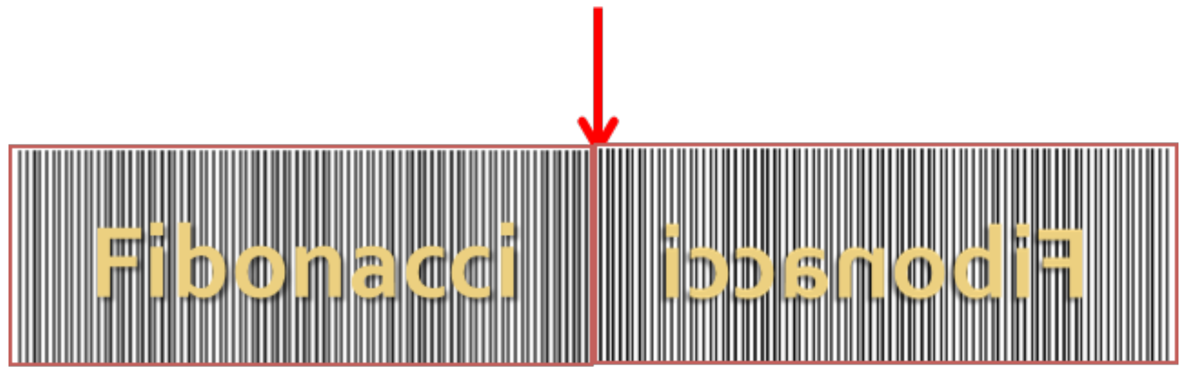
Work with a closed boundary

Equivalent to the artificial palindrome



$$\overrightarrow{F}_N \overleftarrow{F}_N$$

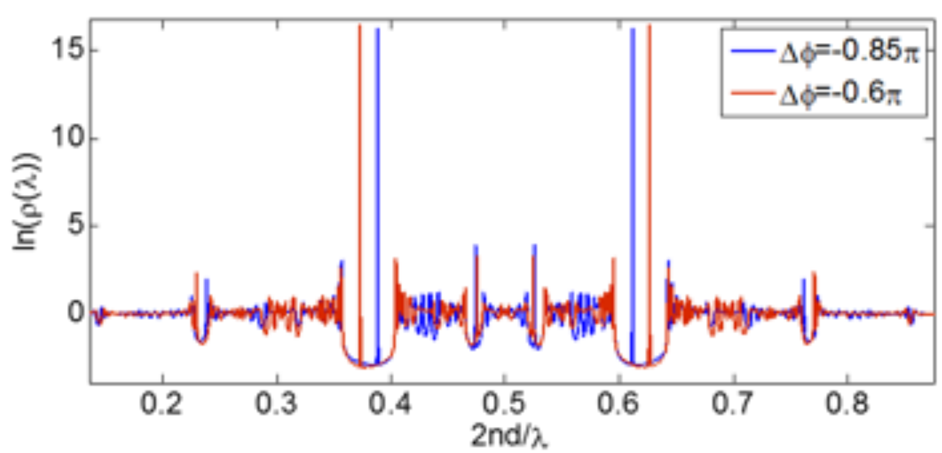
Edge states of the artificial palindrome $\overrightarrow{F}_N \overleftarrow{F}_N$

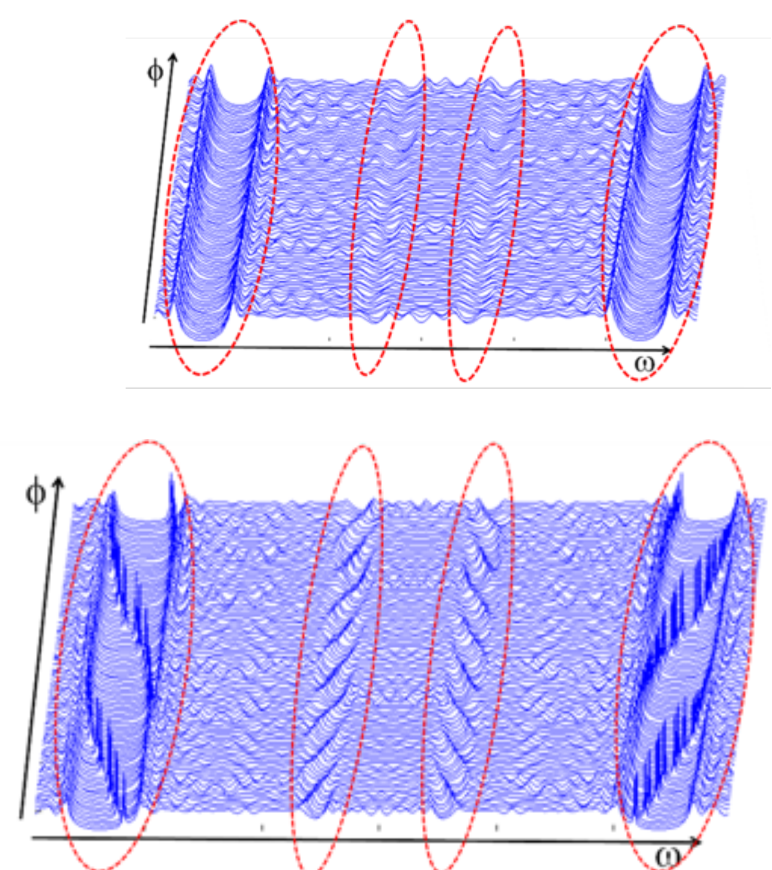


- This structure displays additional modes in the band gaps

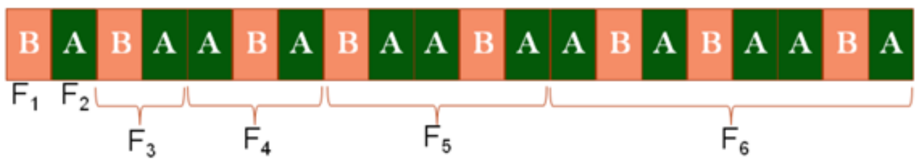
- Gap locations remain unchanged w.r.t. the original structure

