Moiré Dirac semimetals and the role of quasiperiodicity

U.PORTO

FACULDADE DE CIÊNCIAS UNIVERSIDADE DO PORTO

Eduardo V. Castro

Centro de Física do Porto

CF-UM-UP

LaPMET LABORATORY OF PHYSICS FOR MATERIALS AND EMERGENT TECHNOLOGIES

Physics & Astronomy Department

Faculty of Sciences, University of Porto

Centro de Física das Universidades do Minho e do Porto (CF-UM-UP)

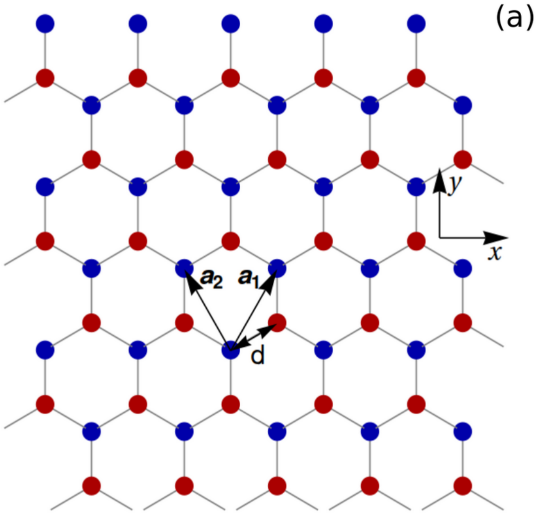
Laboratório de Física para Materiais e Tecnologias Emergentes (LaPMET)

Weyl and Dirac Semimetals as a Laboratory for High-Energy Physics

U. Minho, 27 June 2025

2D Dirac semimetals – Graphene

Monolayer graphene



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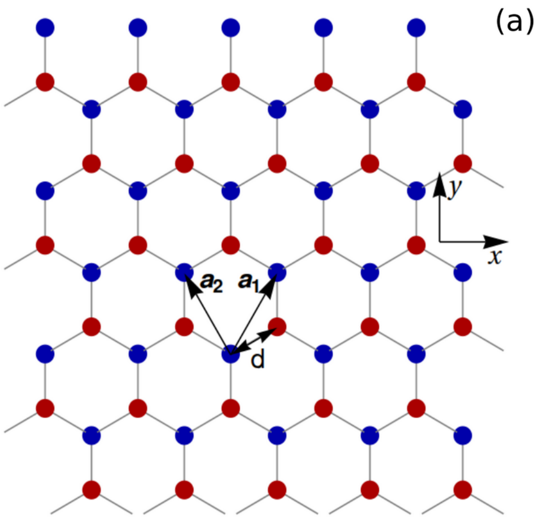

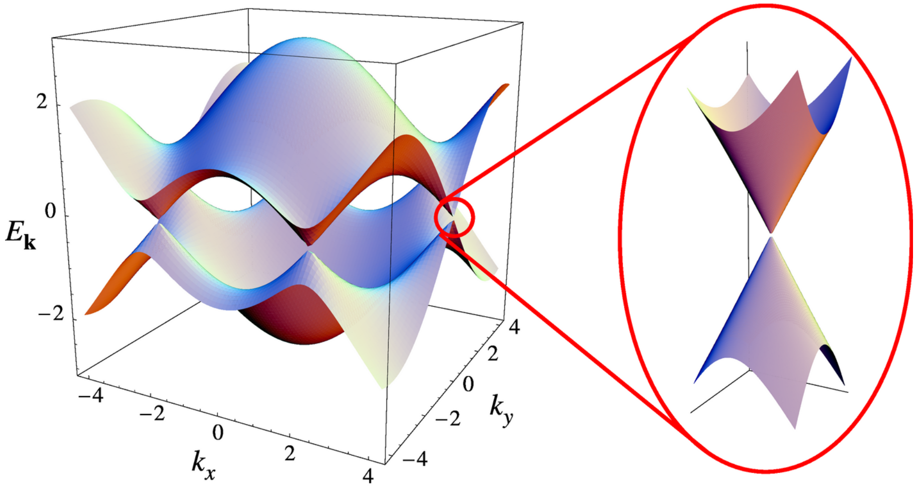

$$\mathcal{H} \simeq v_F \hbar \begin{bmatrix} 0 & k_x - i k_y \\ k_x + i k_y & 0 \end{bmatrix} = v_F \boldsymbol{\sigma} \cdot \mathbf{p}$$

$\boldsymbol{\sigma} \rightarrow$ vector of Pauli matrices

$v_F \rightarrow c/300$

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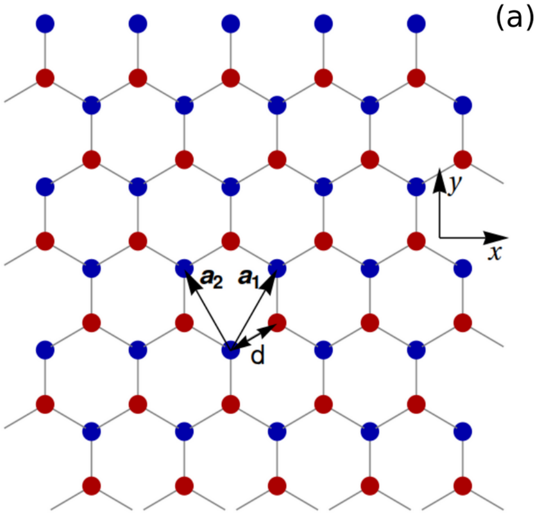

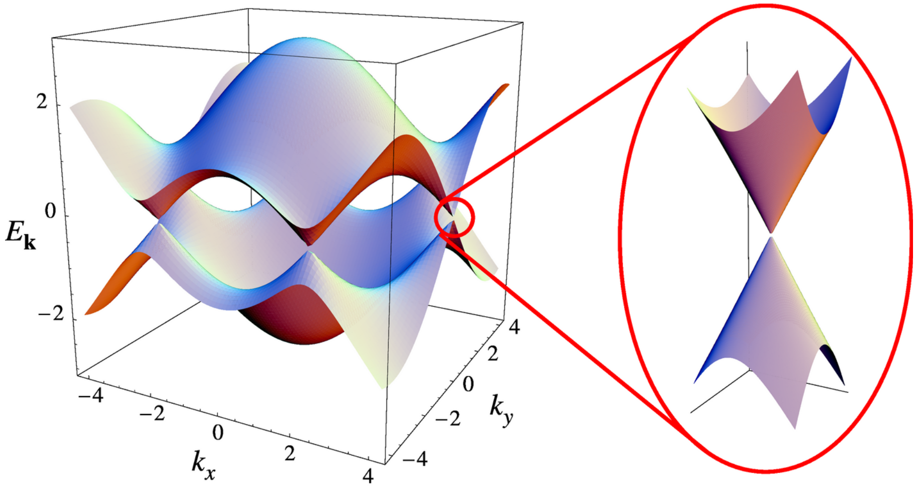

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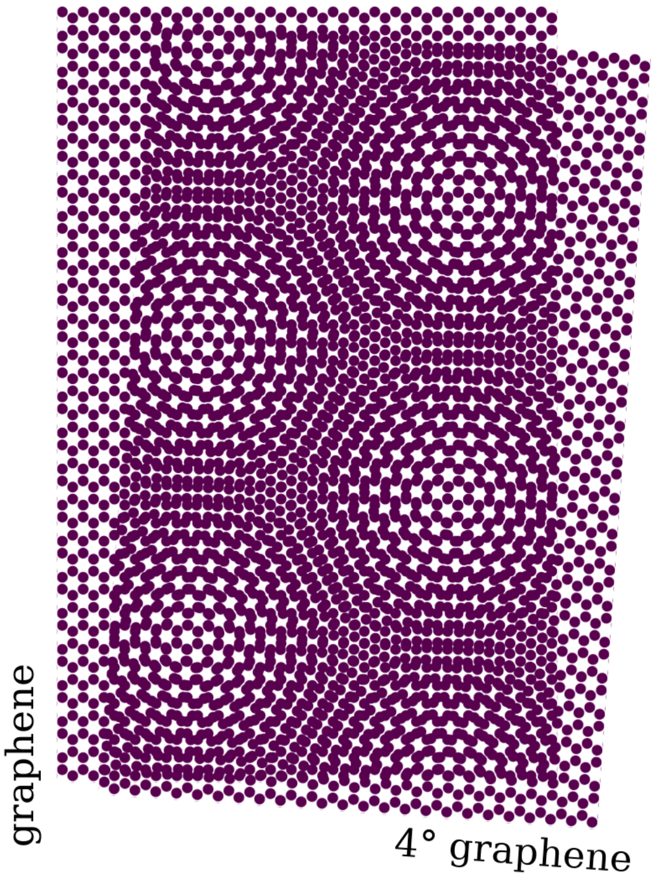
Collapse of Landau levels in Weyl semimetals

Vicente Arjona[1], Eduardo V. Castro[2,3], and María A. H. Vozmediano[1]

Phys. Rev. B **96**, 081110(R) – **Published 17 August, 2017**

Twisted bilayer graphene (tBLG)

Cao et al., Nature **556**, 43-50 (2018)
Cao et al., Nature **556**, 80-84 (2018)



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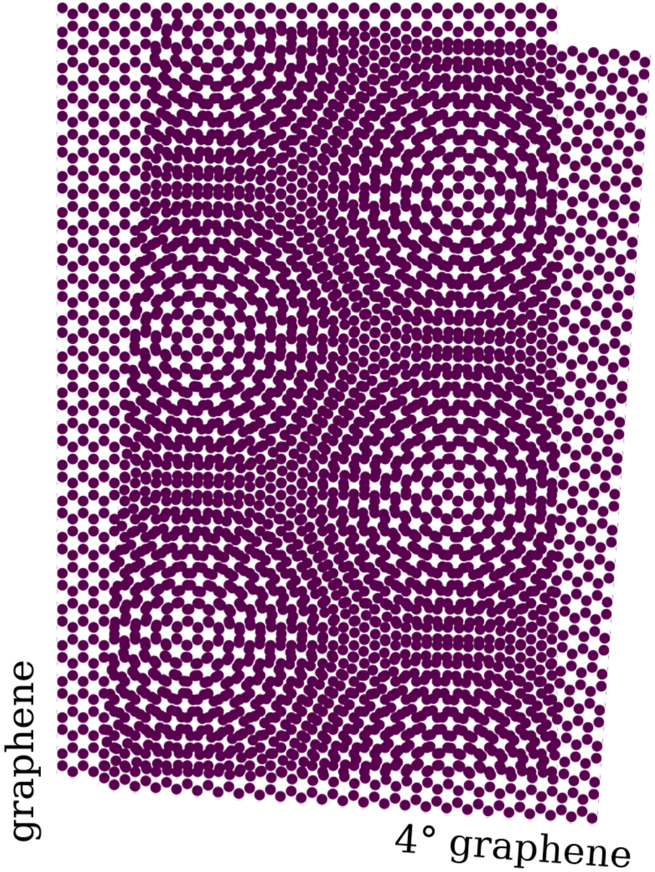

