Orbital magnetic susceptibility of the Rauzy tiling

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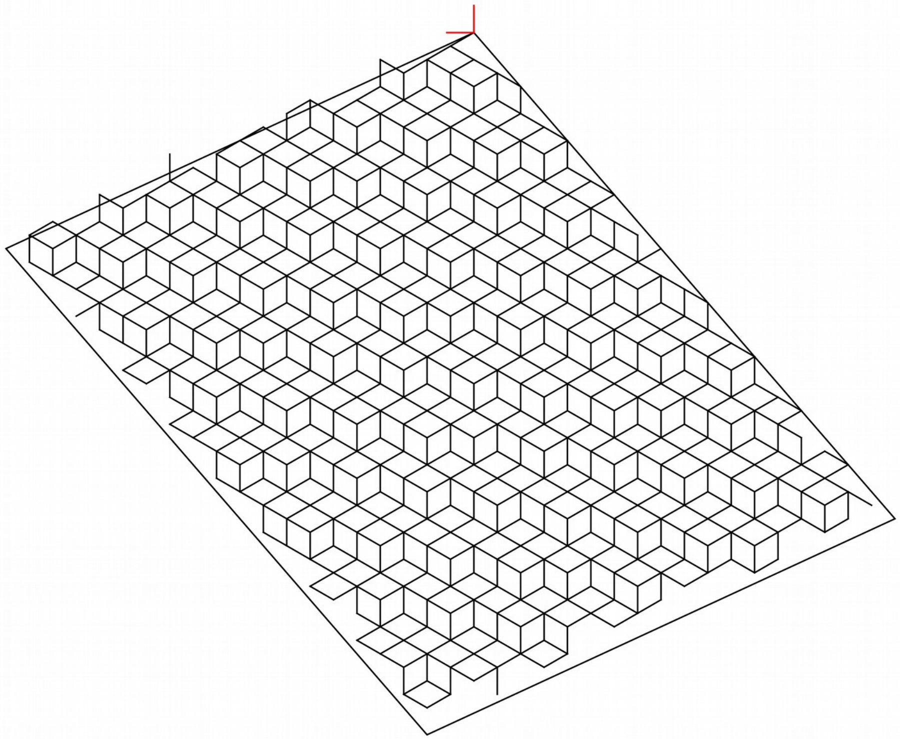
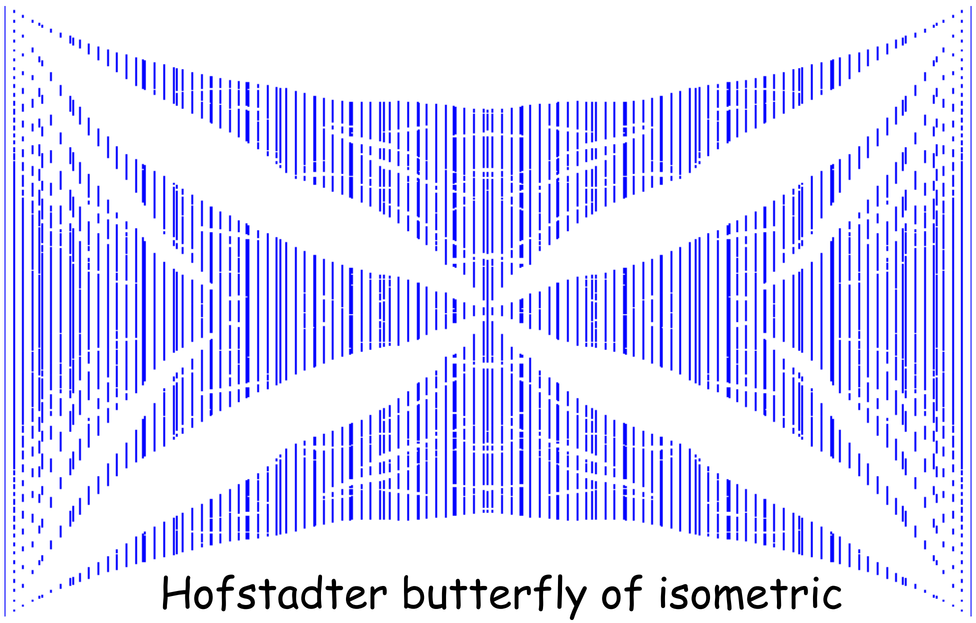


Isometric Rauzy tiling approximant of order k=10



Hofstadter butterfly of isometric Rauzy tiling (order k=14)

30'

Geo-dyn2015, IHP, 01/12/2015

Motivation :
Orbital magnetic susceptibility and band structure

Orbital magnetic susceptibility

2D electrons in free space, no interactions
Perpendicular magnetic field $\rightarrow$ cyclotron motion
Thermodynamic (grand) potential is a function of B

$$\Omega(\mu, T, B) = -T \int d\epsilon \rho(\epsilon, B) \ln(1 + e^{(\mu-\epsilon)/T})$$

First derivative $\rightarrow$ Spontaneous magnetization

$$M = -\left.\frac{\partial \Omega}{\partial B}\right|_{B=0}$$

Second derivative $\rightarrow$ <u>Susceptibility</u> (induced magnetization)

$$\chi = \left.\frac{\partial M}{\partial B}\right|_{B=0} = -\left.\frac{\partial^2 \Omega}{\partial B^2}\right|_{B=0}$$

Landau's diamagnetic susceptibility

Free electrons $\varepsilon(\mathbf{k}) = \dfrac{\hbar^2\mathbf{k}^2}{2m}$

Flat zero-field density of states (DoS) $\dfrac{m}{2\pi\hbar^2}$

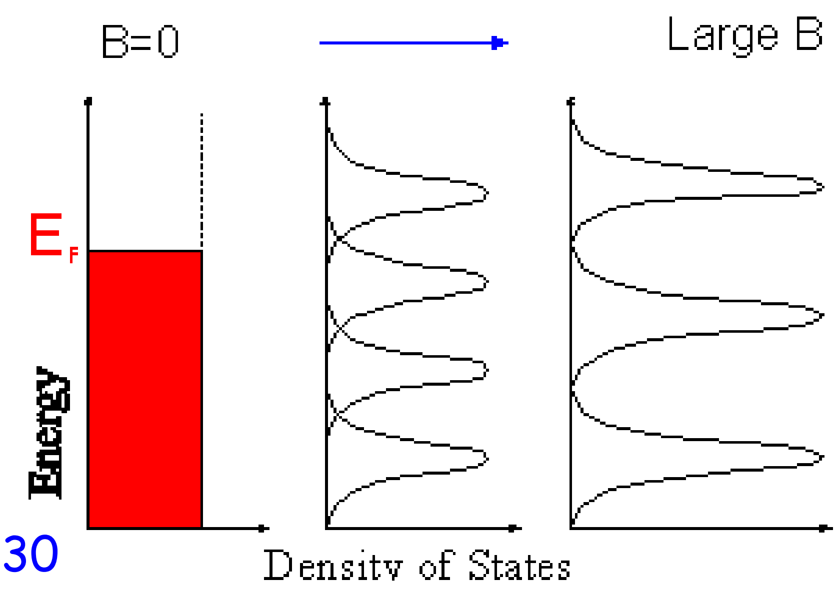
Landau levels (finite B)

$$\epsilon_n = \hbar\frac{eB}{m}(n+1/2)$$

Energy increase with B (due to 1/2 : zero-point motion)
$\rightarrow$ diamagnetism

$$\chi = -\frac{e^2}{24\pi m} < 0$$

Landau 1930



$$\hbar eB/m \ll T \ll \mu$$

Quantum diamagnetism

Orbital suscep. in periodic crystals & QC

Periodic crystals :

Orbital susceptibility can be diamagnetic (parabolic band edges) or paramagnetic (van Hove singularity)

Not only Fermi surface property (also Fermi sea)

Not only zero-field energy spectrum property (inter-band effects). Not just DoS, not just eff. Mass.

For review see Raoux, Morigi, Fuchs, Piéchon & Montambaux, PRB 2015

What about quasi-crystals ?