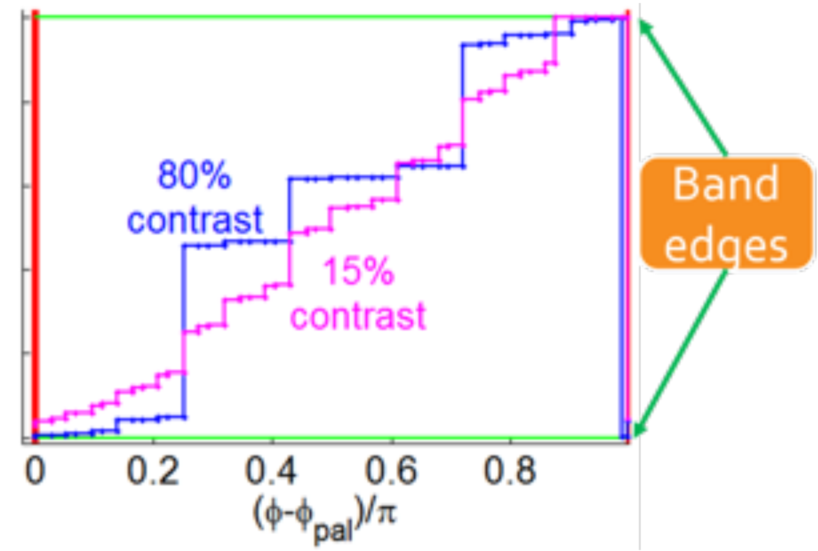
- Frequencies of the gap modes depend on the structural modulation phase $\Delta\phi$





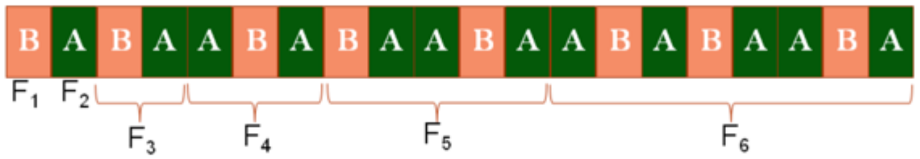
Gap modes move through gaps in a discrete staircase which depends on the contrast of the Fibonacci letters.

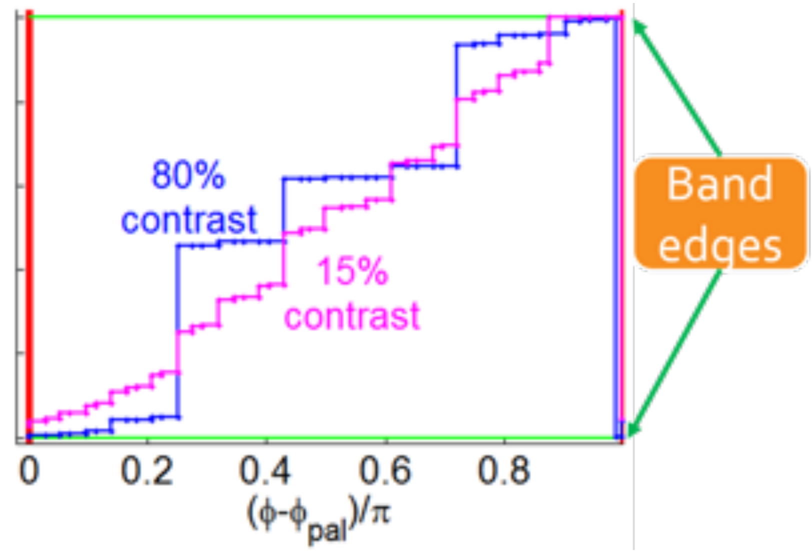




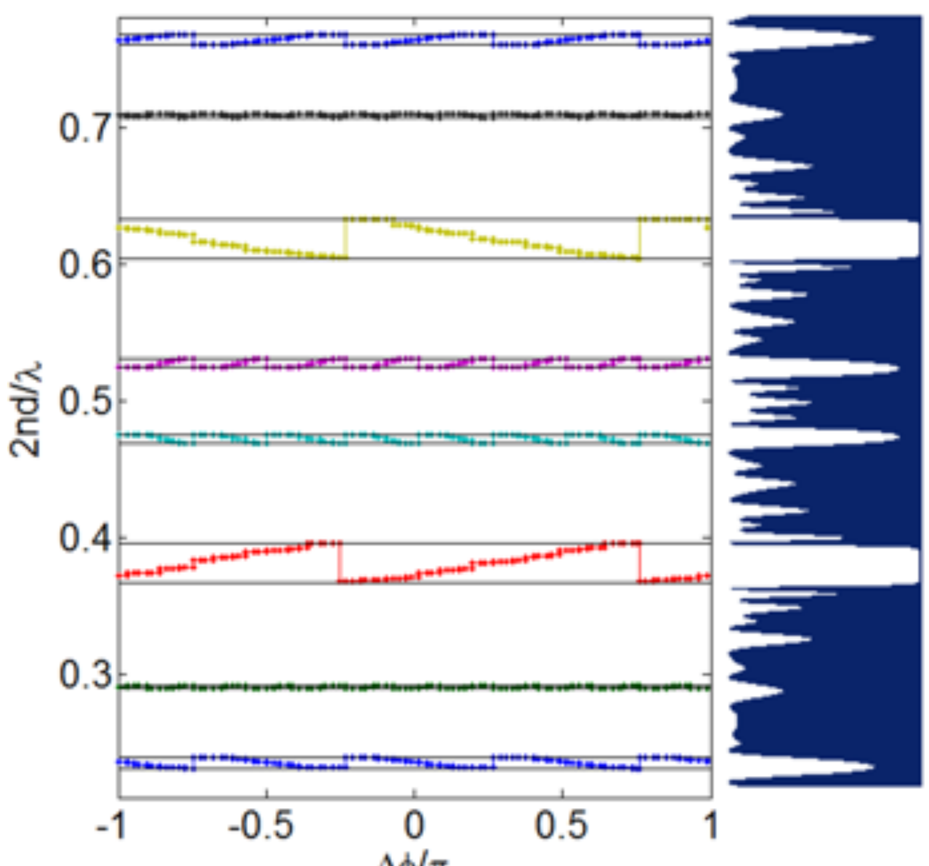
Behaviour intrinsic to the discrete nature of the chain
(unlike Harper or Aubry-Andre models).