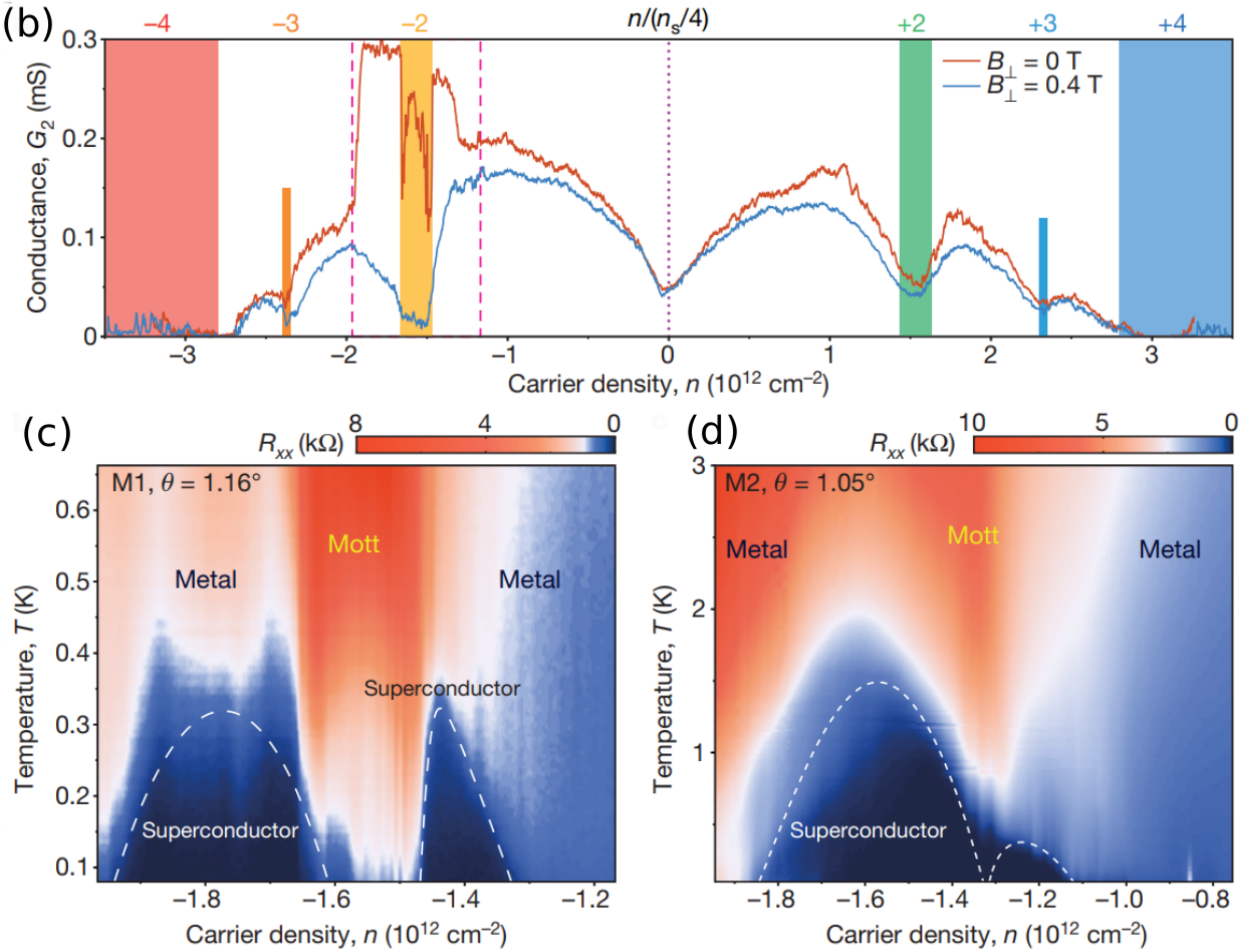

Outline

- *Introduction*
  - 2D Dirac semimetals and moiré physics
- *Motivation*
  - Quasiperiodicity driven sub-ballistic behavior in tBLG

    M. Gonçalves, H. Olyaei, B. Amorim, R. Mondaini, P. Ribeiro, EVC, 2D Mater. **9**, 011001 (2022)
- *Quasiperiodicity effects in interacting 1D moiré systems*
  - Quasi-fractal order: DMRG and Mean-Field

    M. Gonçalves, B. Amorim, F. Riche, EVC, P. Ribeiro, Nat. Phys. **20**, 1933–1940 (2024)
    N. Sobrosa, M. Gonçalves, EVC, P. Ribeiro, B. Amorim [to appear soon]

    M. Gonçalves, B. Amorim, EVC, P. Ribeiro, Scipost Phys. **13**, 046 (2022)
    M. Gonçalves, B. Amorim, EVC, P. Ribeiro, Phys. Rev. B **108**, L100201 (2023)
    M. Gonçalves, B. Amorim, EVC, P. Ribeiro, Phys. Rev. Lett. **131**, 186303 (2023)
    M. Gonçalves, J. H. Pixley, B. Amorim, EVC, P. Ribeiro, Phys. Rev. B **109**, 014211 (2024)
    R. Oliveira, M. Gonçalves, P. Ribeiro, EVC, B. Amorim [arxiv:2303.17656]

The team

Bruno Amorim
U Porto

Pedro Ribeiro
U Lisbon

Students:

Nicolau Sobrosa
U Porto

Ricardo Oliveira
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Raul Liquito
U Porto

Flávio Riche
U Lisbon

Former Students:

Miguel Gonçalves
Before: U Lisbon; LANL
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Collaborators:

Rubem Mondaini
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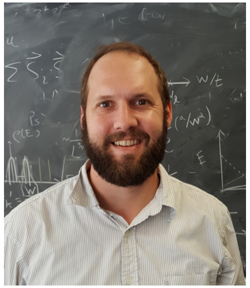

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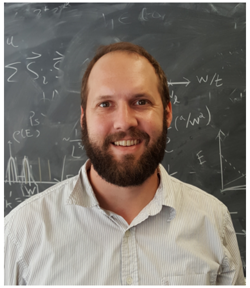

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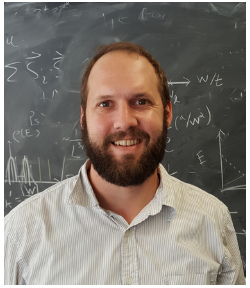

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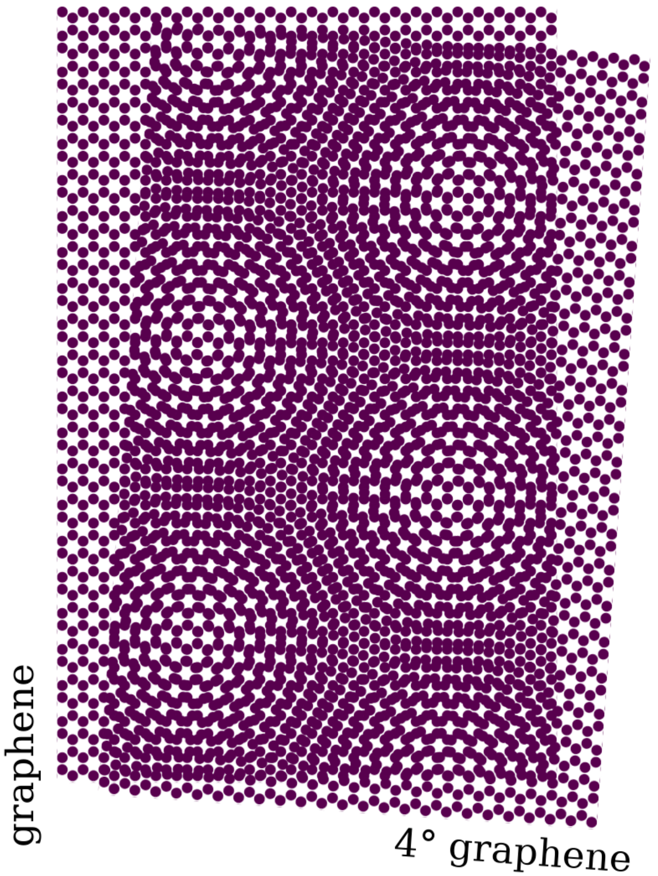
tBLG – A moiré Dirac semimetal



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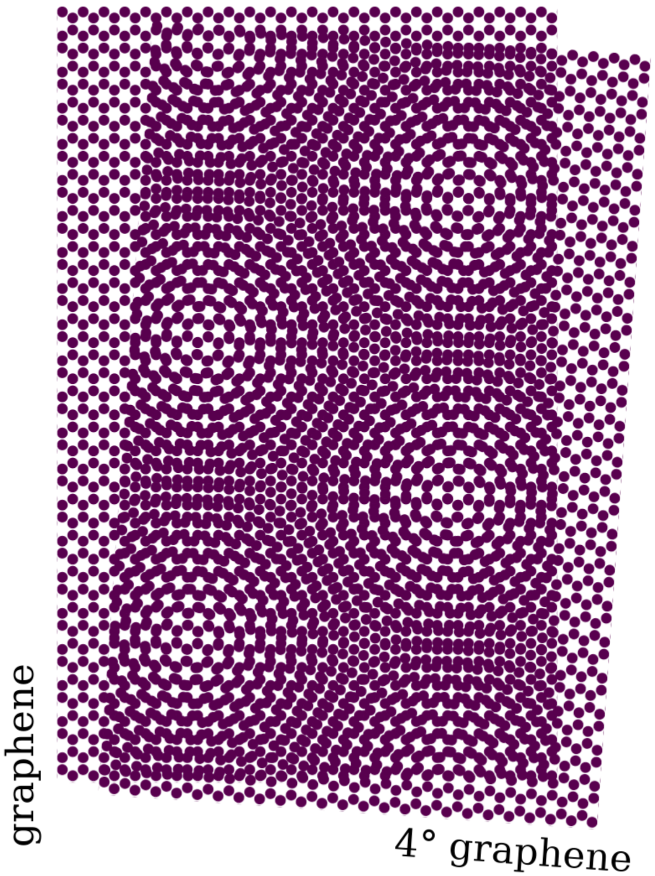
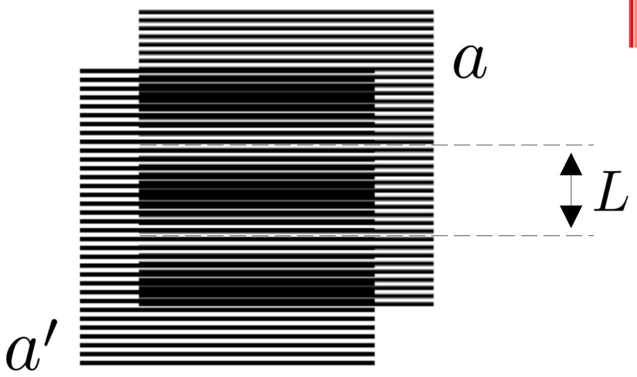
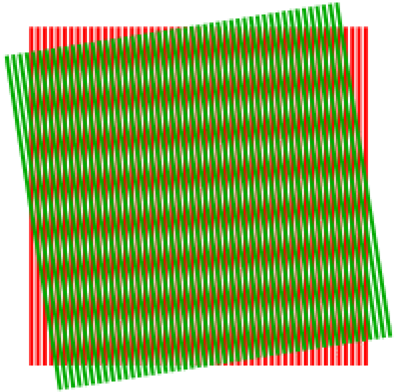