« Diamagnetism of quasicrystals » (experiments)

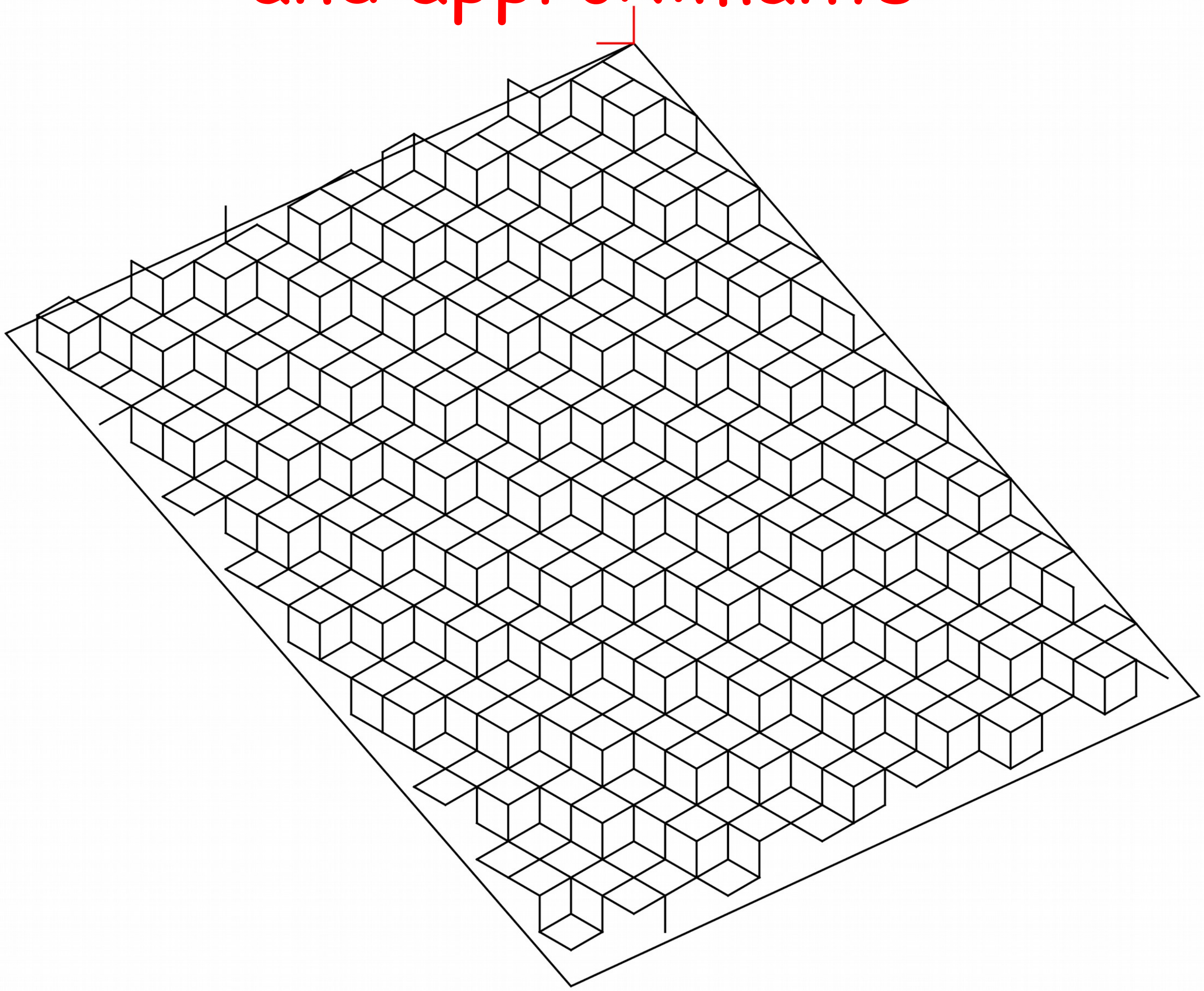
EITHER attributed to very low effective masses (Landau-Peierls formula) Cyrot-Lackmann, SSC 1997

OR attributed to atomic-like diamagnetism (no LP contribution due to very large effective masses)

Vekilov, Isaev & Johansson, SSC 2004

Unclear situation...

Isometric Rauzy tiling in 2D and approximants



Isometric Rauzy tiling in 2D: construction

Cut & project method 3 $\rightarrow$ 2 (co-dim 1)
Isometric = identical rhombic tiles
Sequence of Rauzy numbers to build approximants
(similar to Fibonacci chain but in 2D)

$R_{k+1} = R_k + R_{k-1} + R_{k-2}$ with $R_{-1} = 0, R_0 = 1, R_1 = 1$

Pisot root of

$$x^3 = x^2 + x + 1 \rightarrow \theta = 1.839... = \lim_{k\rightarrow\infty} R_{k+1}/R_k$$

(similar to golden mean)

Approximant of order k has N = R_{k+1} sites. Typically :

From k = 10, N = R_{11} = 927

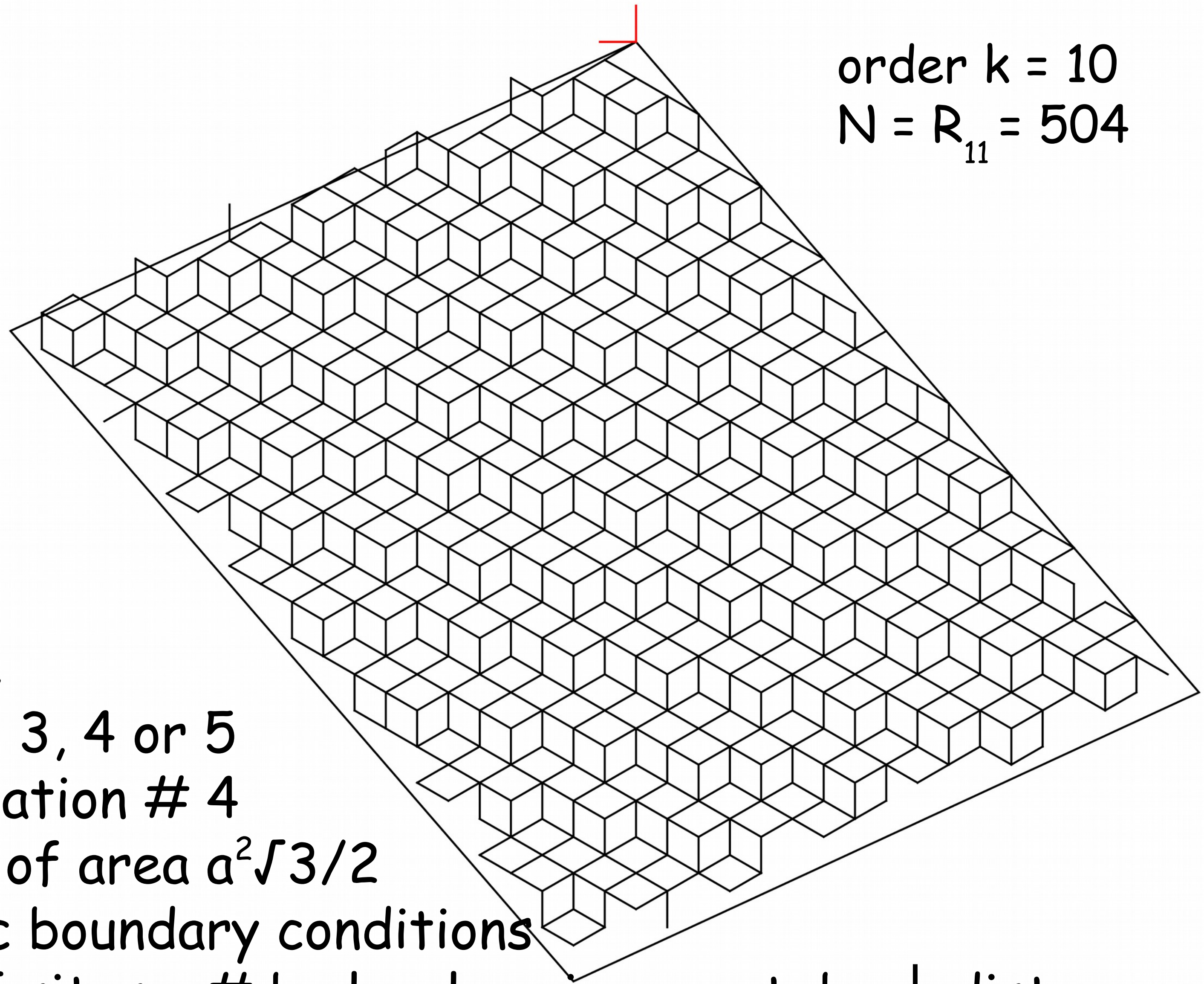
To k = 18, N = R_{19} = 66012

Vidal & Mosseri, J. Phys. A 2001 and J. Non-crys. Sol. 2004

Isometric Rauzy tiling in 2D: geometry

order k = 10

$N = R_{11} = 504$



Bipartite lattice

Coordination # : 3, 4 or 5

Average coordination # 4

Tiles = rhombus of area $a^2\sqrt{3}/2$

Open or periodic boundary conditions

Co-numbering of sites = # by local environment, by $\perp$ distance

Vidal & Mosseri, JPA 2001 and JNCS 2004

Isometric Rauzy tiling in 2D: TB model

Nearest-neighbor TB Hamiltonian $H = -t \sum_{\langle i,j \rangle} |i\rangle\langle j|$