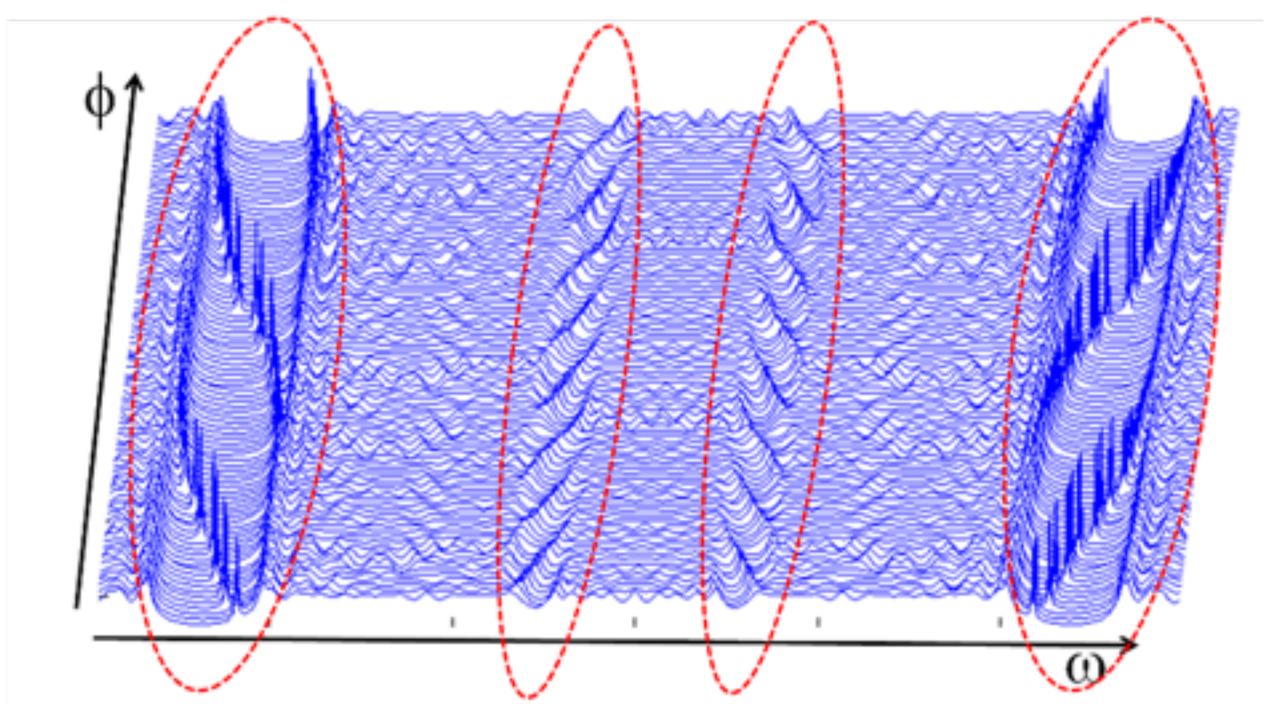
Gap modes move through gaps in a discrete staircase which depends on the contrast of the Fibonacci letters.