Moiré patterns





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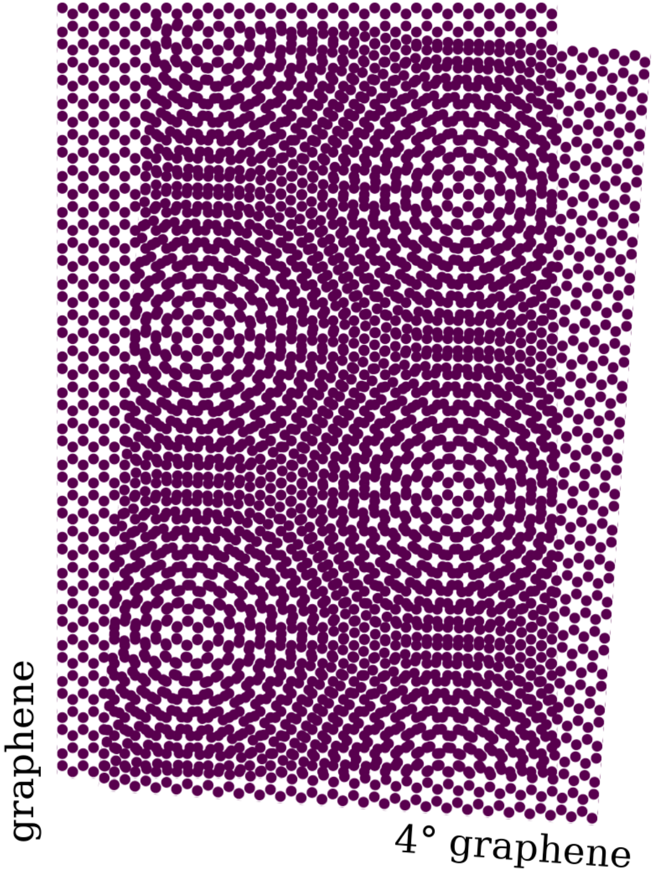

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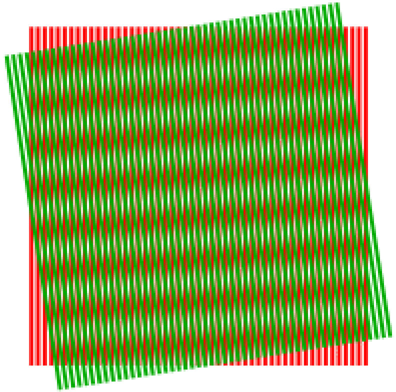

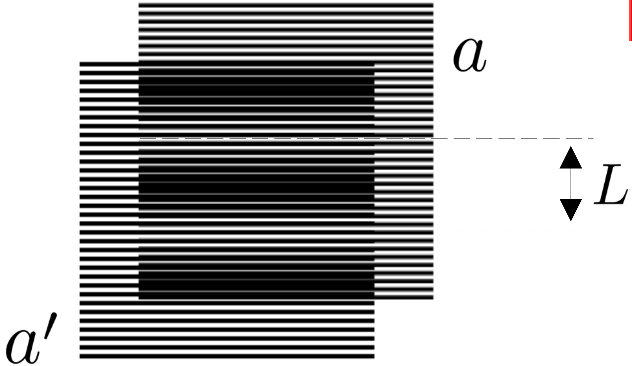

$$L = \frac{a}{|\tau - 1|}, \quad \tau = \frac{a}{a'}$$

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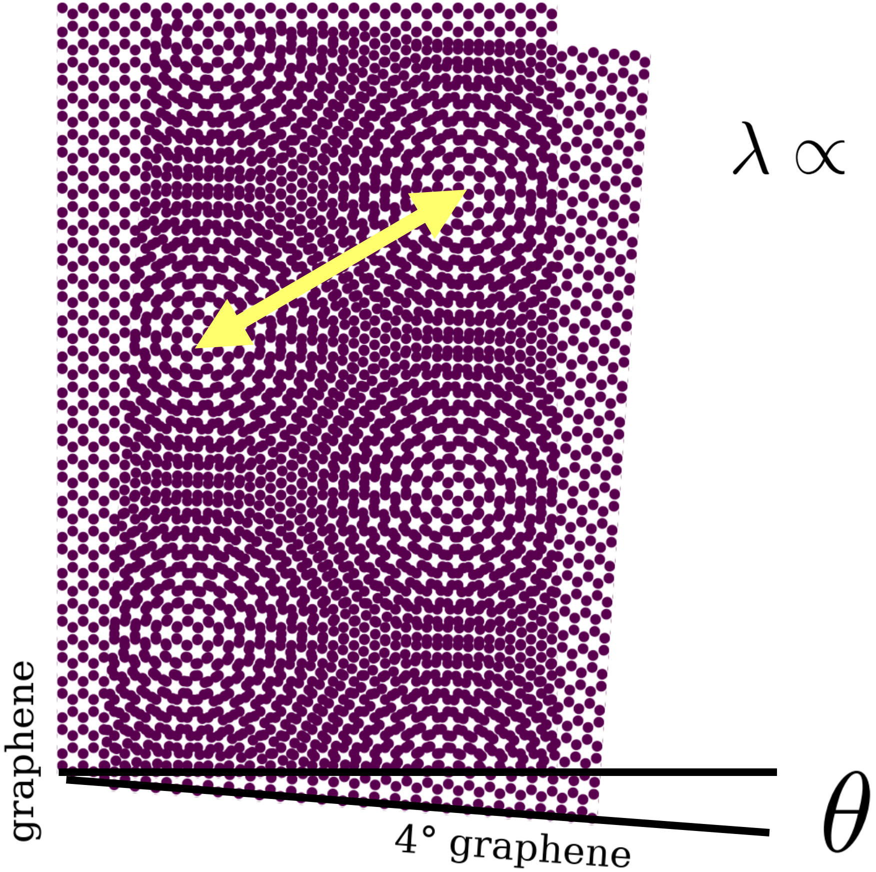

$$\lambda \propto \frac{a}{\sin(\theta/2)}$$

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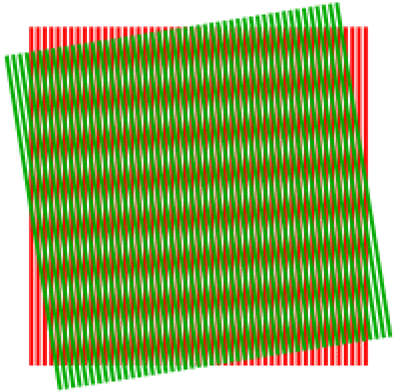

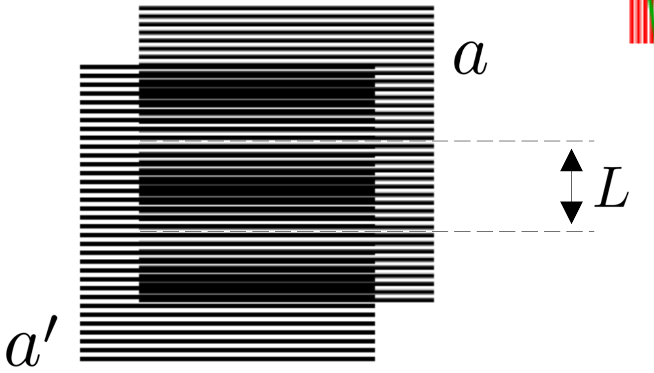

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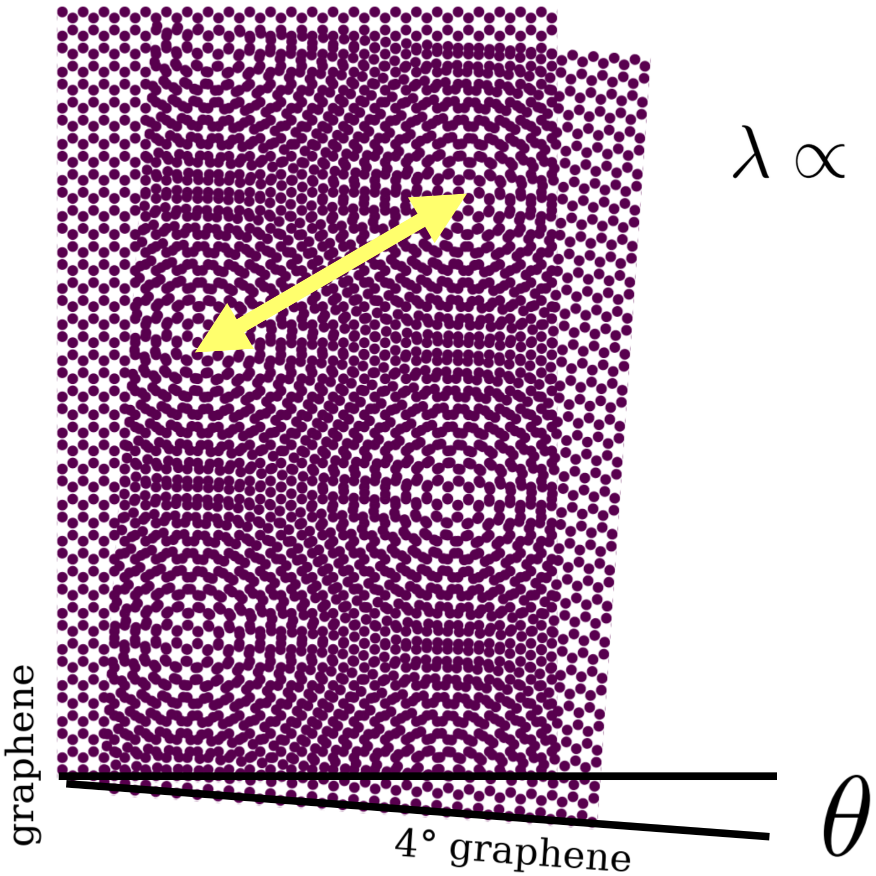
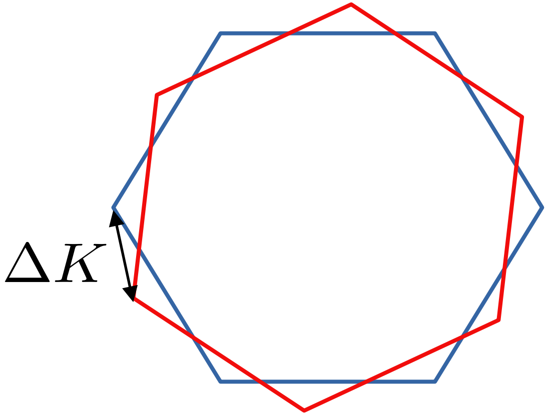
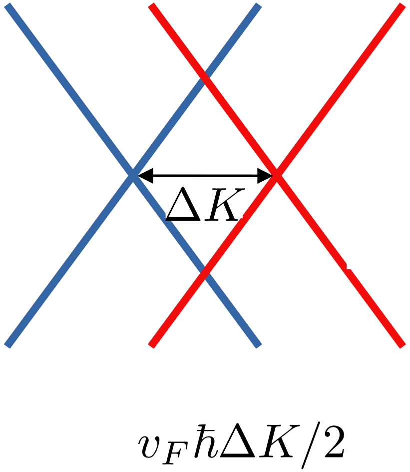


$$\lambda \propto \frac{a}{\sin(\theta/2)} \propto 1/\Delta K$$





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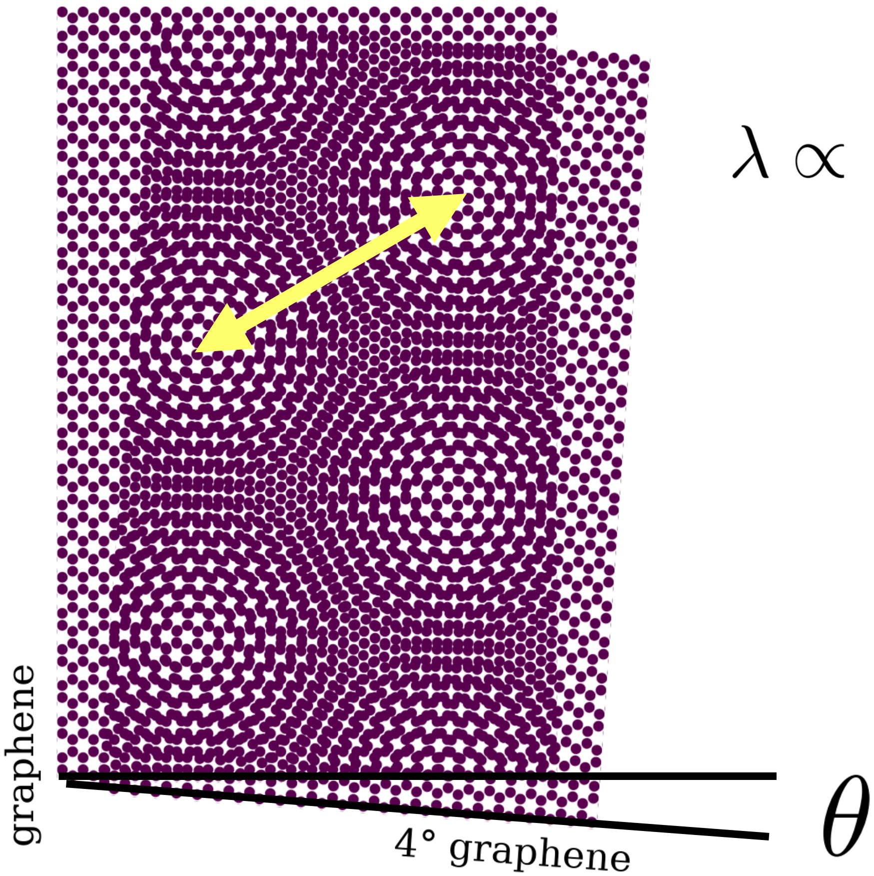