Co-numbering of sites according to their perpendicular space coordinate. Connectivity matrix is Toeplitz-like.
Ex: approximant k = 4, N = R_5 = 13 sites, H is NxN matrix

$$H_{PBC}/\text{-}t = \begin{pmatrix}
0&0&1&0&1&0&0&1&0&0&0&0&0\\
0&0&0&1&0&1&0&0&1&0&0&0&0\\
1&0&0&0&1&0&1&0&0&1&0&0&0\\
0&1&0&0&0&1&0&1&0&0&1&0&0\\
1&0&1&0&0&0&1&0&1&0&0&1&0\\
0&1&0&1&0&0&0&1&0&1&0&0&1\\
0&0&1&0&1&0&0&0&1&0&1&0&0\\
1&0&0&1&0&1&0&0&0&1&0&1&0\\
0&1&0&0&1&0&1&0&0&0&1&0&1\\
0&0&1&0&0&1&0&1&0&0&0&1&0\\
0&0&0&1&0&0&1&0&1&0&0&0&1\\
0&0&0&0&1&0&0&1&0&1&0&0&0\\
0&0&0&0&0&1&0&0&1&0&1&0&0
\end{pmatrix}
\qquad
H_{OBC}/\text{-}t = \begin{pmatrix}
0&0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&0&0&1&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0\\
0&1&0&0&0&1&0&1&0&0&1&0&0\\
1&0&1&0&0&0&1&0&1&0&0&1&0\\
0&0&0&1&0&0&0&0&0&1&0&0&1\\
0&0&0&0&1&0&0&0&0&0&1&0&0\\
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0&0&0&0&0&1&0&1&0&0&0&0&0\\
0&0&0&1&0&0&1&0&1&0&0&0&1\\
0&0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&1&0&0
\end{pmatrix}$$

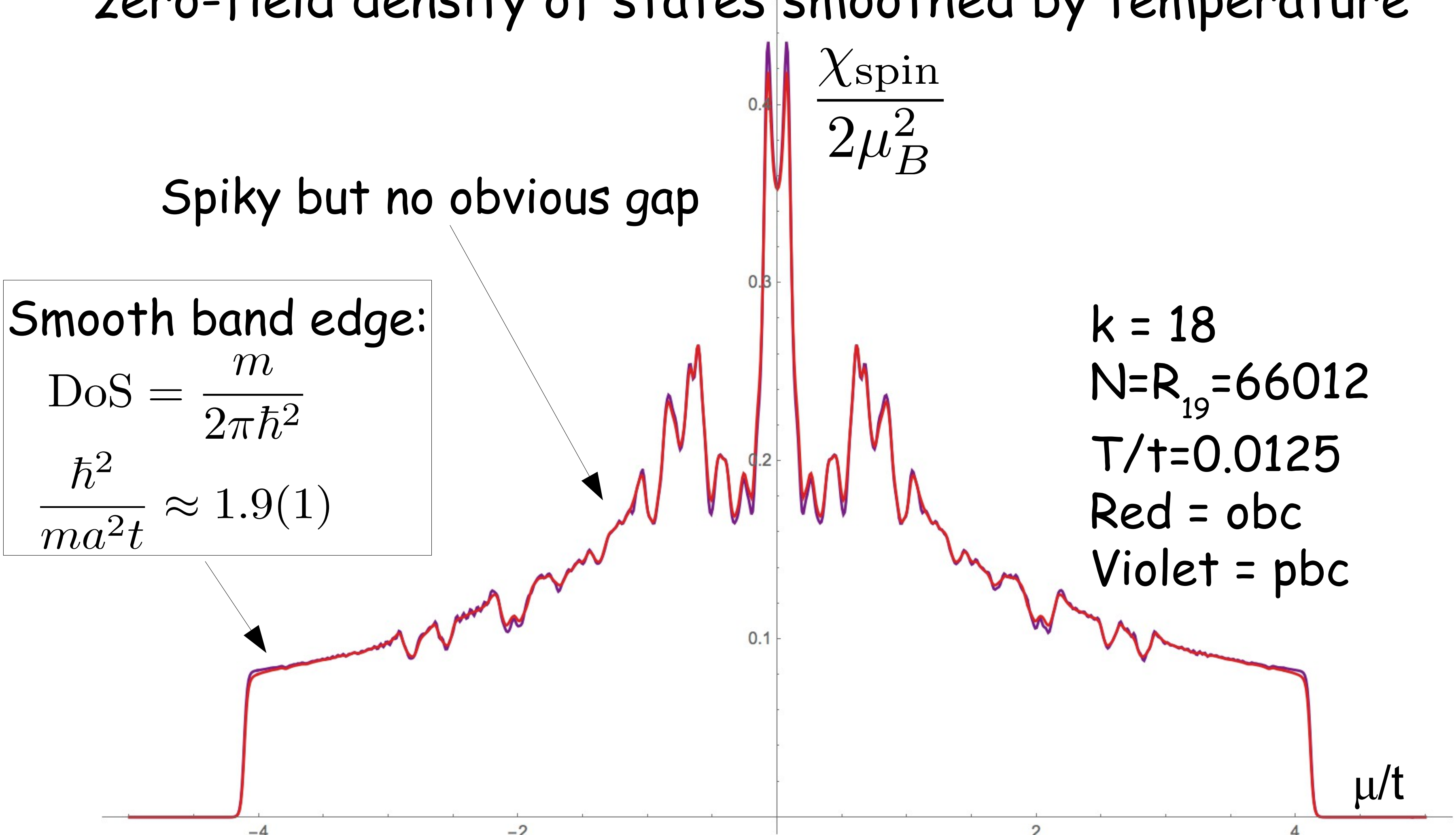
Vidal & Mosseri, JPA 2001 and JNCS 2004

Tight-binding model in zero field : density of states (DoS) & ground-state

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

Spin susceptibility (T-smoothed DoS)

Zeeman coupling , no spin-orbit → spin susceptibility is zero-field density of states smoothed by temperature



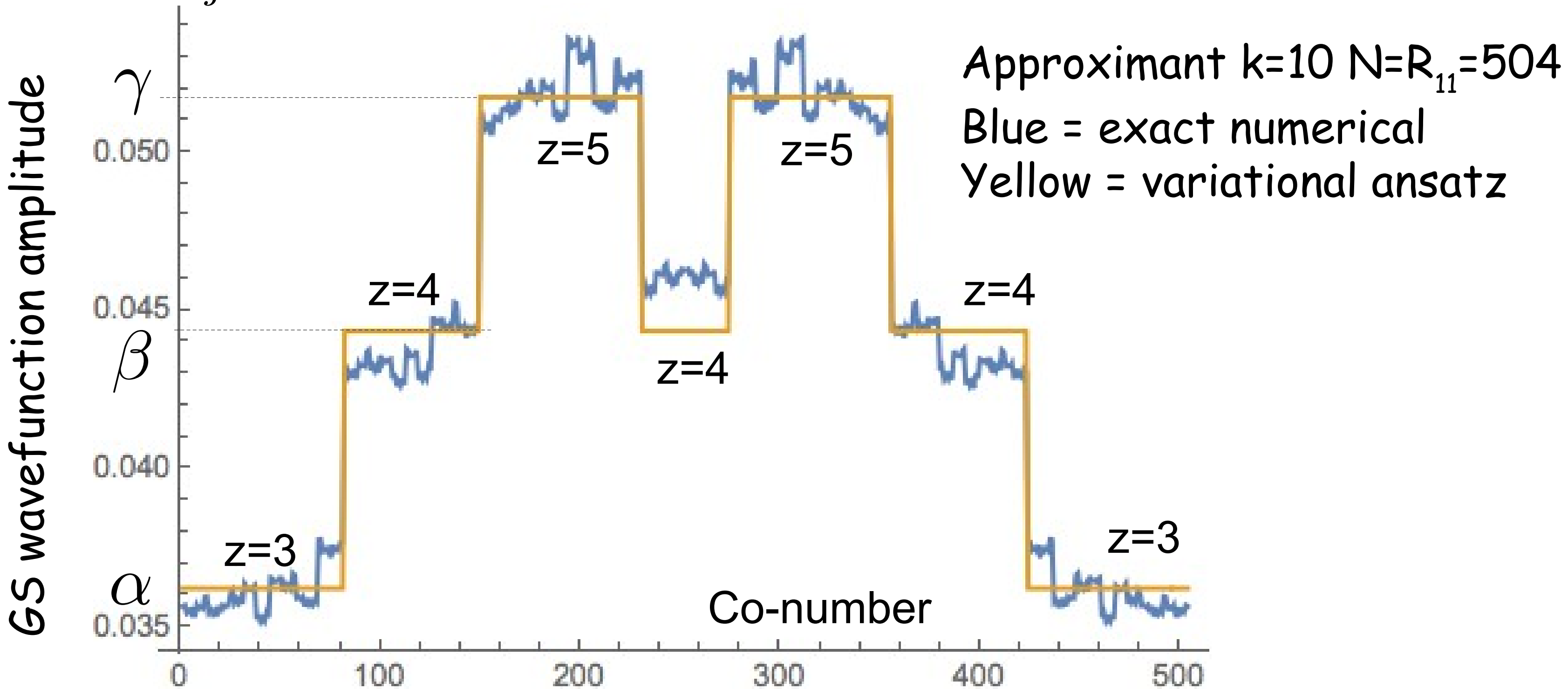
Bandwidth $W \approx 8.22t$

See also Jagannathan, PRB 2001
Triozon, Vidal, Mosseri & Mayou, JNCS 2004

Ground-state energy and wavefunction

Exact num. calculation for approximant (order up to k= 20) with PBC vs variational ansatz with «3» parameters (coordination #)

$$|\psi_{\rm var}\rangle = \sum_{j \text{ conum}} \psi(z_j)|j\rangle \text{ with } \psi(z_j) = \alpha, \beta, \gamma \text{ if } z_j = 3, 4, 5$$