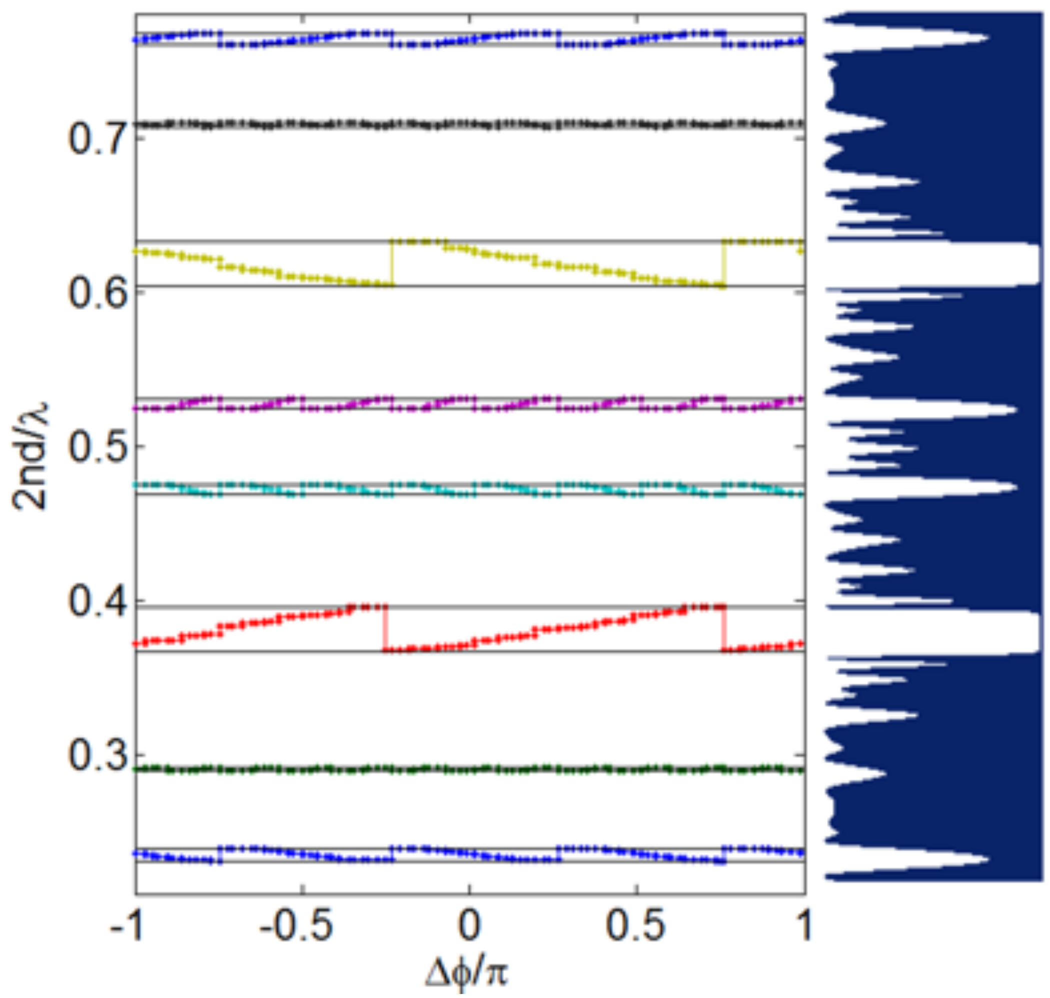


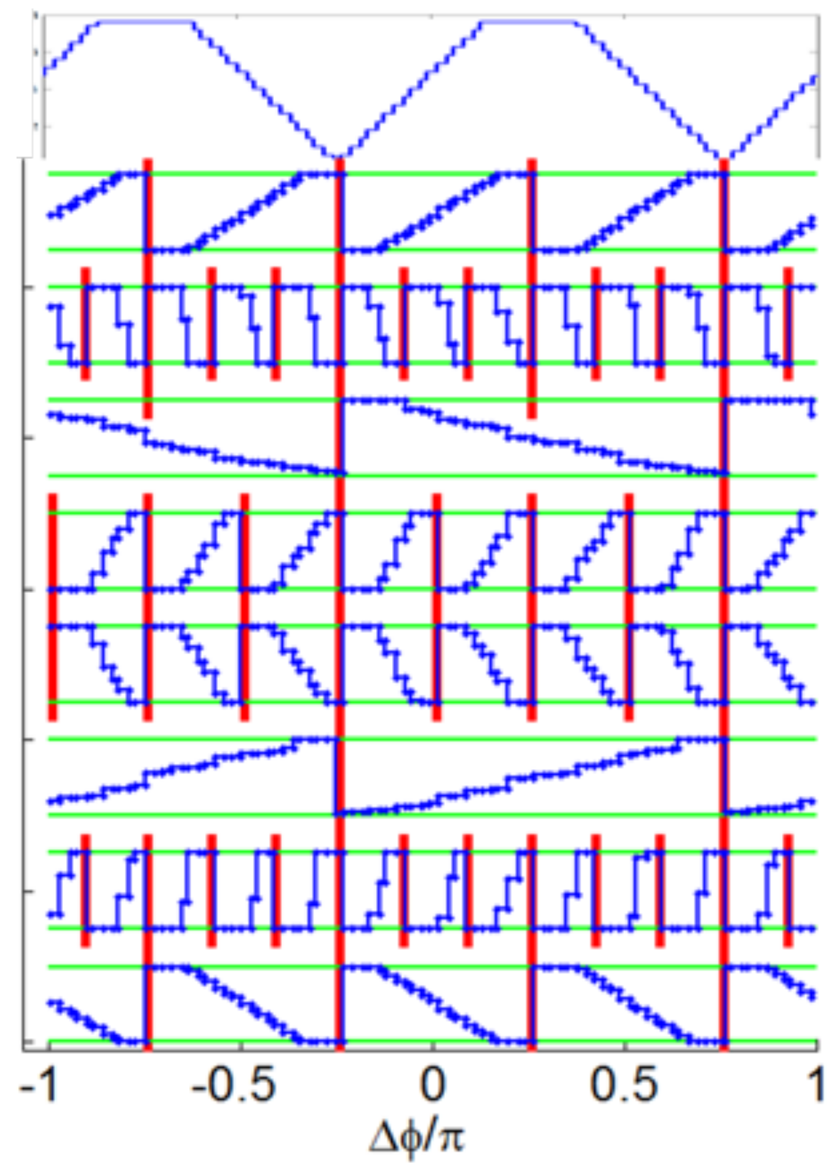
Dwell ”time” of the gap modes is periodic with the modulation phase $\Delta\phi$ with a period which depends on the gap.