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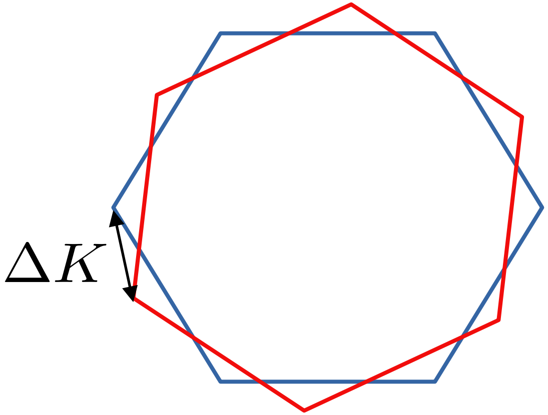

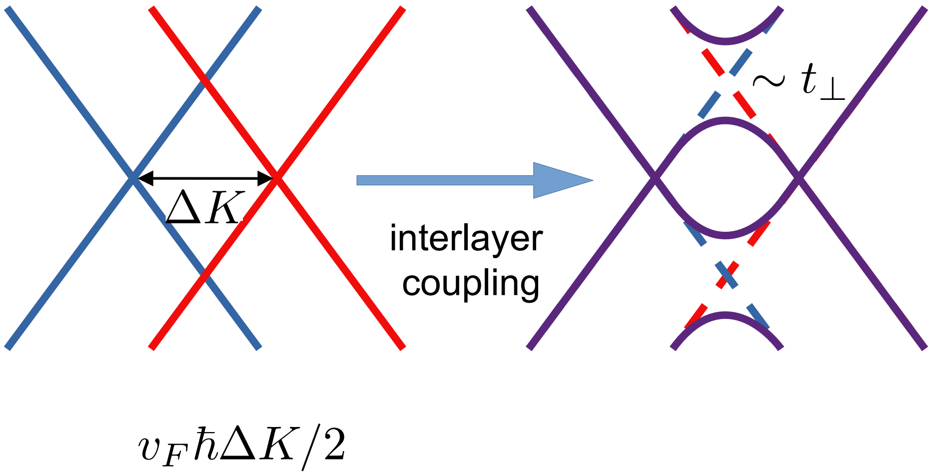

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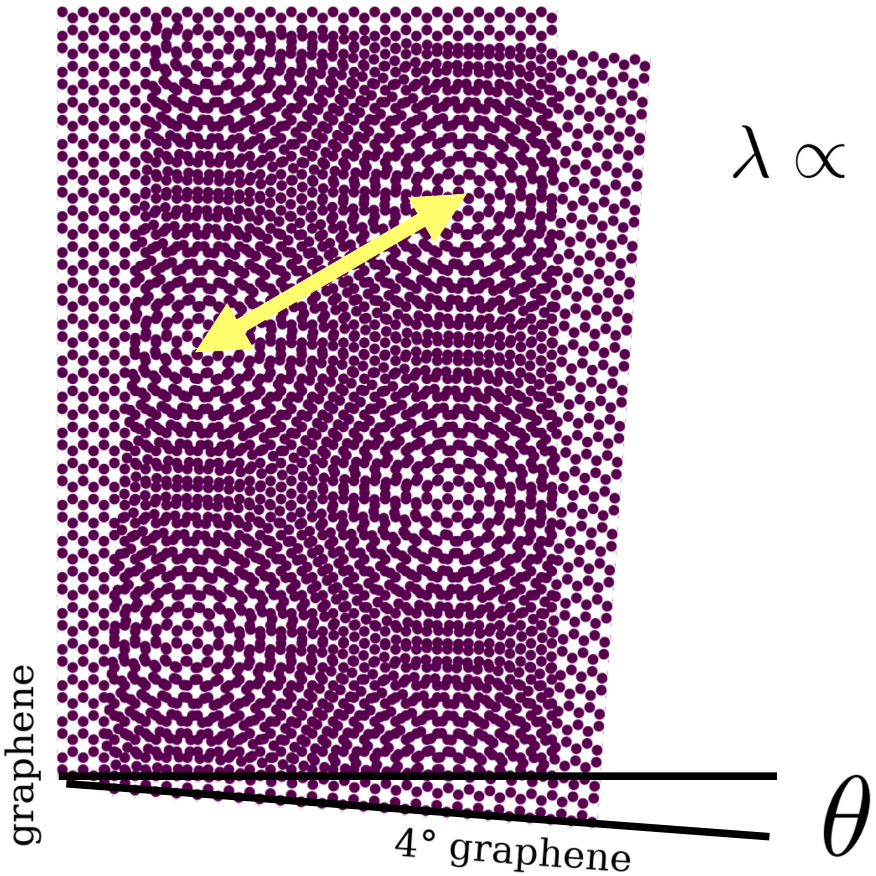

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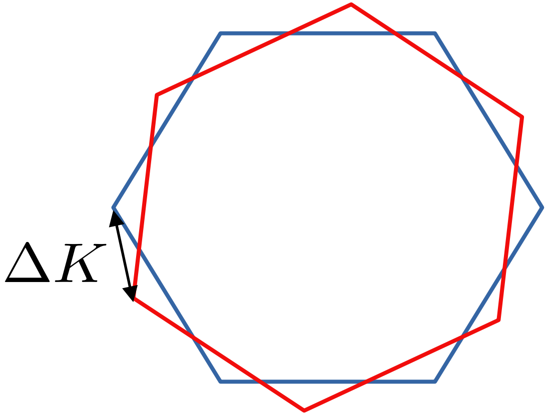
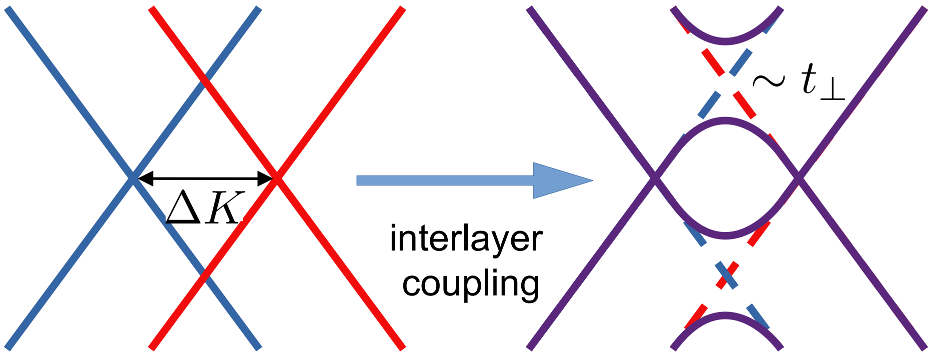




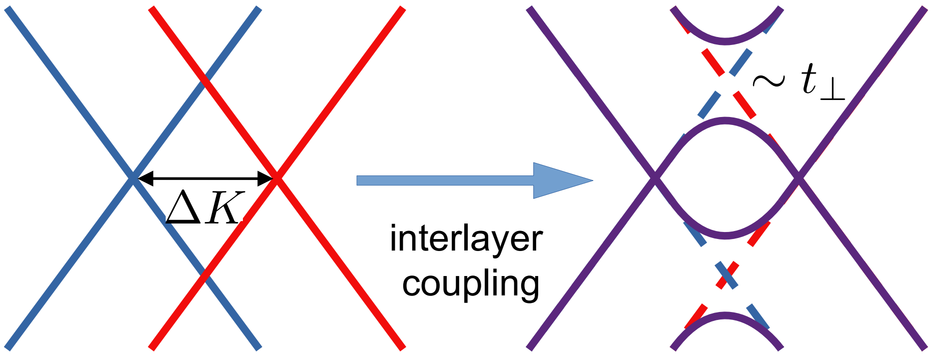
$v_F \hbar \Delta K/2 \sim t_\perp$ → **Flatband**

tBLG – A moiré Dirac semimetal

PRL **99**, 256802 (2007) PHYSICAL REVIEW LETTERS week ending 21 DECEMBER 2007

Graphene Bilayer with a Twist: Electronic Structure

J. M. B. Lopes dos Santos,[1] N. M. R. Peres,[2] and A. H. Castro Neto[3]



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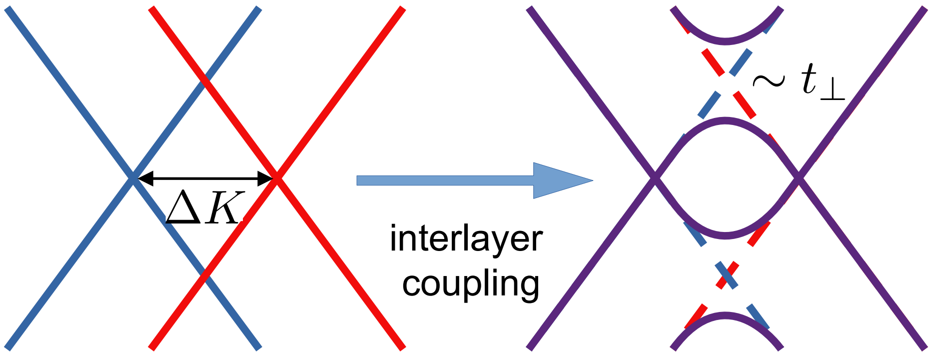
$v_F \hbar \Delta K \gg t_\perp$



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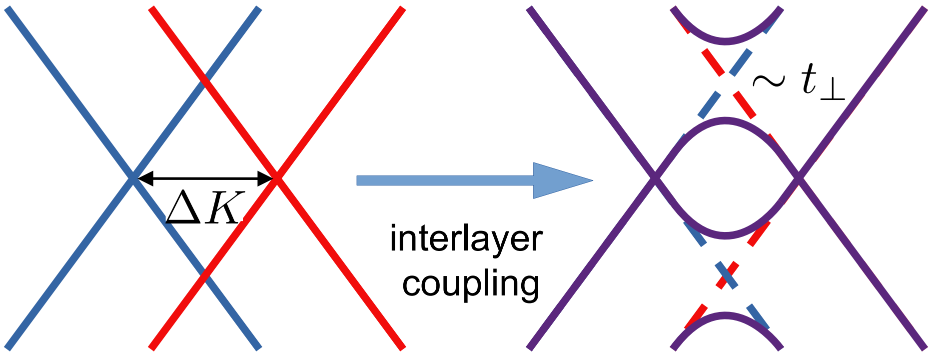
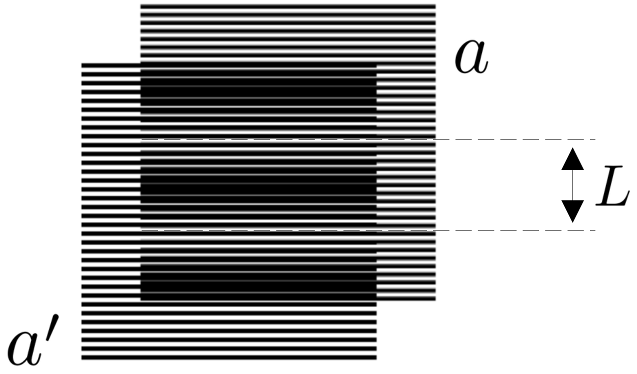


tBLG at small angles:

- reduction of Fermi velocity
- formation of narrow bands

$v_F \hbar \Delta K/2 \sim t_\perp$ → **Flatband**

Moiré physics and Quasiperiodicity



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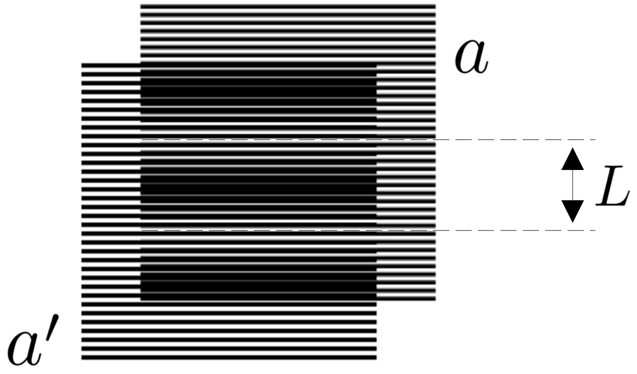
Moiré physics and Quasiperiodicity



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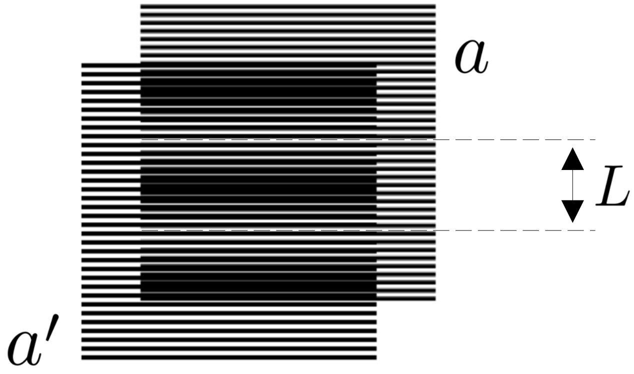
$$\tau = \frac{p}{q} \in \mathbb{Q}$$ **Periodic system**

$$\tau \neq \frac{p}{q} \in \mathbb{Q}$$ **Quasiperiodic system**

Moiré physics and Quasiperiodicity



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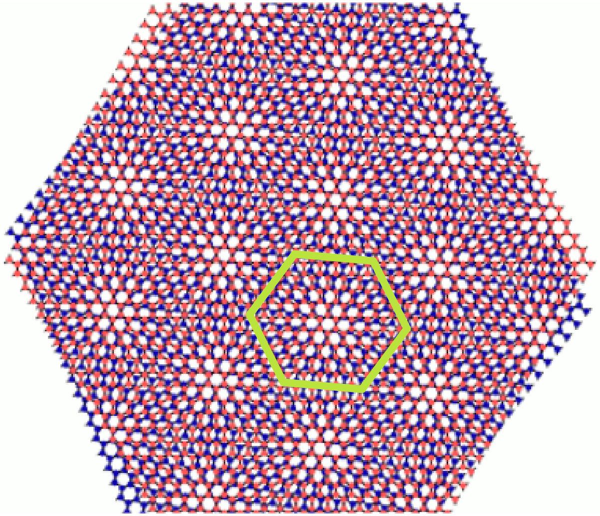

Periodic structure only when:

$$\cos\theta_{m,r} = \frac{3m^2 + 3mr + r^2/2}{3m^2 + 3mr + r^2}$$

(for $r = 1$, moiré = unit cell)

dos Santos, Peres, Neto, PRB 86 155449 (2012)

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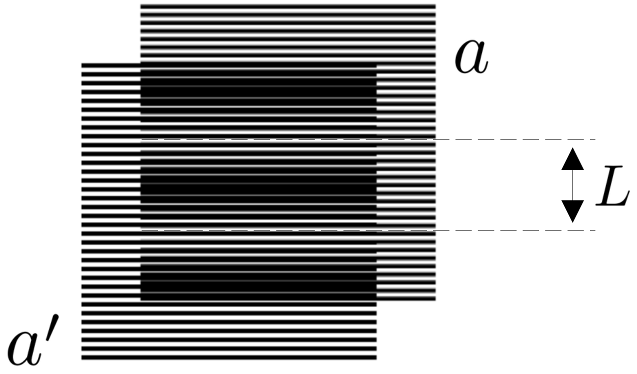

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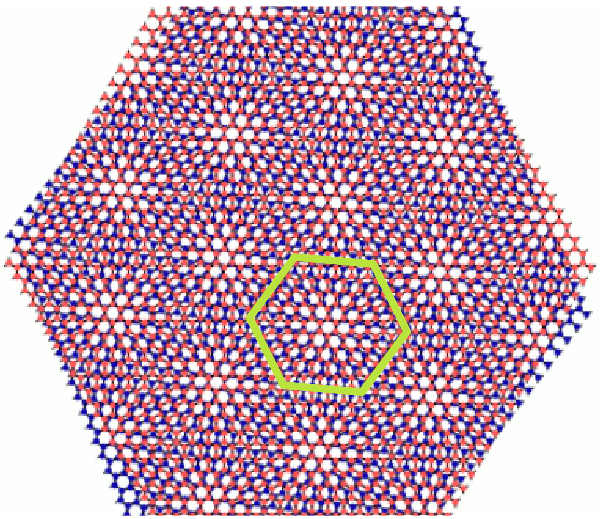

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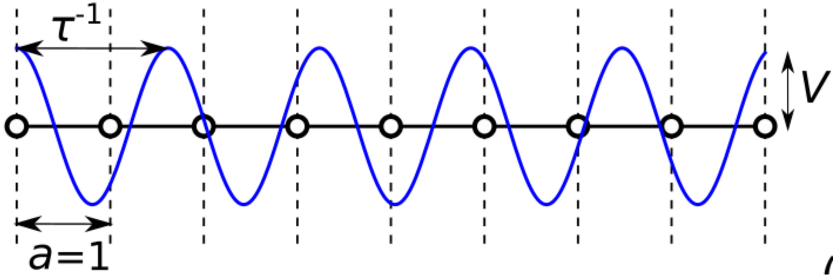
For any other angle: quasiperiodic structure!

Quasiperiodicity matters

Famous example in 1D

$\tau \notin \mathbb{Q}$



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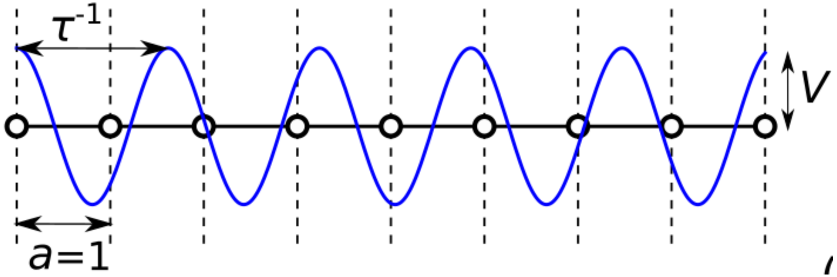

$$H = -t \sum_n \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + V \sum_n \cos(2\pi\tau n) c_n^\dagger c_n$$

1D: Aubry-André model

S. Aubry and G. André,
Ann. Isr. Phys. Soc. 3, 133 (1980)

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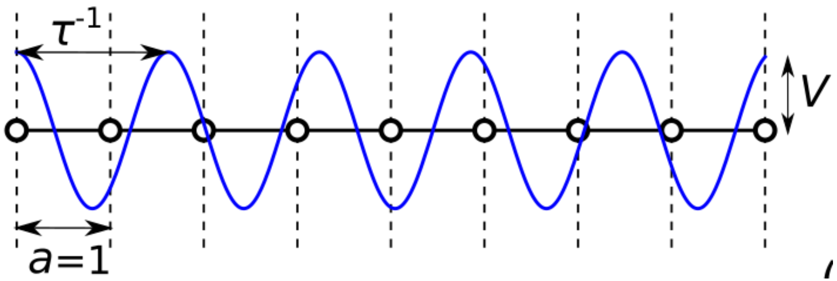

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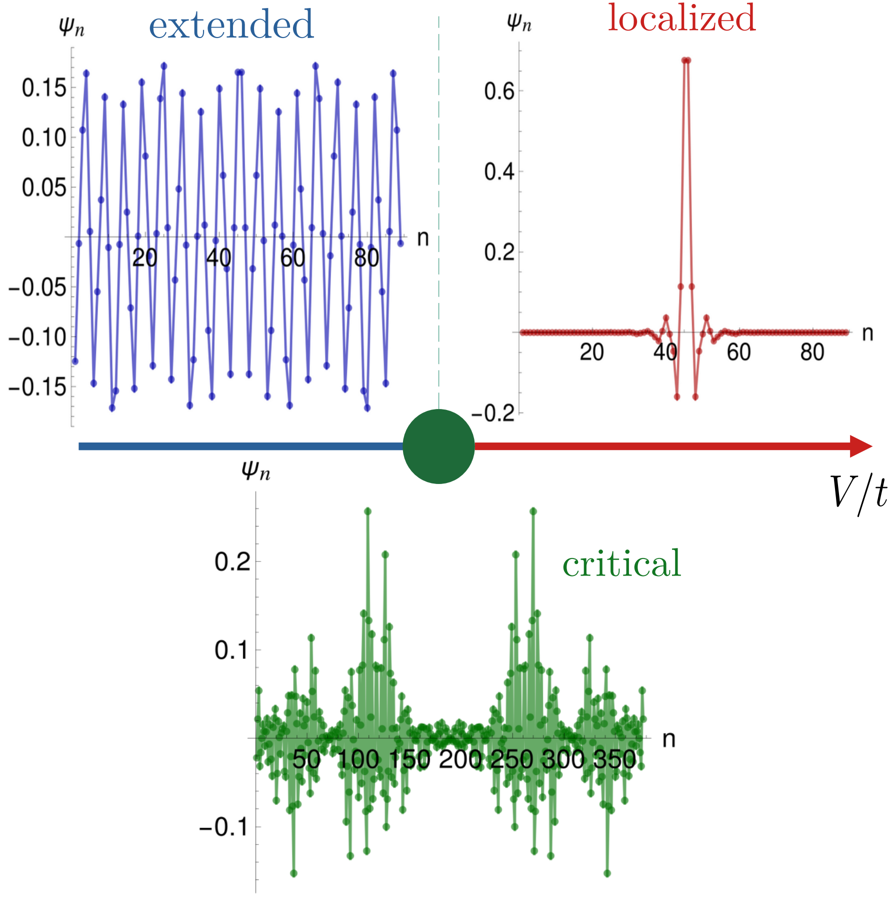
Localization