Thermodynamic limit : wf overlap = 0.999777

& GS energy $E_{\rm exact} = -4.11501t$ and $E_{\rm var} = -4.11297t(0.05\%)$

See also Triozon, Vidal, Mosseri & Mayou, JNCS. 2004 ; Kalugin & Katz, JPA 2014

Tight-binding model in a field : OBC butterfly & orbital susceptibility

$$H_A = -t \sum_{\langle i,j \rangle} e^{-i\frac{e}{\hbar}\int_j^i d\boldsymbol{r}\cdot\boldsymbol{A}} |i\rangle\langle j|$$

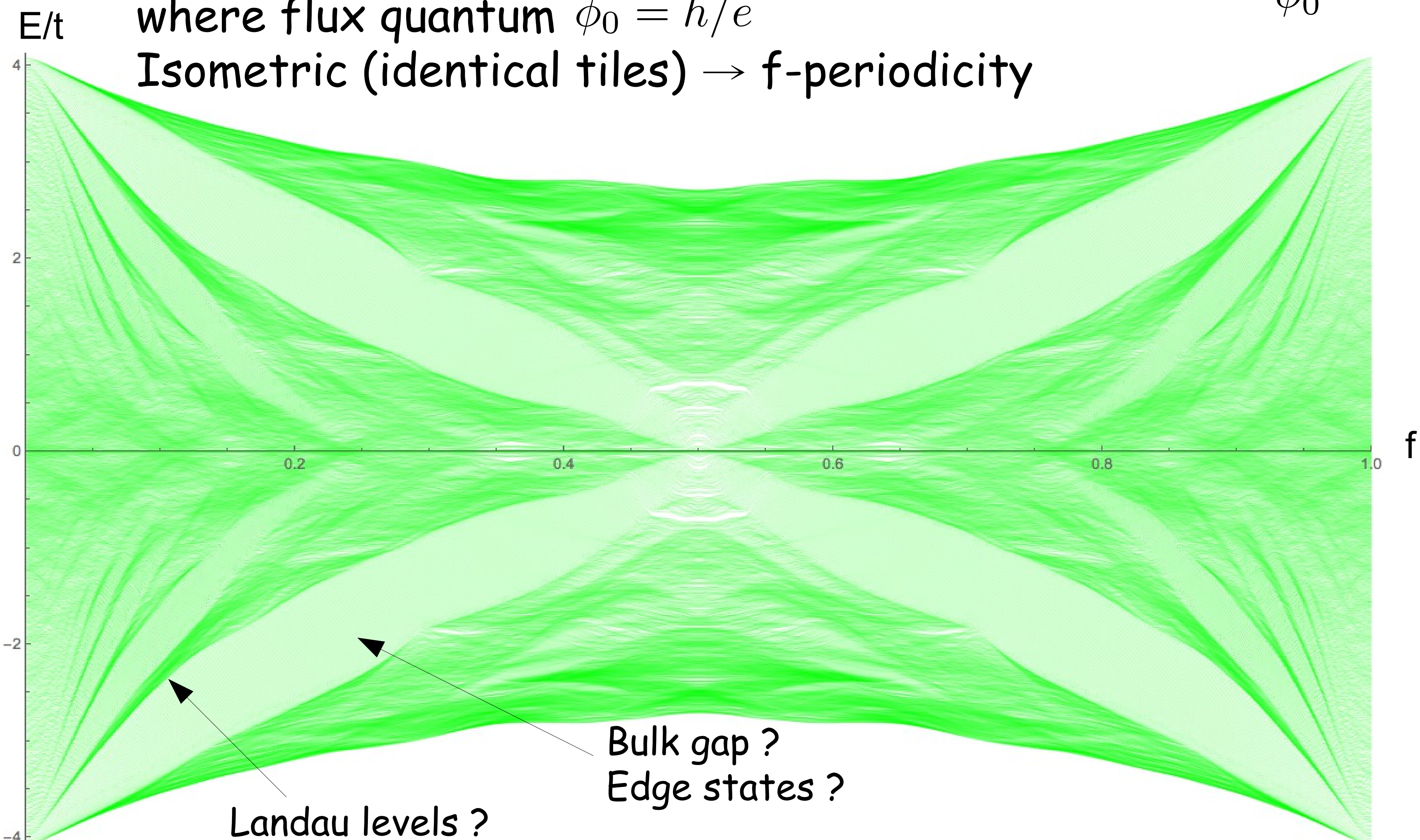
OBC Rauzy butterfly

Order k = 11, N= R_{12} = 927. Finite size, edges, any flux.

Energy spec. vs dimensionless flux/plaquette $f = \dfrac{Ba^2\sqrt{3}/2}{\phi_0}$

where flux quantum $\phi_0 = h/e$

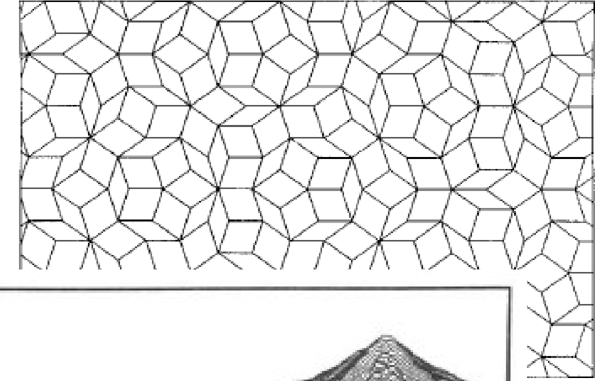
Isometric (identical tiles) $\rightarrow$ f-periodicity



See also Vidal & Mosseri, JNCS 2004; Tran, Dauphin, Goldman & Gaspard, PRB 2015

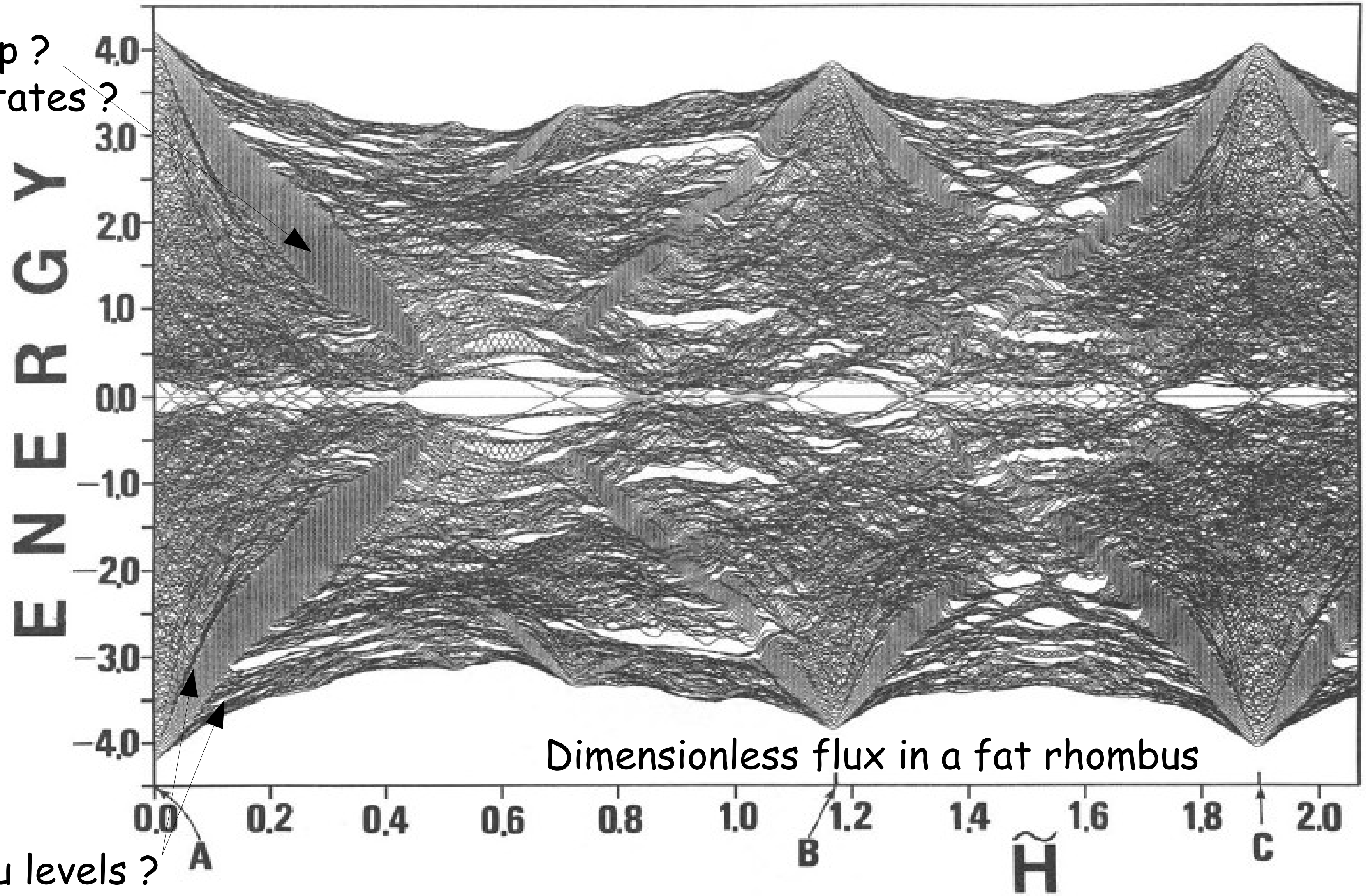
OBC Penrose butterfly

N=536. Two incommensurate tiles (thin and fat rhombi).