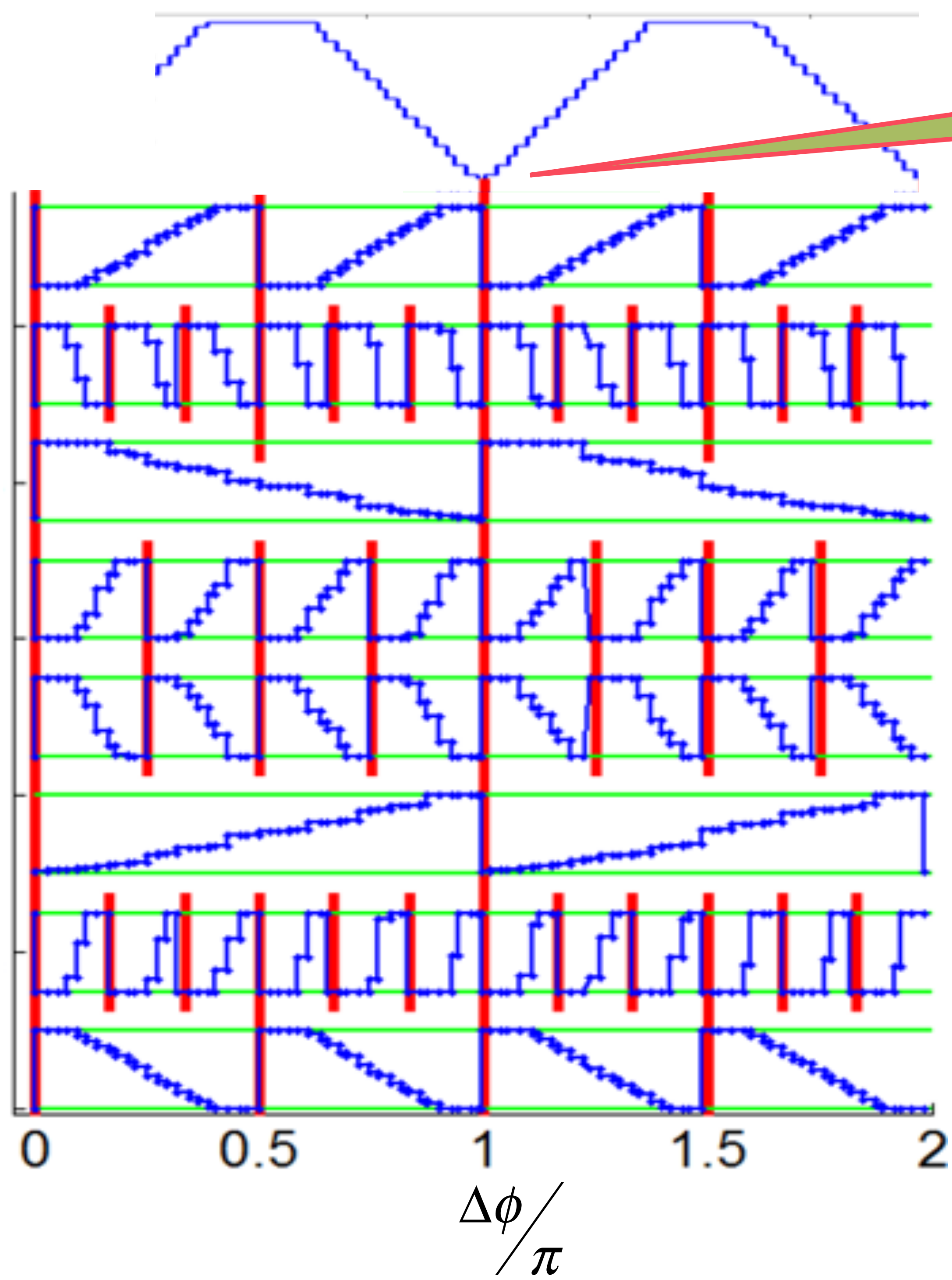


Relation to the palindromic cycle





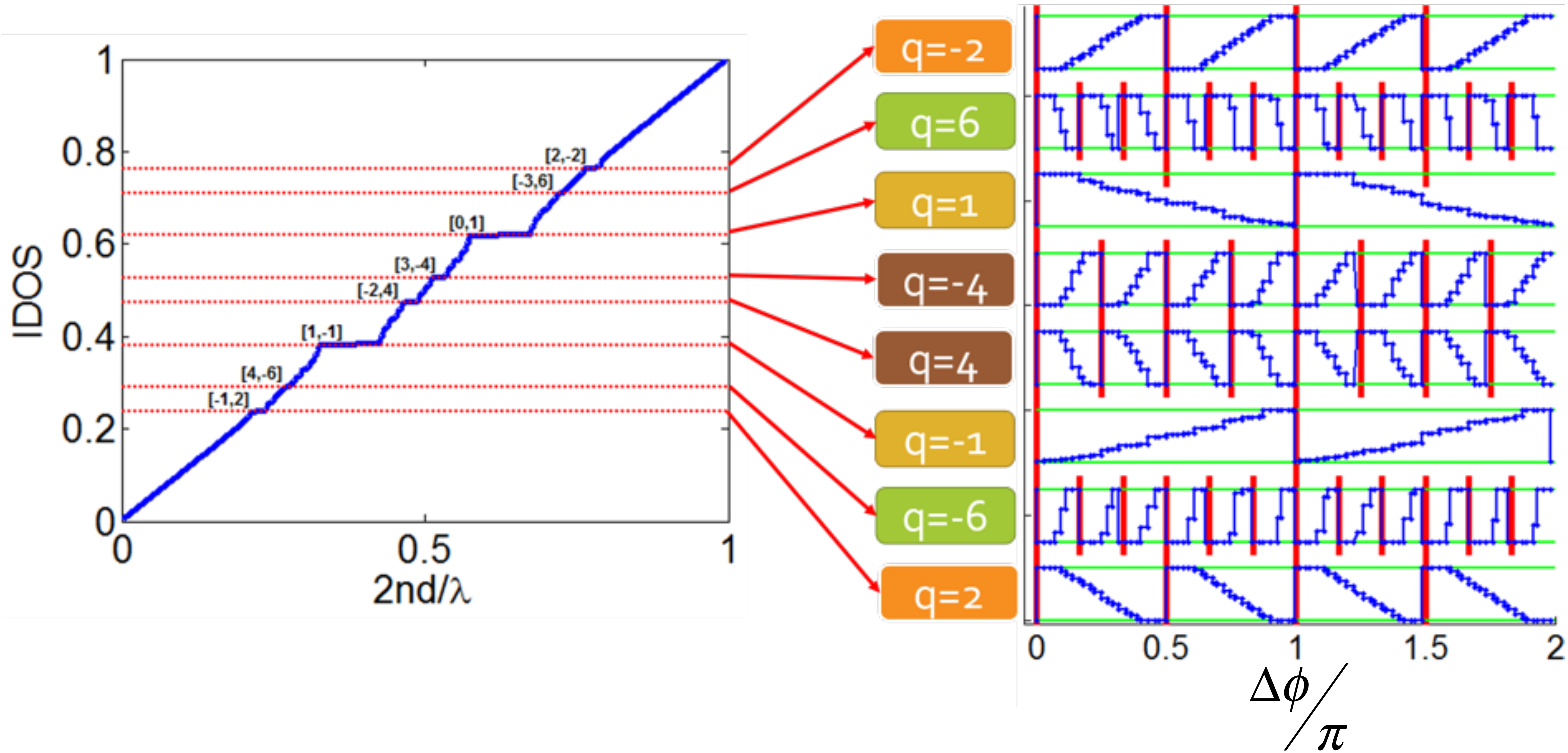
Relation to the palindromic cycle



No topological edge states at structural palindromicity

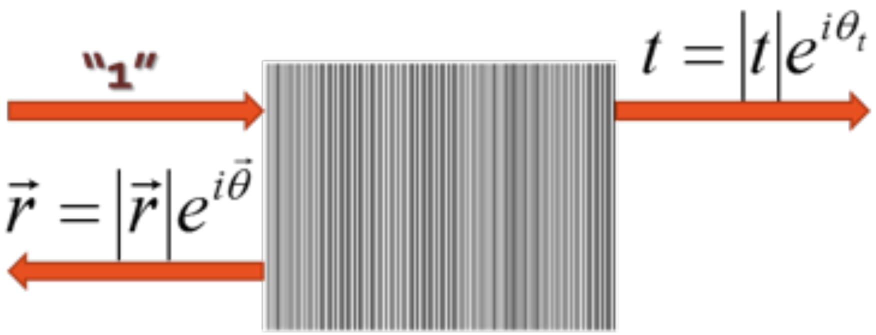
for all gaps

Relation to the gap labelling and Chern numbers



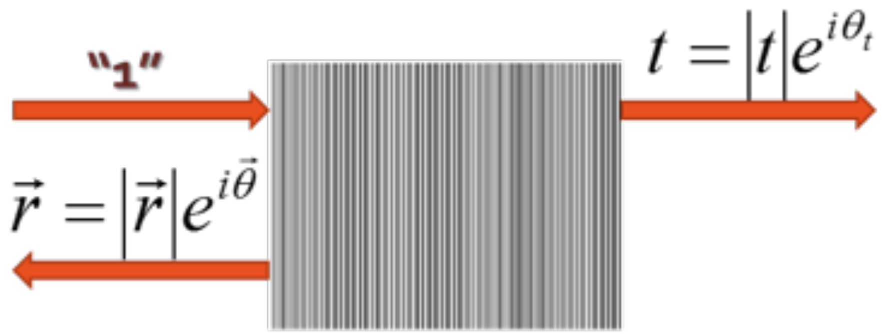