Motivation:
Sub-ballistic behavior in tBLG

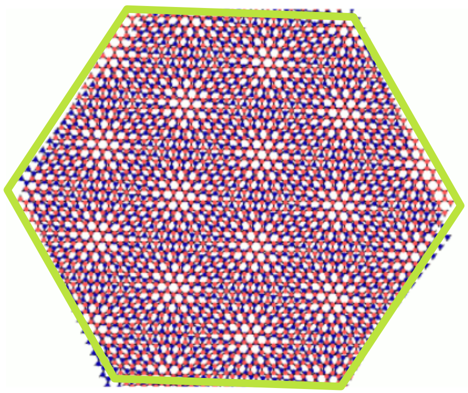
Model

To capture quasiperiodicity:

- Real-space tight-binding Hamiltonian for tBLG

$$\cos\theta_{m,r} = \frac{3m^2 + 3mr + r^2/2}{3m^2 + 3mr + r^2}$$

Quasiperiodic



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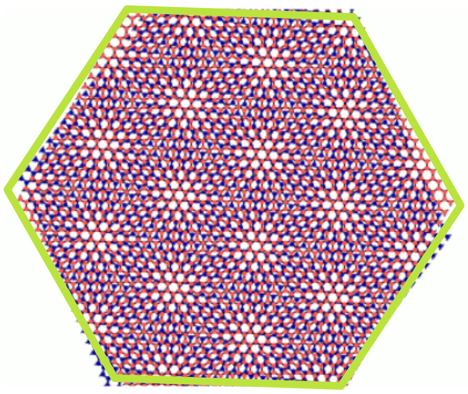
- Real-space tight-binding Hamiltonian for tBLG
- Sequence of approximants: pairs (m_i, r_i), twist angle $\theta_i = \theta_c(m_i, r_i)$

$$\cos\theta_{m,r} = \frac{3m^2 + 3mr + r^2/2}{3m^2 + 3mr + r^2}$$

- $|\theta_{i+1} - \theta_i|$ decreases
- N_i increases

Quasiperiodic



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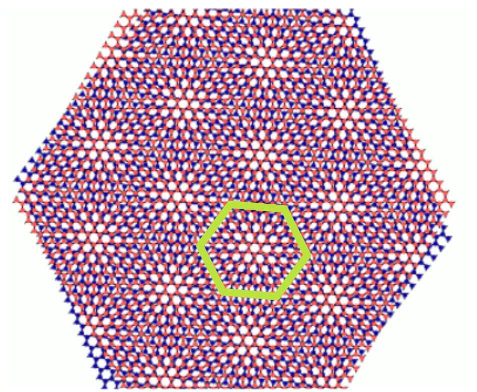

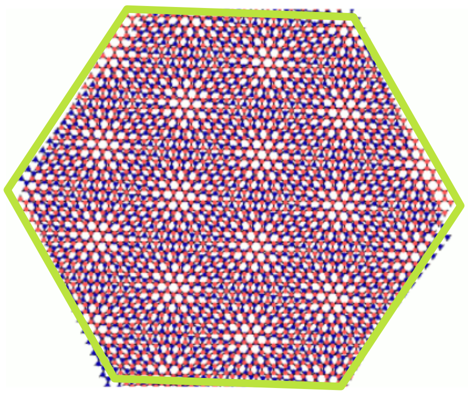

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Real space

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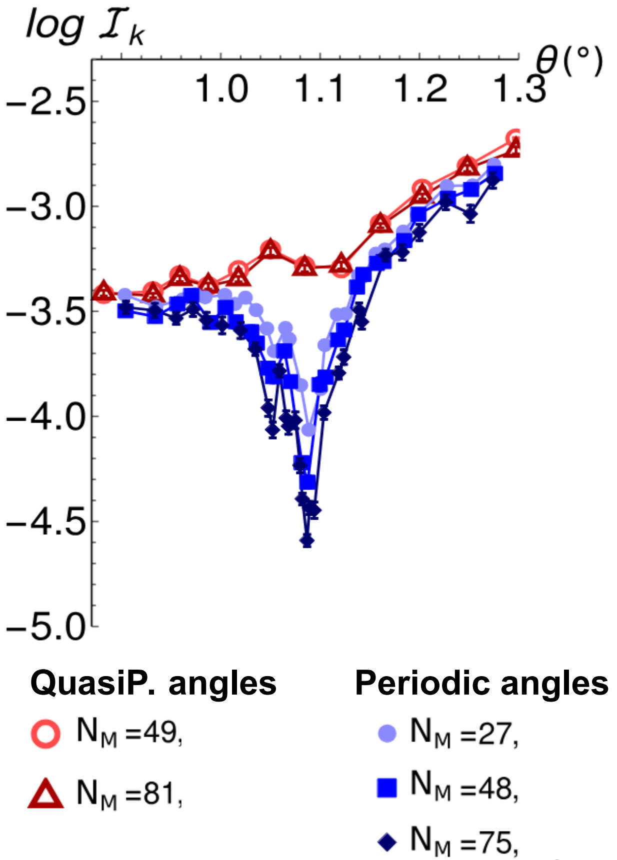
IPR-k in tBLG narrow band

2D Mater. **9**, 011001 (2022)

IPR-k: QuasiP. vs Periodic



IPR-k in tBLG narrow band and beyond

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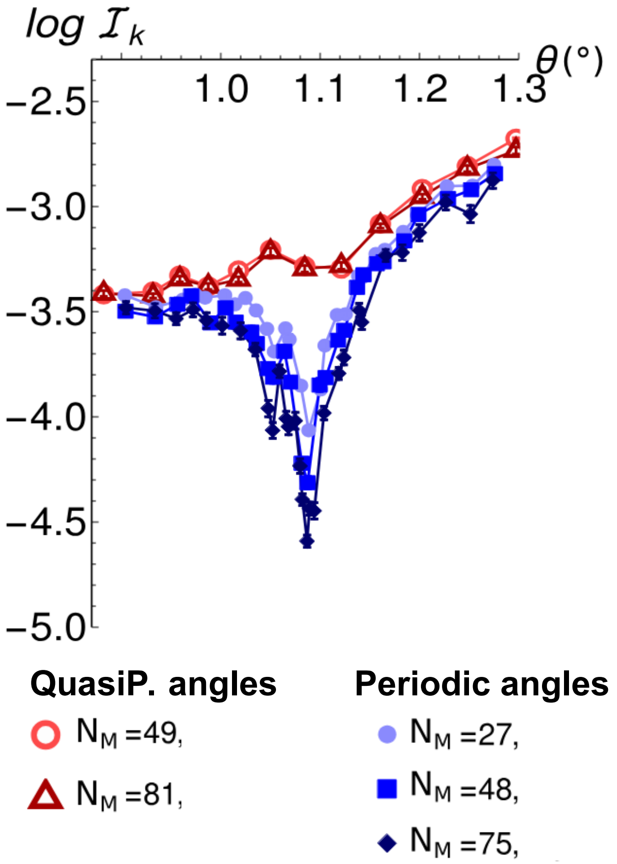
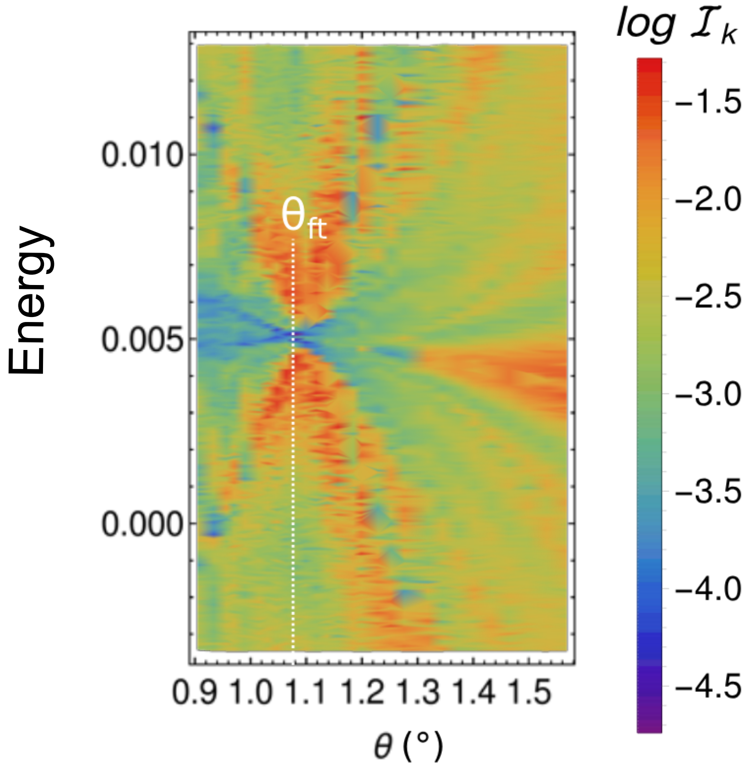


IPR-k for QuasiP.



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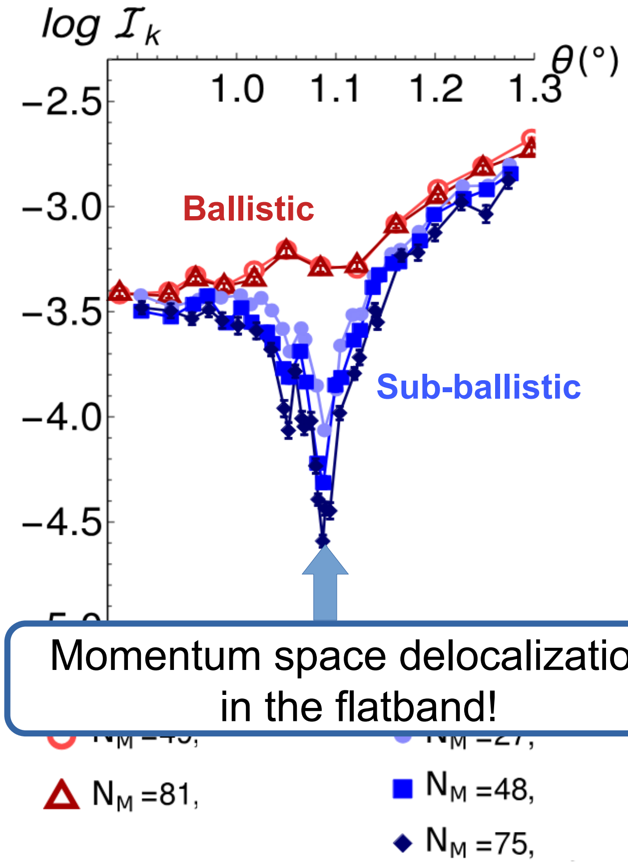

Momentum space delocalization in the flatband!