Bulk gap ?

Edge states ?

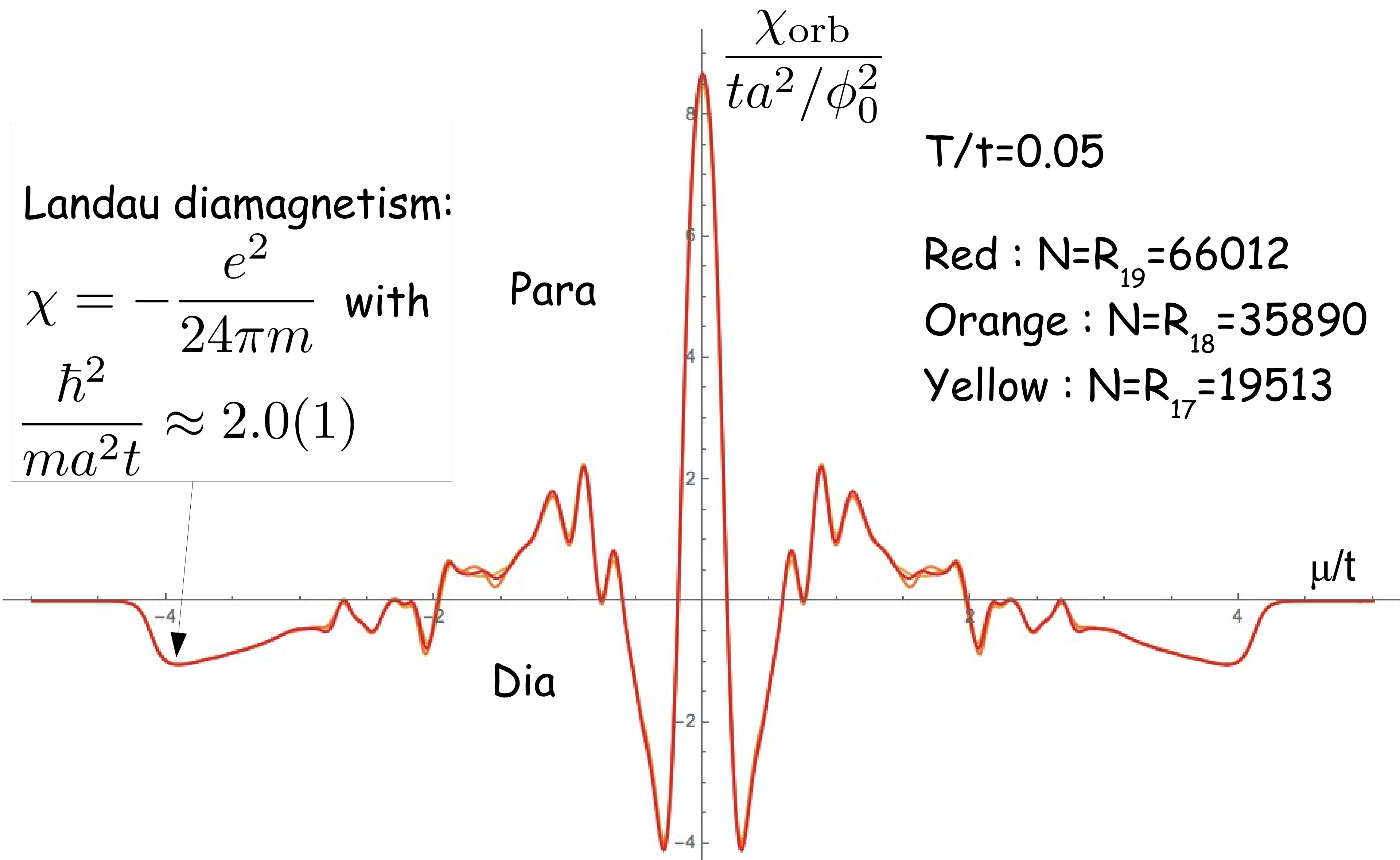


Dimensionless flux in a fat rhombus

Landau levels ?

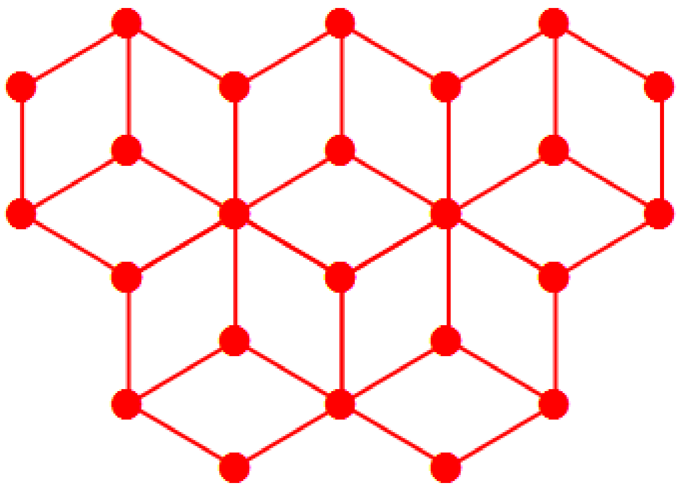
Hatakeyama, Kamimura, SSC. 1987

Orbital susceptibility of Rauzy tiling

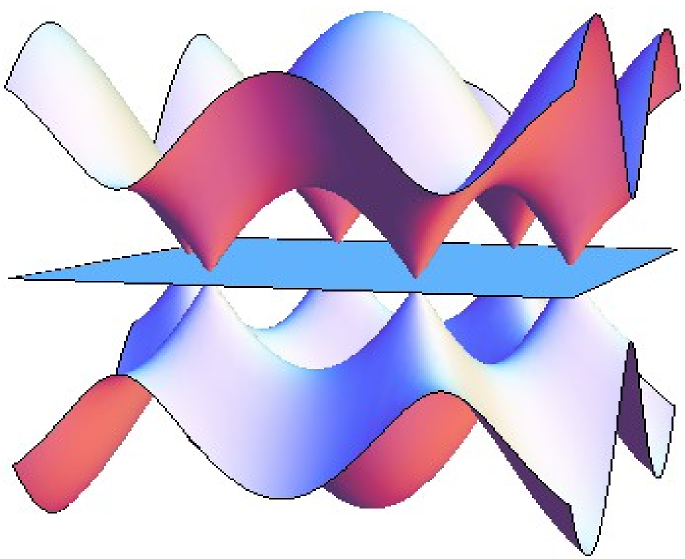


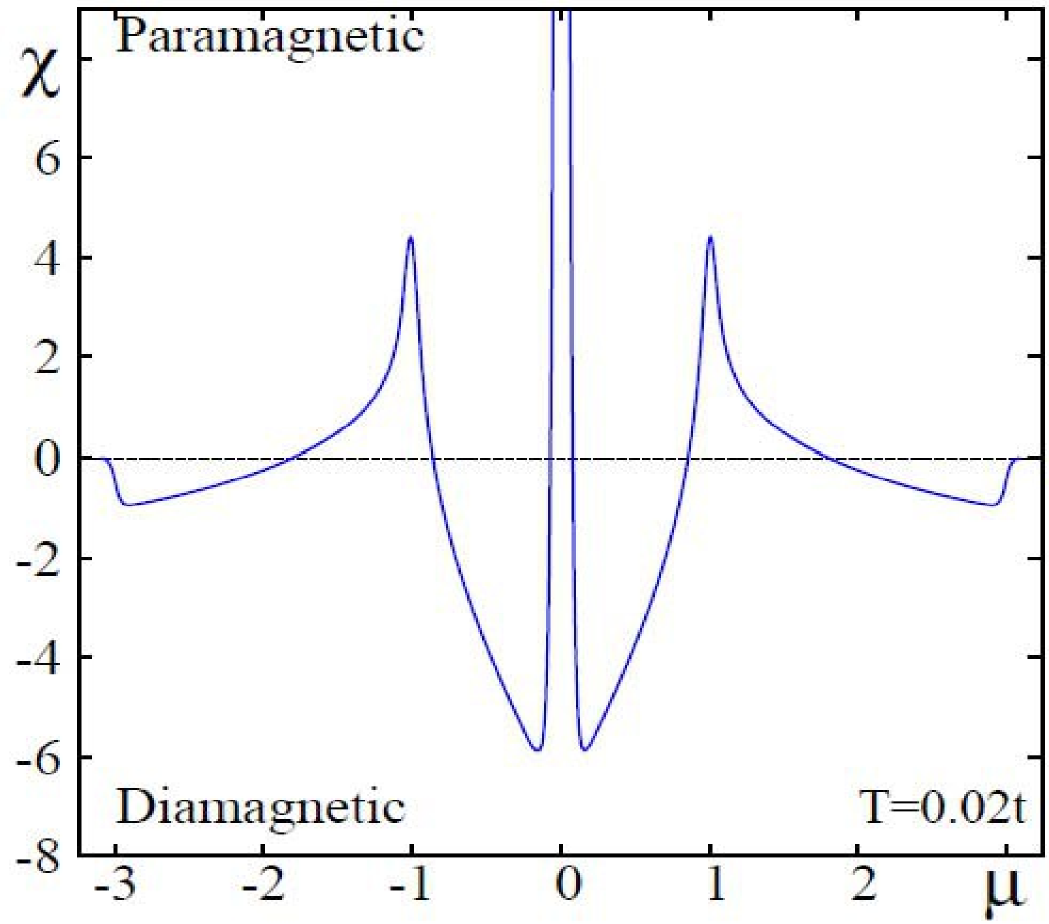
$T \gg$ Landau level spacing $\sim W/N_\phi \gg$ level spacing $\sim W/N$