Chern numbers [p,q] describe the behaviour of topological edge states in the gaps when changing the structural phase angle $\Delta\phi$ i.e., while moving away from palindromicity.

Relation between the Chern numbers (for each gap) and the scattering matrix



$$\overleftarrow{r} = \overrightarrow{r}\, e^{i\alpha}$$

The chiral angle α depends on the structural phase $\Delta\phi$



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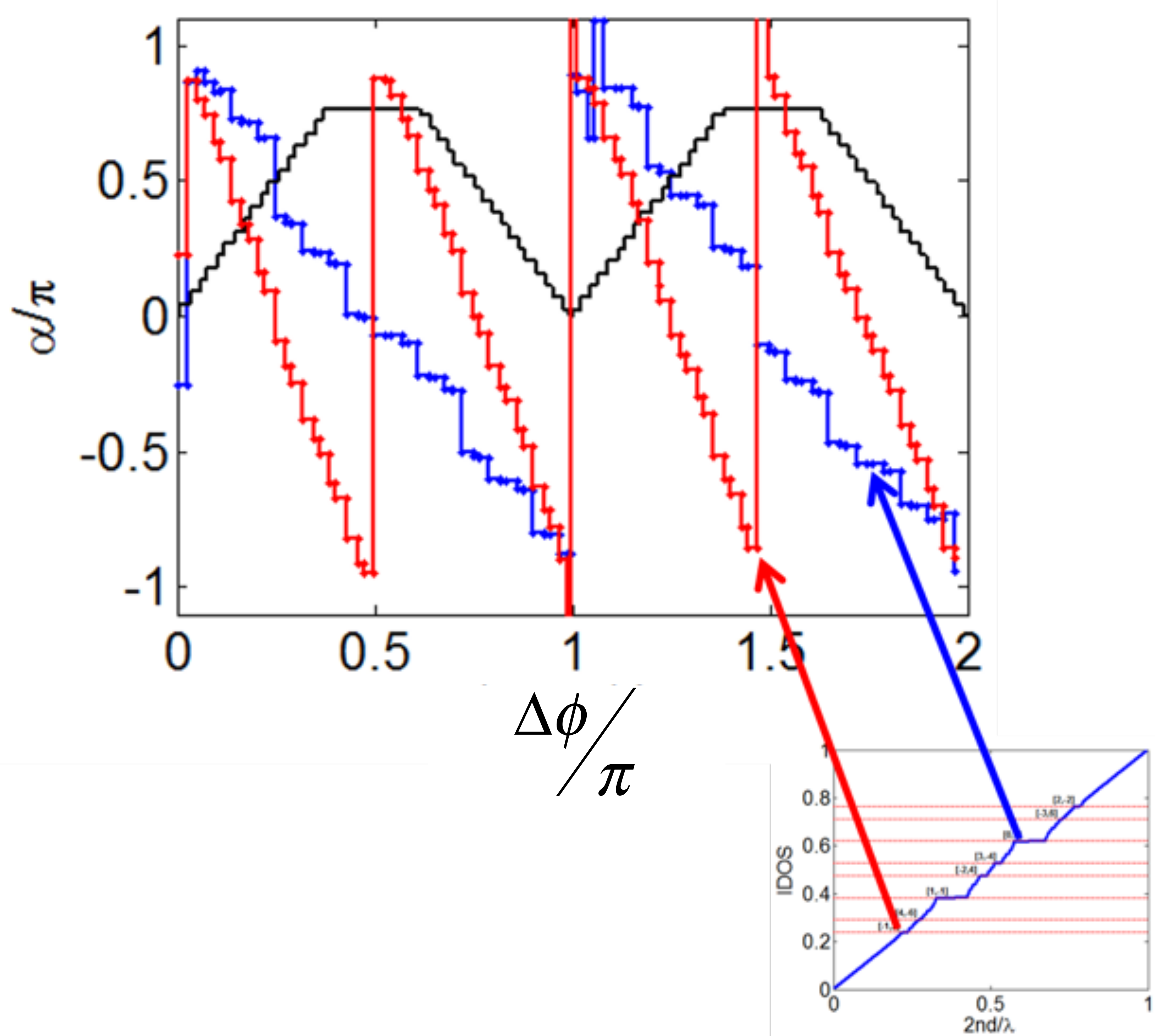