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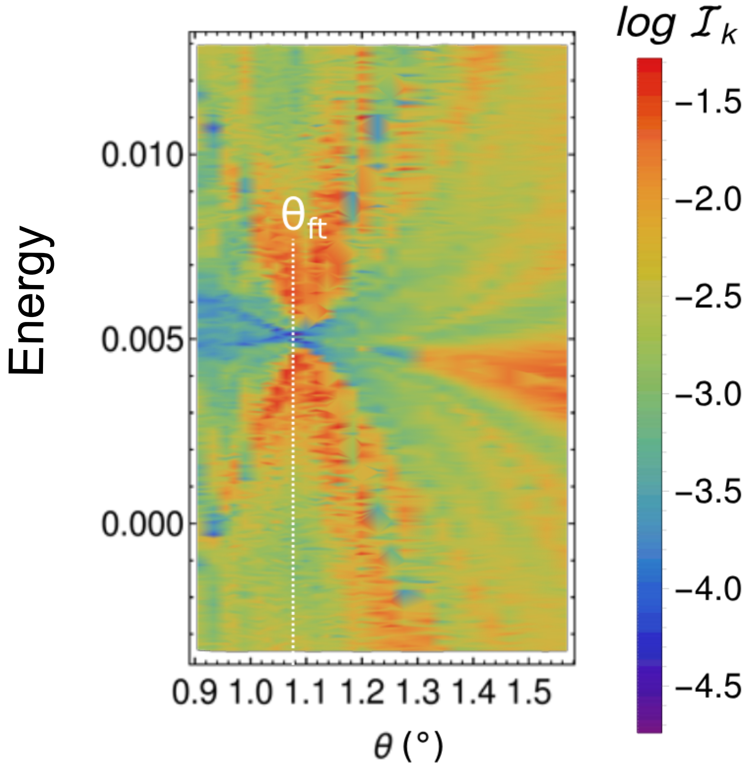

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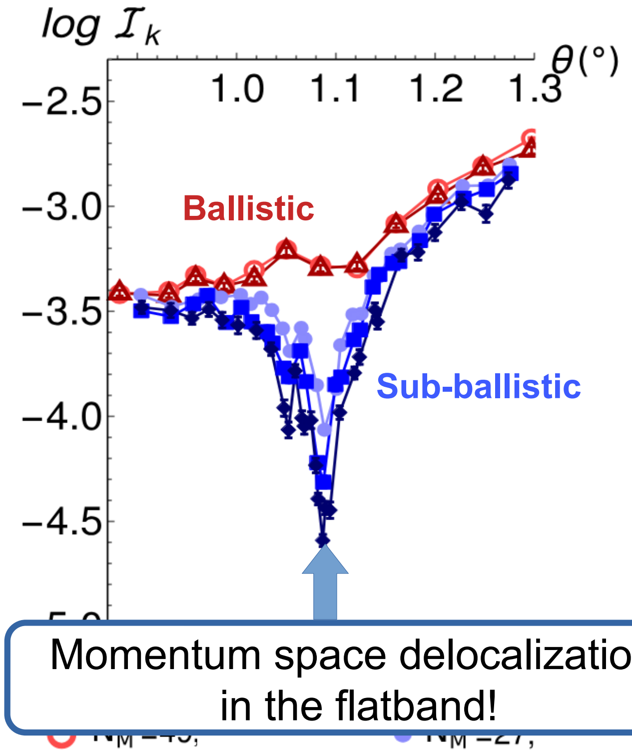

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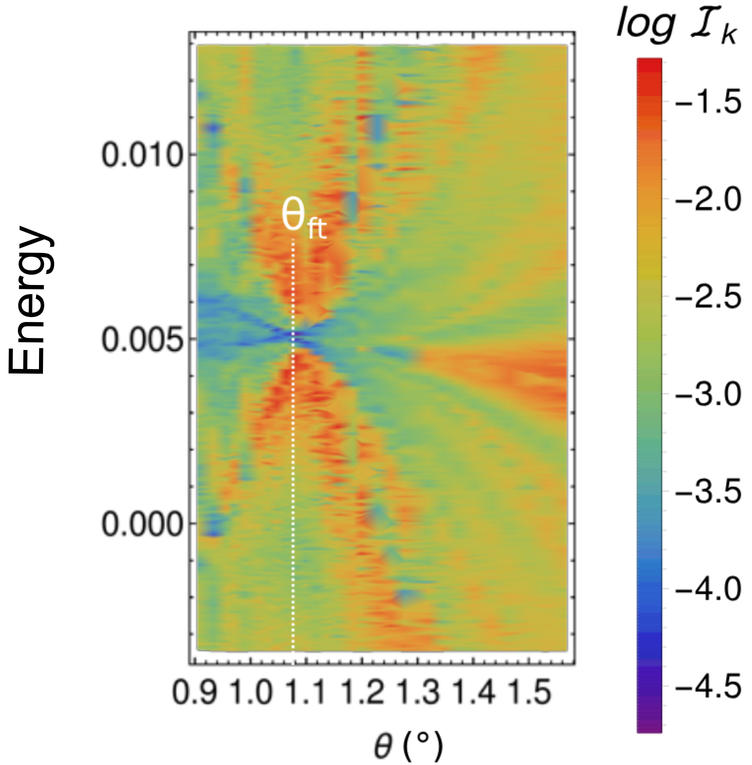


tBLG belongs to the class of "magic angle semimetals"

Fu, König, Wilson, Chou & Pixley npj Quantum Mater. **5**, 71 (2020)

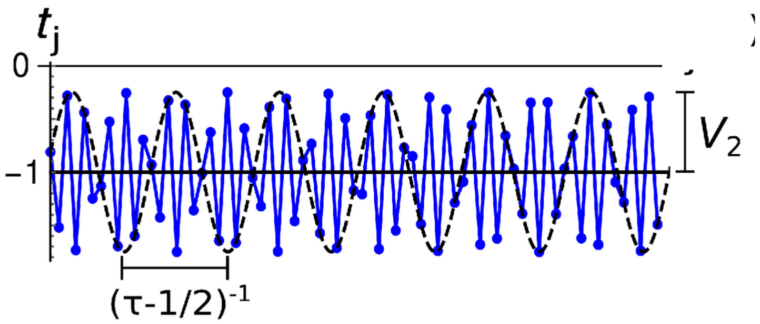
Quasi-fractal order in 1D narrow band quasiperiodic moiré

1D model with narrow band + critical phase

$$H_0 = -\sum_j \left[t + \underbrace{V_2 \cos(2\pi\tau(j+1/2)+\phi)}\right] c_j^\dagger c_{j+1} + h.c.$$

modulation with period $1/\tau$

Moiré pattern:



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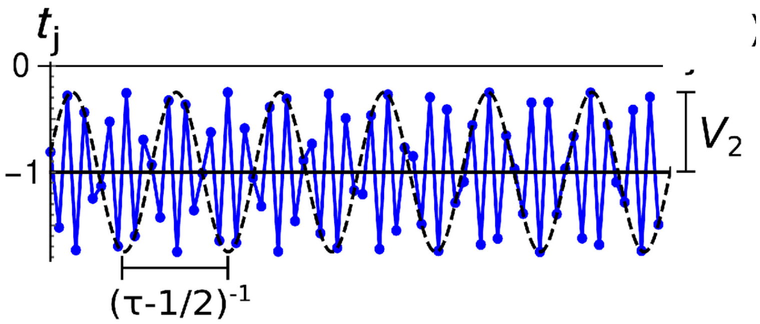
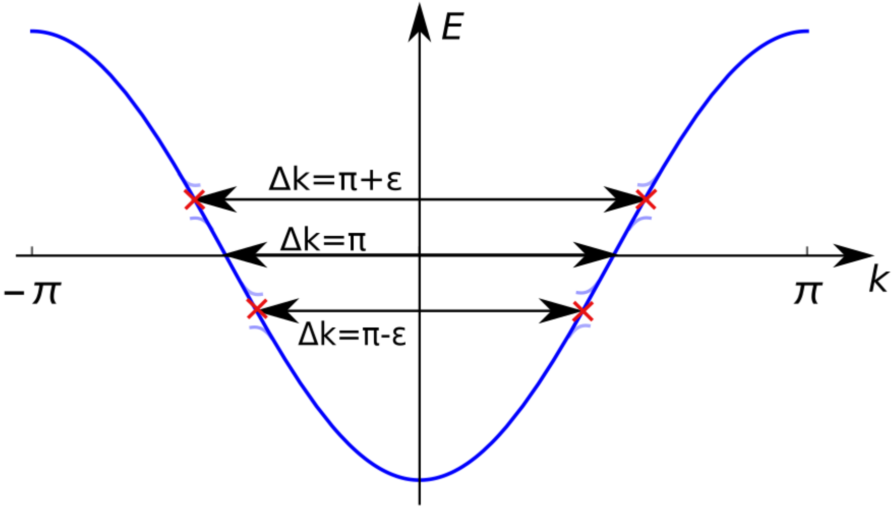


hopping couples k and $k \pm 2\pi\tau n$

n-th order perturbation theory

$\tau = 1/2 + \epsilon$

$\Delta k = \pi \pm \epsilon$



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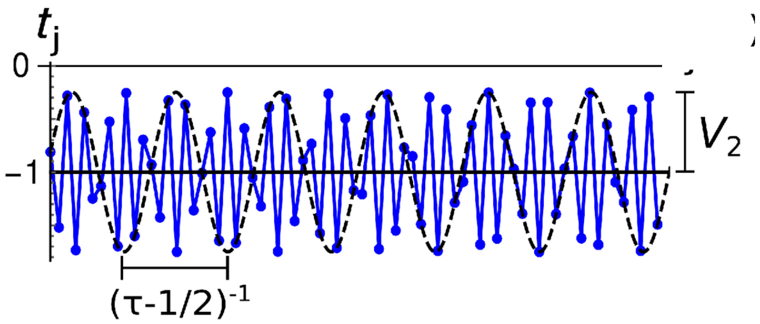
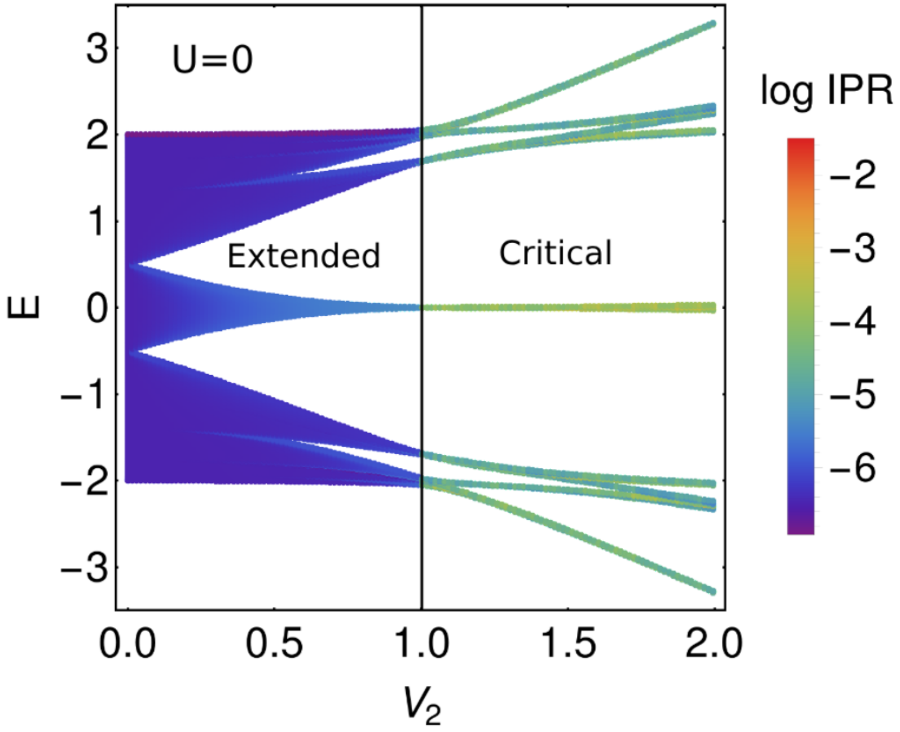


Extended phase for $V_2 < t$

Critical phase for $V_2 > t$



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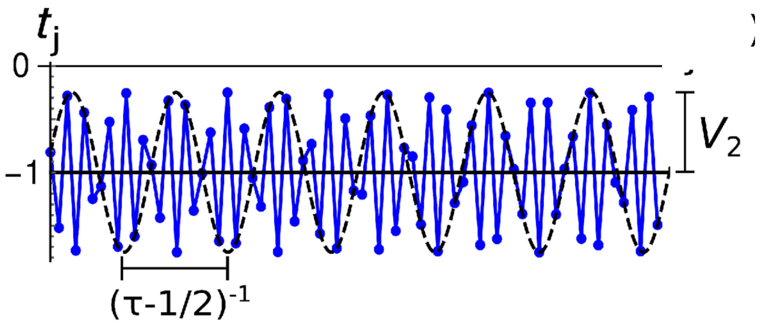