Orbital susceptibility of T3 (dice) crystal



Dice crystal (3 atoms/unit cell)
(sublattice spin 1)



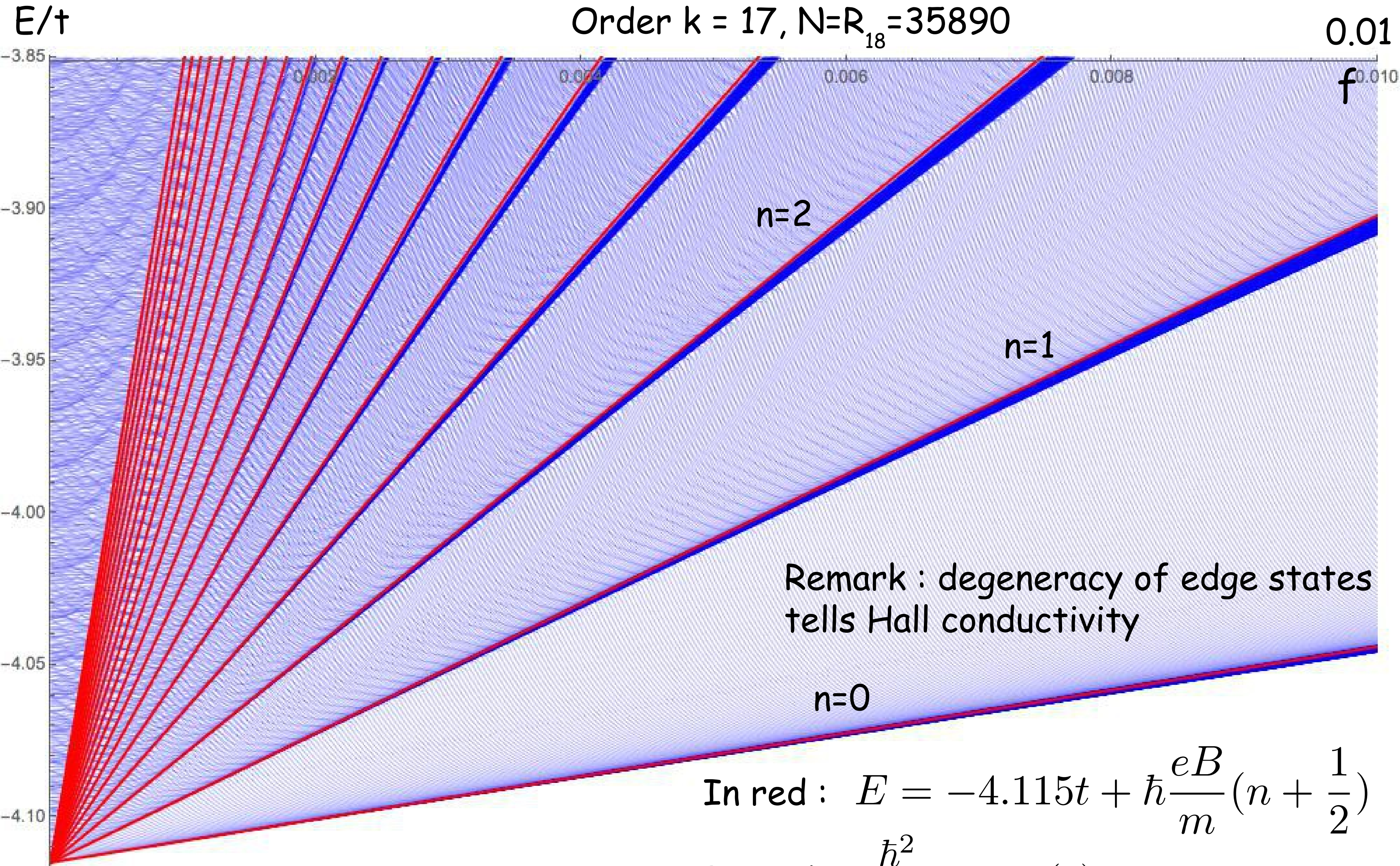


Raoux, Morigi, Fuchs, Piéchon & Montambaux, PRL 2014

Landau levels and effective mass

$$E = \hbar \frac{eB}{m}(n + \frac{1}{2})$$

Landau levels and effective mass ?



In red : $E = -4.115t + \hbar \frac{eB}{m}(n + \frac{1}{2})$

Fit with $\frac{\hbar^2}{ma^2 t} \approx 1.9(1)$

Vicinity of band bottom

Effective mass tensor

Approximant k as large unit cell ($N=R_{k+1}$ sites) of crystal $\rightarrow$ mini-bands and mini Brillouin zone (BZ). Numerical diagonalization for k = 12 to 16.

$$H(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} H e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \text{ where } \boldsymbol{x} \text{ is position operator}$$

$$E_n(\boldsymbol{k}) \qquad n = 1, \ldots, N; \; \boldsymbol{k} \text{ in mini-BZ}$$

(Inverse) effective mass tensor of the lowest mini-band

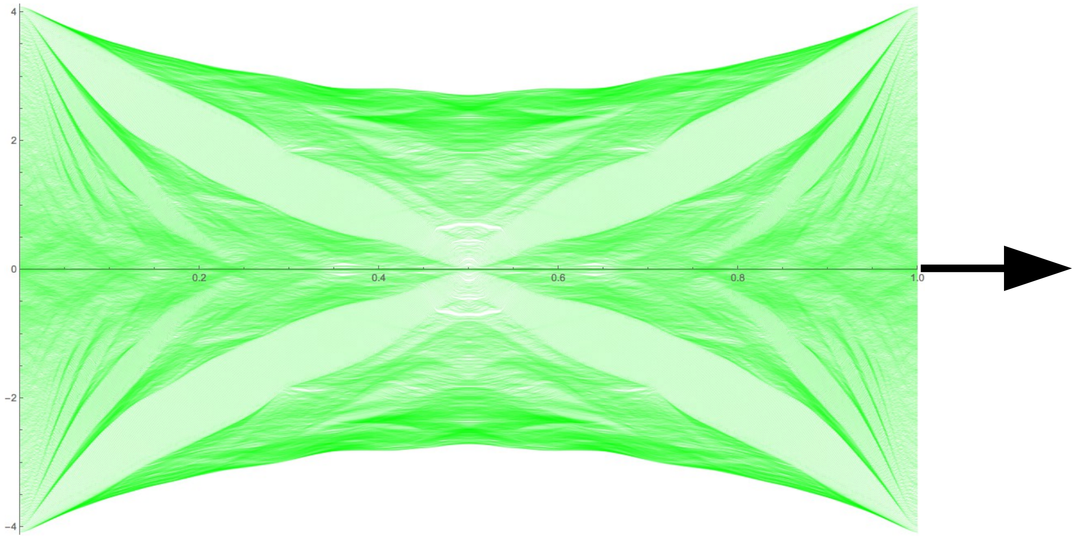
$$E_1(\boldsymbol{k}) - E_1(0) \approx \frac{1}{2}\alpha_{ij} t a^2 k_i k_j$$

$$\mathrm{IDoS} = N(E) = \frac{E}{2\pi t a^2 \sqrt{\det \underline{\alpha}}} = \frac{mE}{2\pi\hbar^2} \quad \text{defines eff. mass}$$