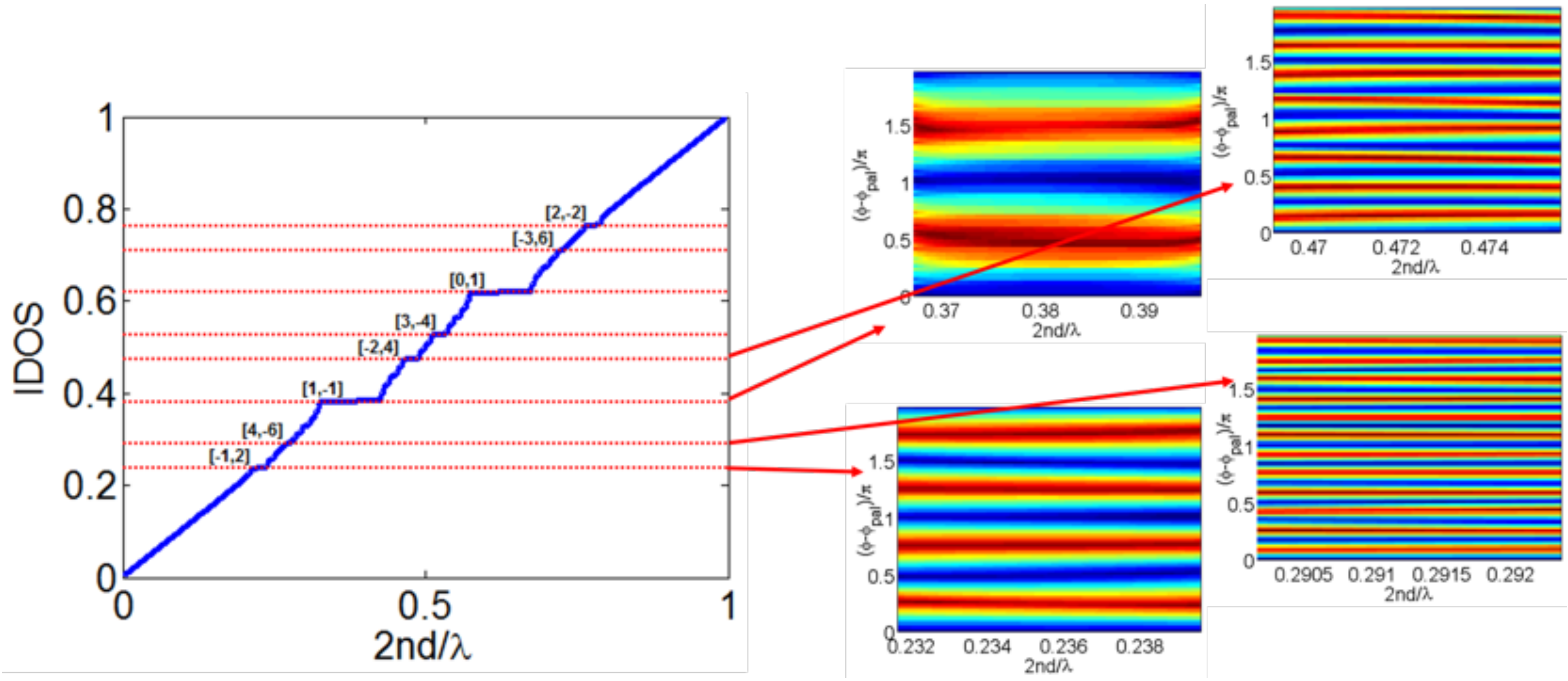
$\alpha_q(\omega,\Delta\phi)$ defines the spectral deviation from palindromicity

It depends on :

- the Chern number q in a gap
- on the frequency in the gap (spectral quantity)
- the structural phase angle $\Delta\phi$
- it does not saturate unlike structural palindromicity

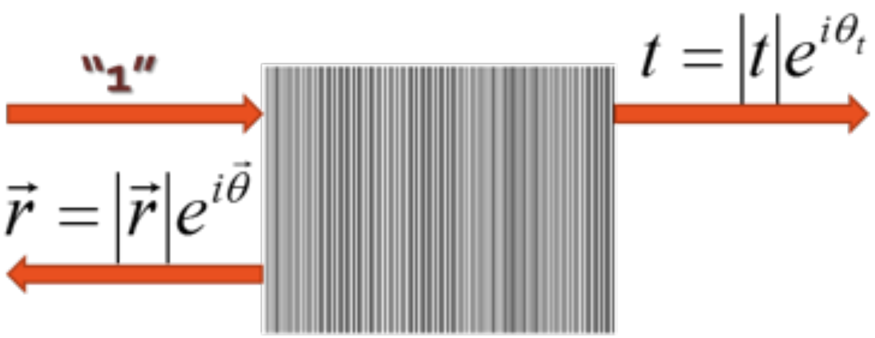
Winding number of the spectral deviation from palindromicity

$$\alpha_q\left(\omega_{gap},\Delta\phi\right)$$



The Chern number q of a gap and $\alpha_q\left(\omega_{gap},\Delta\phi\right)$ are related.

Relation between the Chern numbers (for each gap) and the scattering matrix



$$\overleftarrow{r} = \overrightarrow{r} e^{i\alpha}$$

α depends on the structural phase $\Delta\phi$:

$$\alpha_q(\omega, \Delta\phi) = \overleftarrow{\theta}_q - \vec{\theta}_q = 2\theta_q$$

The Chern number q is the winding number of the reflected phase shift $\theta_q(\Delta\phi)$ associated to the structural phase.

$$q = \frac{\theta_q(\Delta\phi = 2\pi) - \theta_q(\Delta\phi = 0)}{2\pi}$$

The <u>Chern number q</u> is half the winding number of the spectral deviation from palindromicity $\alpha_q(\omega_{gap}, \Delta\phi)$ associated to the structural phase.