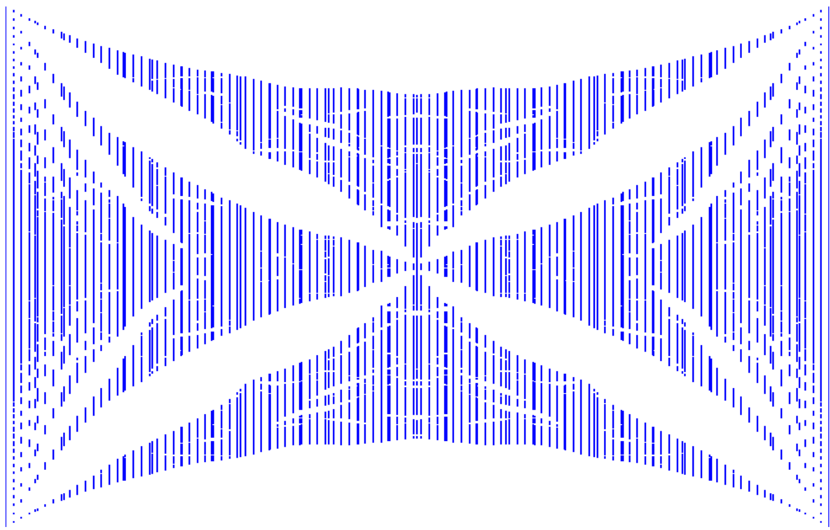
$$\alpha_{ij} = \begin{pmatrix} \alpha_{xx} & \alpha_{xy} \\ \alpha_{xy} & \alpha_{yy} \end{pmatrix} \approx \begin{pmatrix} 1.61702 & 0.0803396 \\ 0.0803396 & 2.37328 \end{pmatrix}$$

$$\frac{\hbar^2}{ma^2 t} = \sqrt{\det \underline{\alpha}} \approx 1.95735(1)$$

PBC butterfly and gap labeling



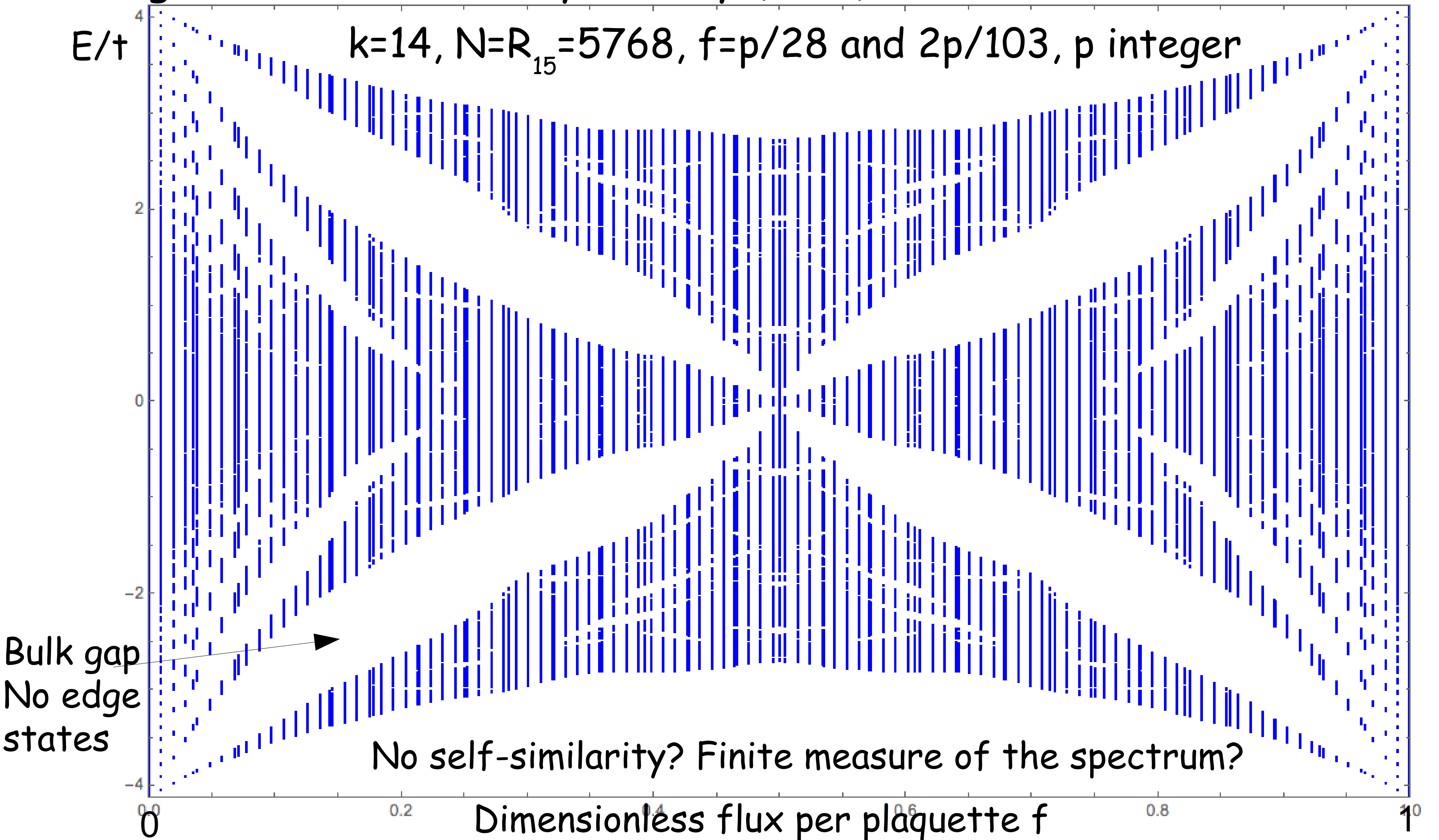
OBC



PBC

PBC Rauzy butterfly

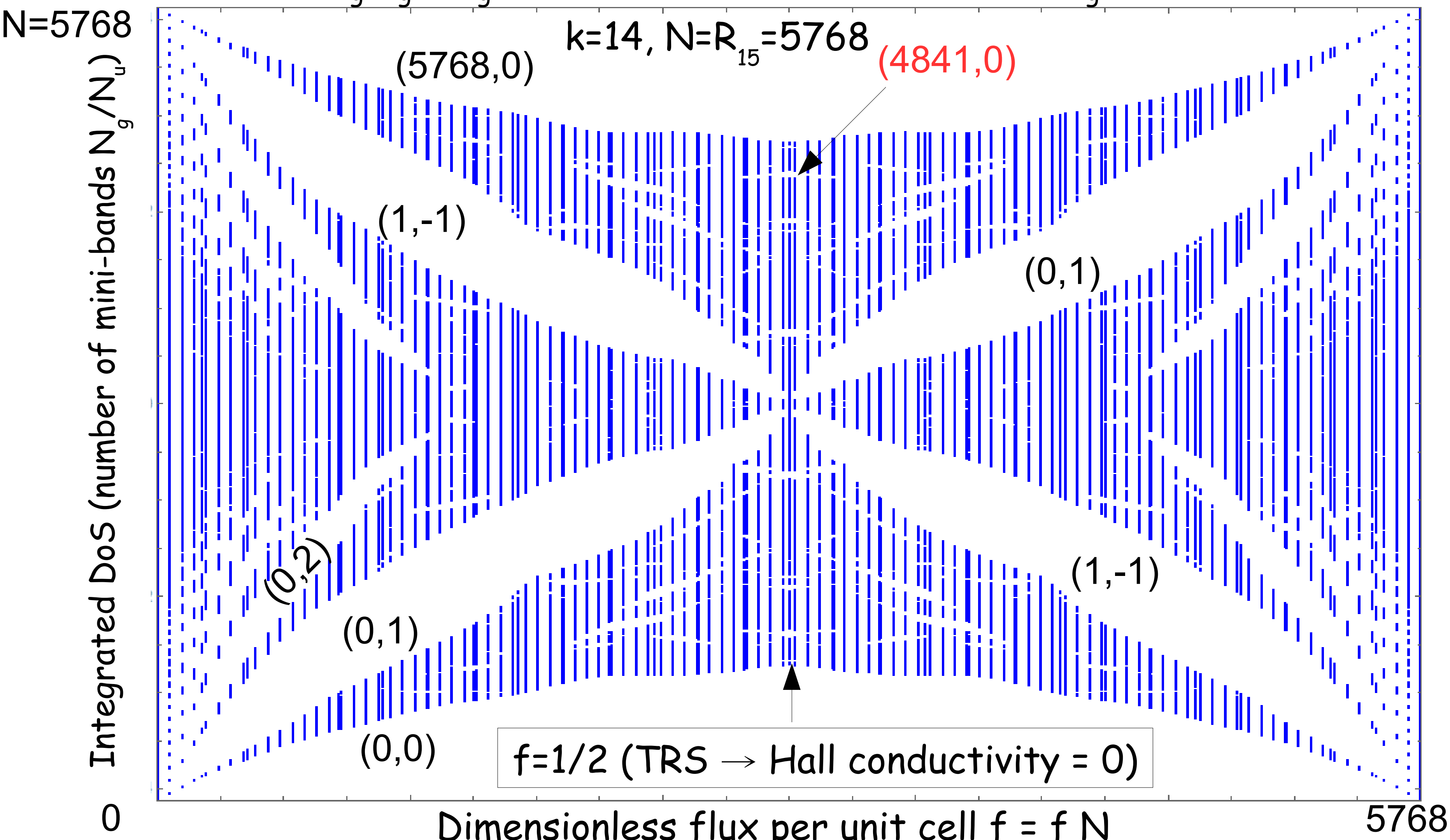
Some gauge choices allows one to study the system on a torus and for a "large" # of fluxes. Single unit cell. Finite size, no edges. Time reversal symmetry (TRS) when f = 0 or ½ modulo 1.



TKNN gap labeling for Rauzy butterfly

Number of mini-bands below a gap : $N_g/N_u = s_g + t_g f_u$ in [0,N]

Two integers (s_g,t_g): t_g = Hall conductivity [e^2/h], s_g = modulo

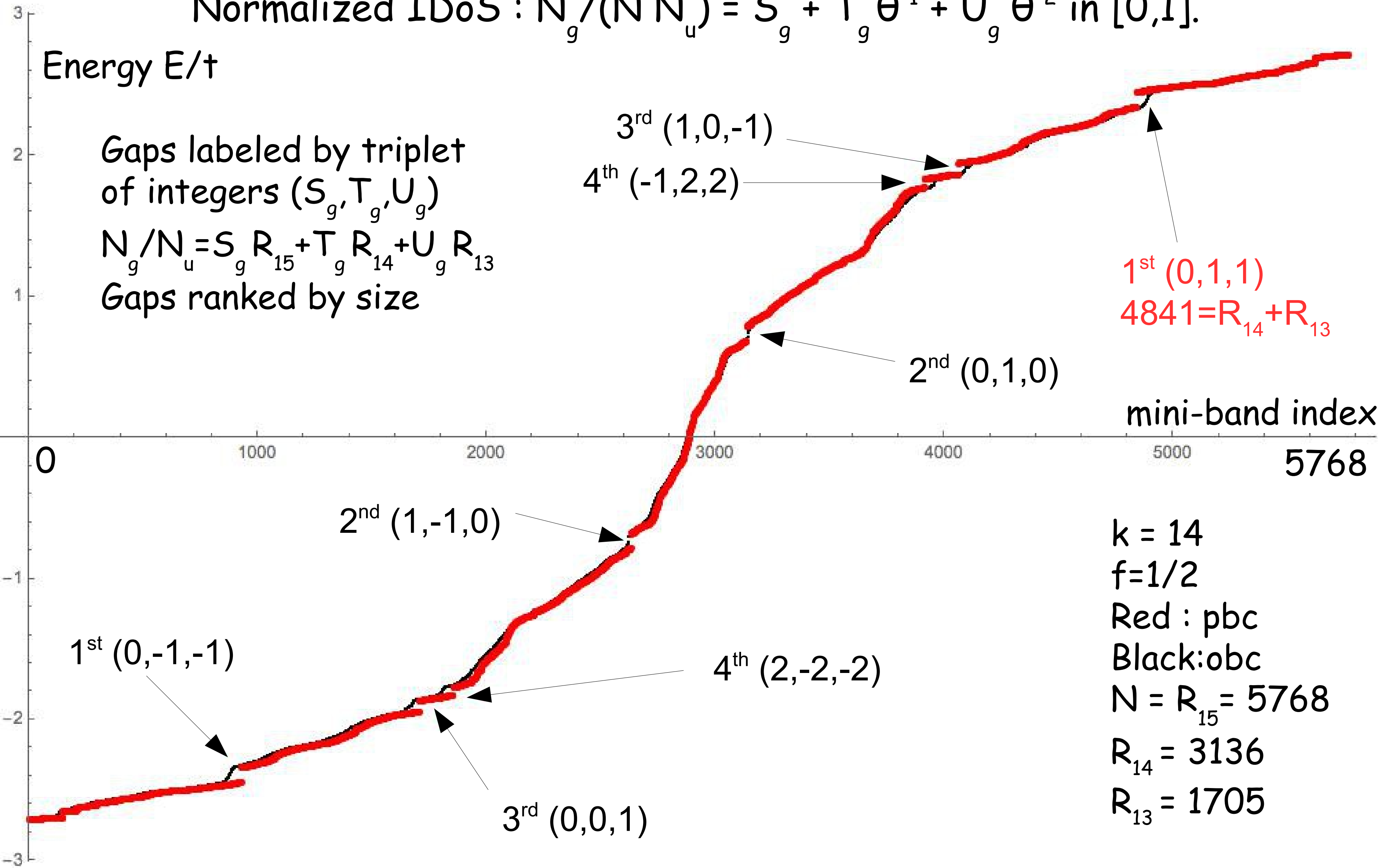


Thouless, Kohmoto, Nightingale, den Nijs, PRL 1982 ; Wannier 1978

QC gap labeling : Rauzy at f=1/2 (TRS)

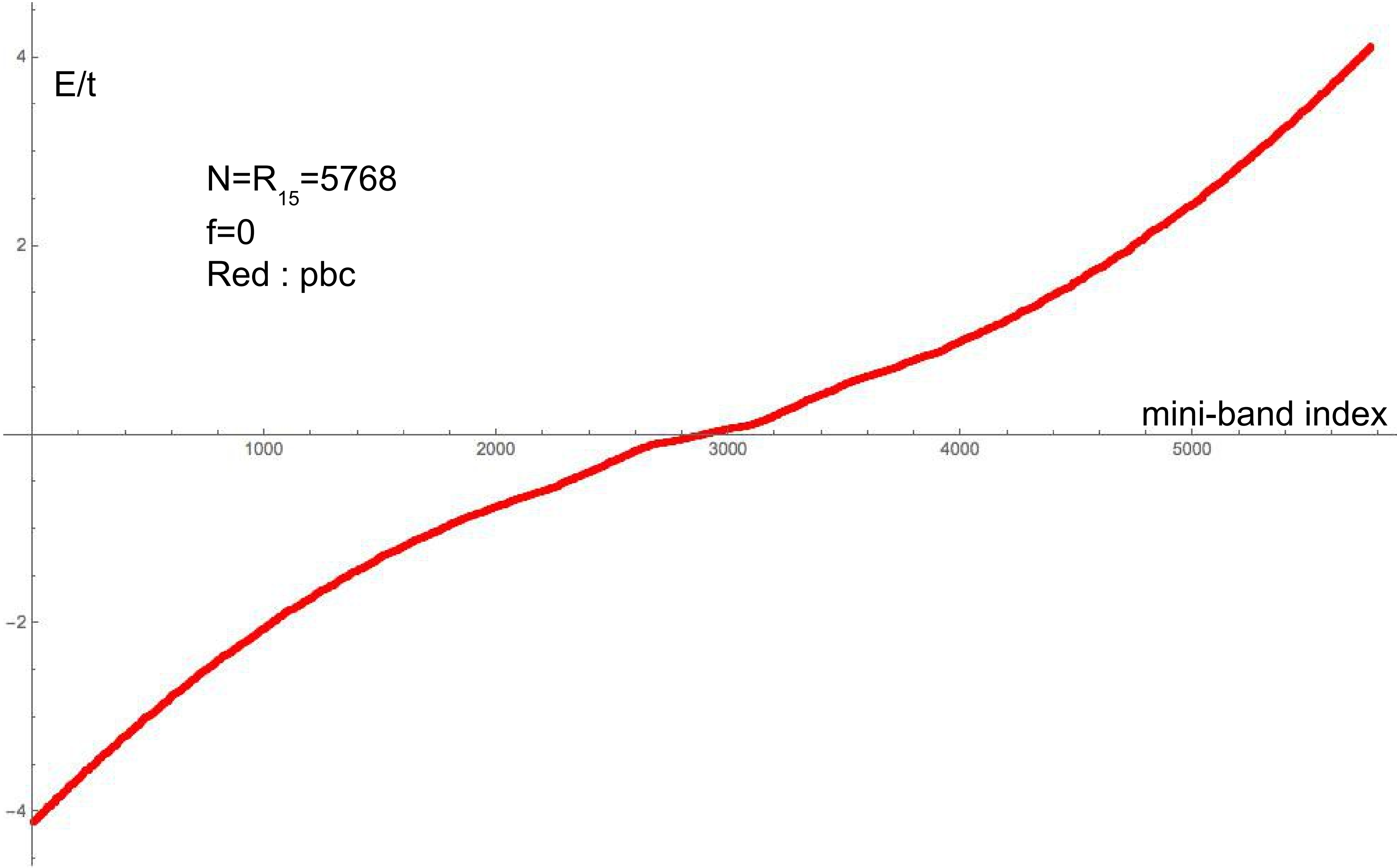
Number of mini-bands below a gap : $N_g/N_u = S_g R_{k+1} + T_g R_k + U_g R_{k-1}$ in [0,N]

Normalized IDoS : $N_g/(N N_u) = S_g + T_g \theta^{-1} + U_g \theta^{-2}$ in [0,1].



QC gap labeling : Rauzy at f=0 (TRS)

Nothing to label... no gaps



Conclusion/perspectives

Orbital susceptibility of Rauzy tiling :

As much dia as para; sum rule $\int d\mu \chi_{\mathrm{orb}}(T,\mu) = 0$

Closest to dice's susceptibility, para peak at half-filling, several sign changes as function of doping

Band edges eff. mass neither small nor large $m \sim \frac{\hbar^2}{ta^2}$

Rauzy butterfly :

Two types of gaps. TKNN labeling (1 relevant int. = Hall conductivity) or QC labeling (2 relevant integers) ?

Physical meaning of the integers ? Bragg peak co-num ?

Spectrum appears dense : measure ? Open orbits ?

No self-similarity ?

Two origins for incommensurability: magnetic flux f and C&P slope (related to Rauzy number θ)

Robustness of gap labeling vs flux or vs C&P slope ?

Acknowledgments

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