Summary-Further directions

- Topological structure of finite size quasi-periodic chains induced by the palindromic symmetry (non trivial fiber bundle)

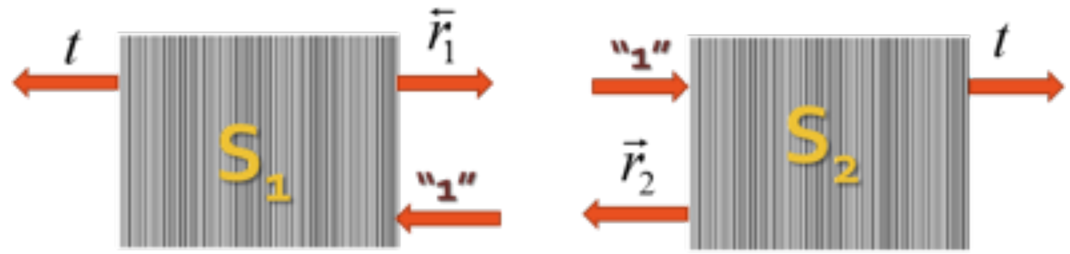
- Direct relation between scattering data (chiral reflection phase)

$$\boxed{\alpha_q(\omega,\Delta\phi)=\overleftarrow{\theta}_q-\overrightarrow{\theta}_q=2\theta_q}$$

and the gap labelling Chern numbers.

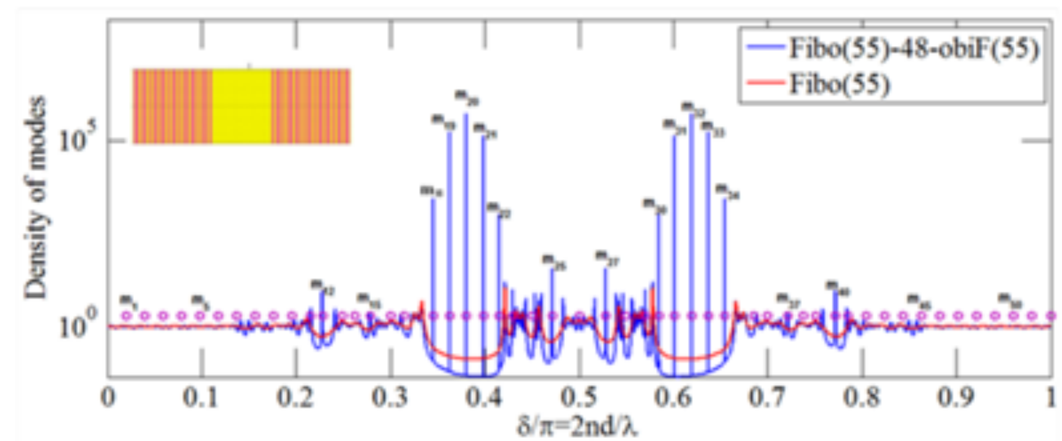
- C&P and scattering theory give a simple way to calculate/measure Chern numbers.

- Effective Fabry-Perot condition : systematic and simple design of topological mirrors.

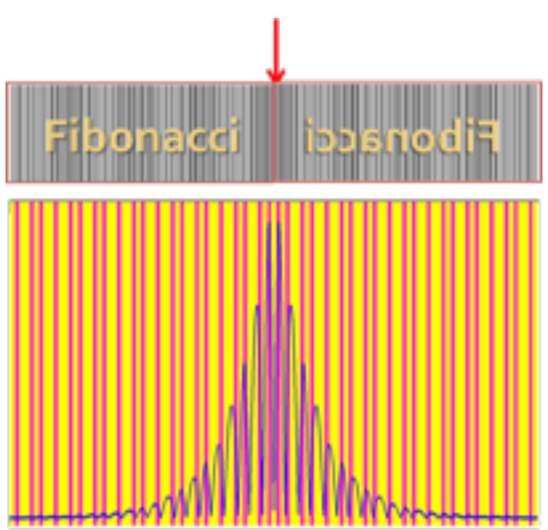


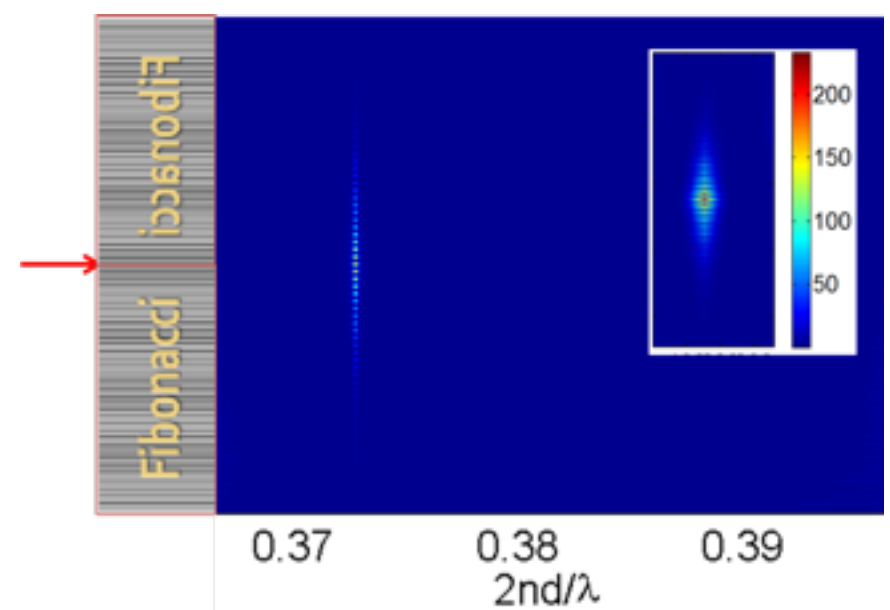
- A simple resonance condition allows to calculate the position of the gap modes.

$$L^{FP}(k) = \frac{\lambda(k)}{4}\frac{\overleftarrow{\theta}_1 + \vec{\theta}_2}{\pi} = m\frac{\lambda(k)}{2}, \quad m \in \mathbb{Z}$$



- Spatial structure of the topological modes.





- Casimir effect between topological mirrors.
- Topological origin of fractional charge (polyacetylene, SSH)
- Quantum anomaly for relativistic fermions (Jackiw, Rebbi)
- Topological invariants (Atiyah-Singer index theorem), relation to scattering theory.

Thank you for your attention.