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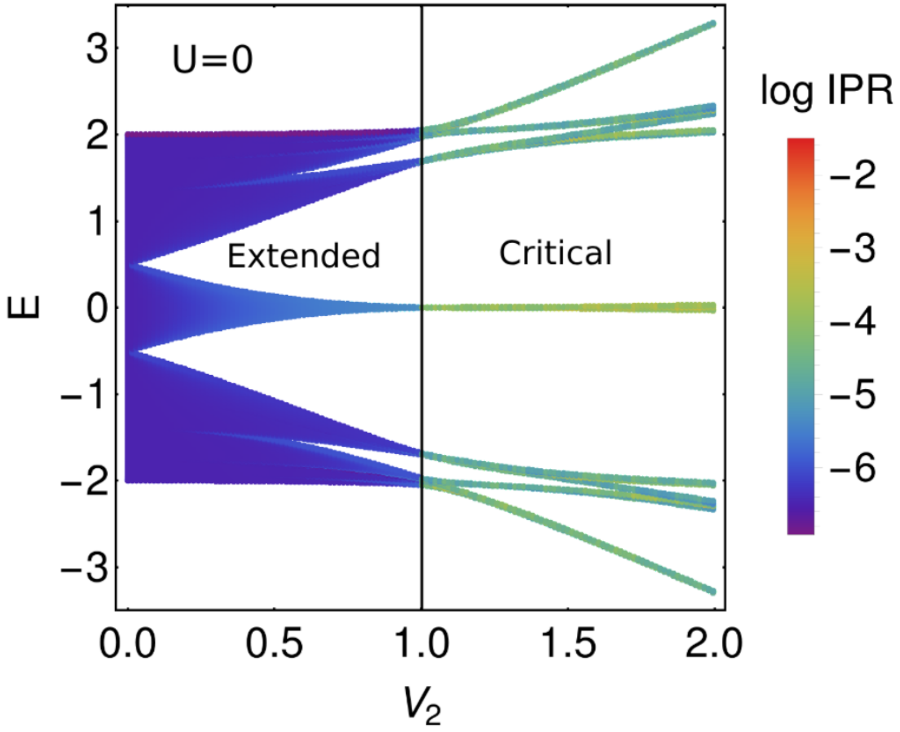

The critical phase hosts:

- multifractal states concomitant with a narrow energy band
- eigenstates delocalized both in real and momentum-space

Adding interactions

Nearest-neighbour repulsion:
(half-filling, spinless electrons)

$$H = H_0 + U \sum_j n_j n_{j+1}$$

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system sizes up to N=2500

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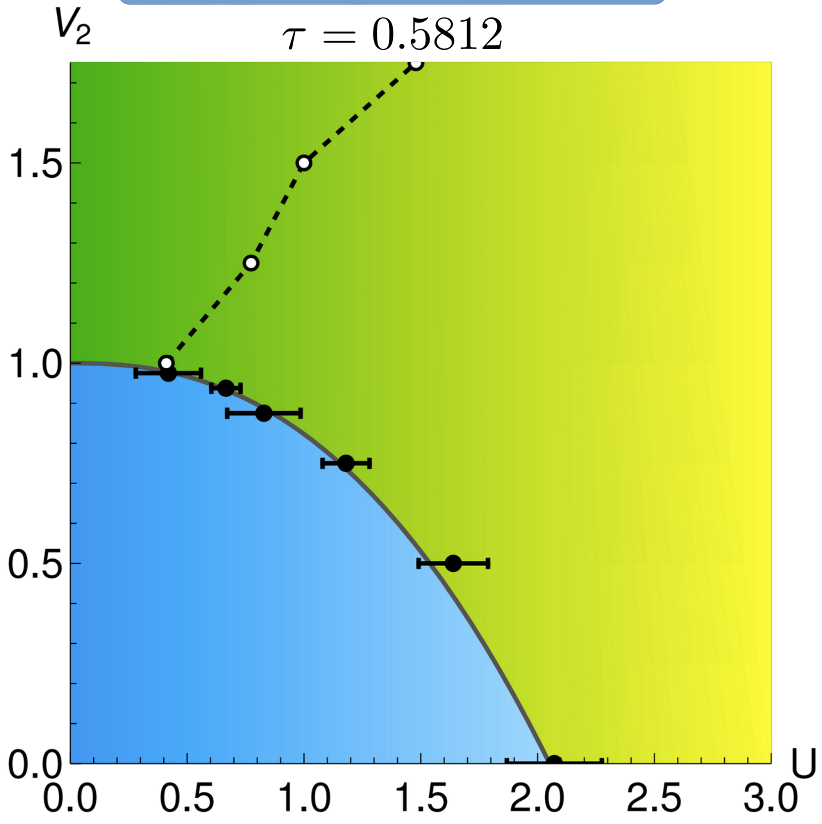
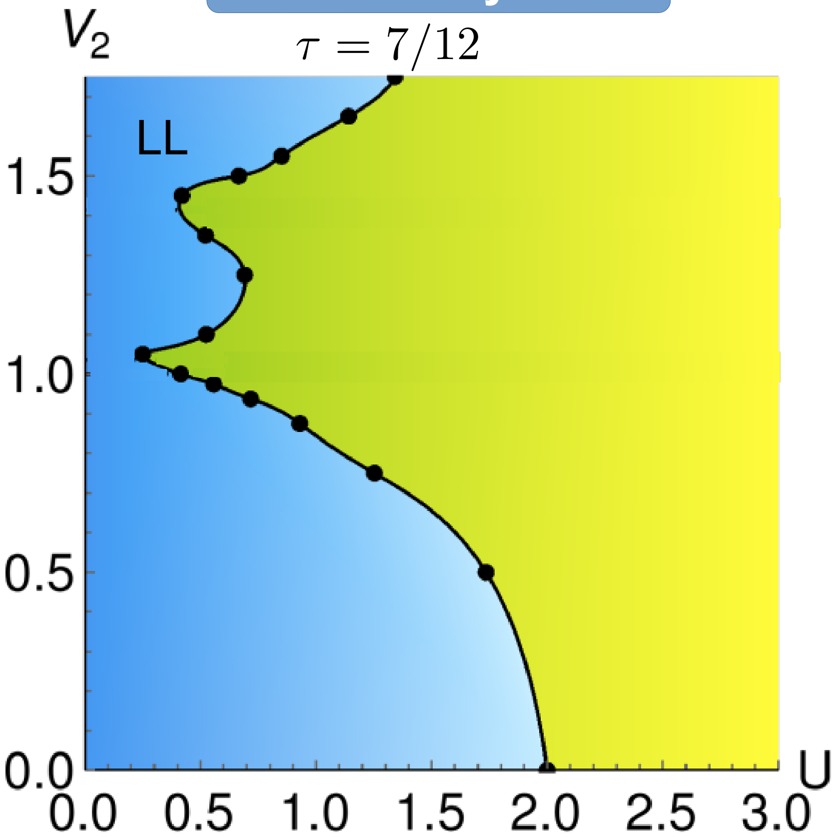
Quasiperiodic system



Periodic system



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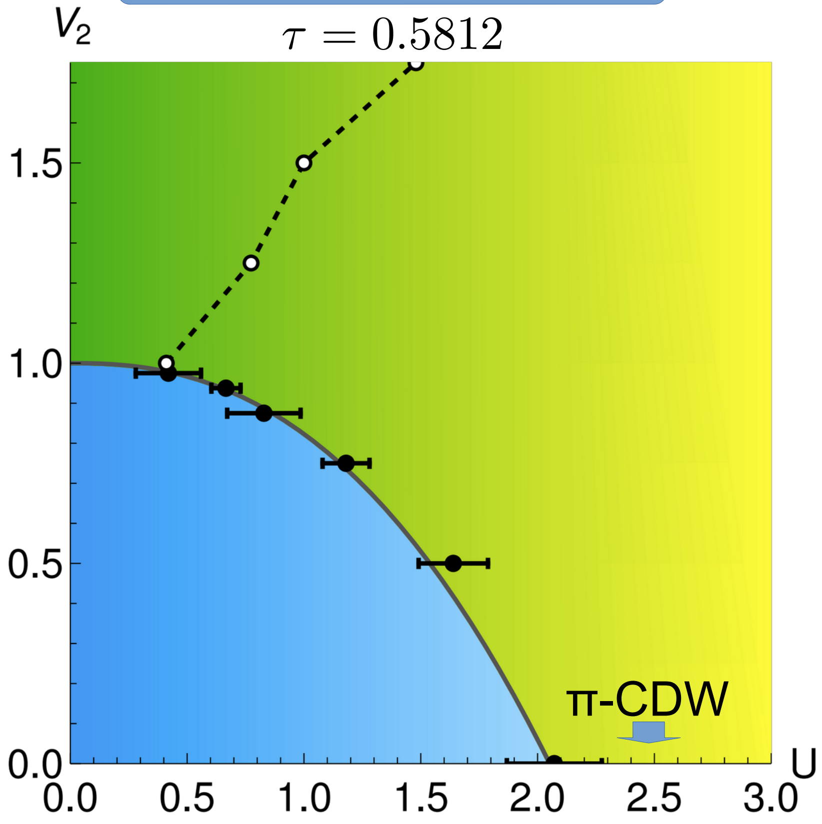

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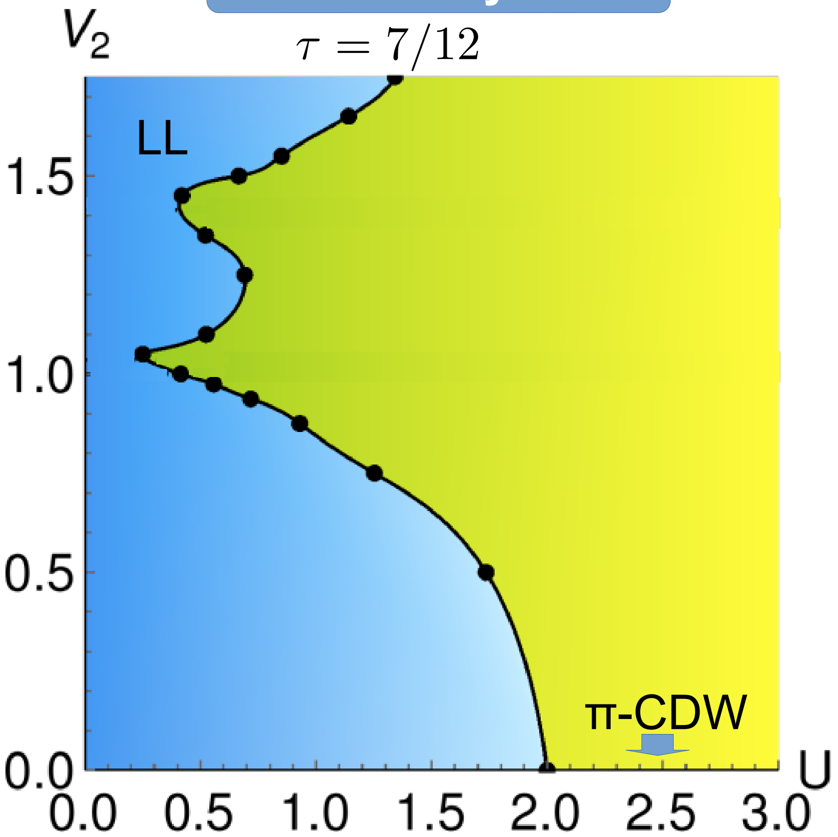

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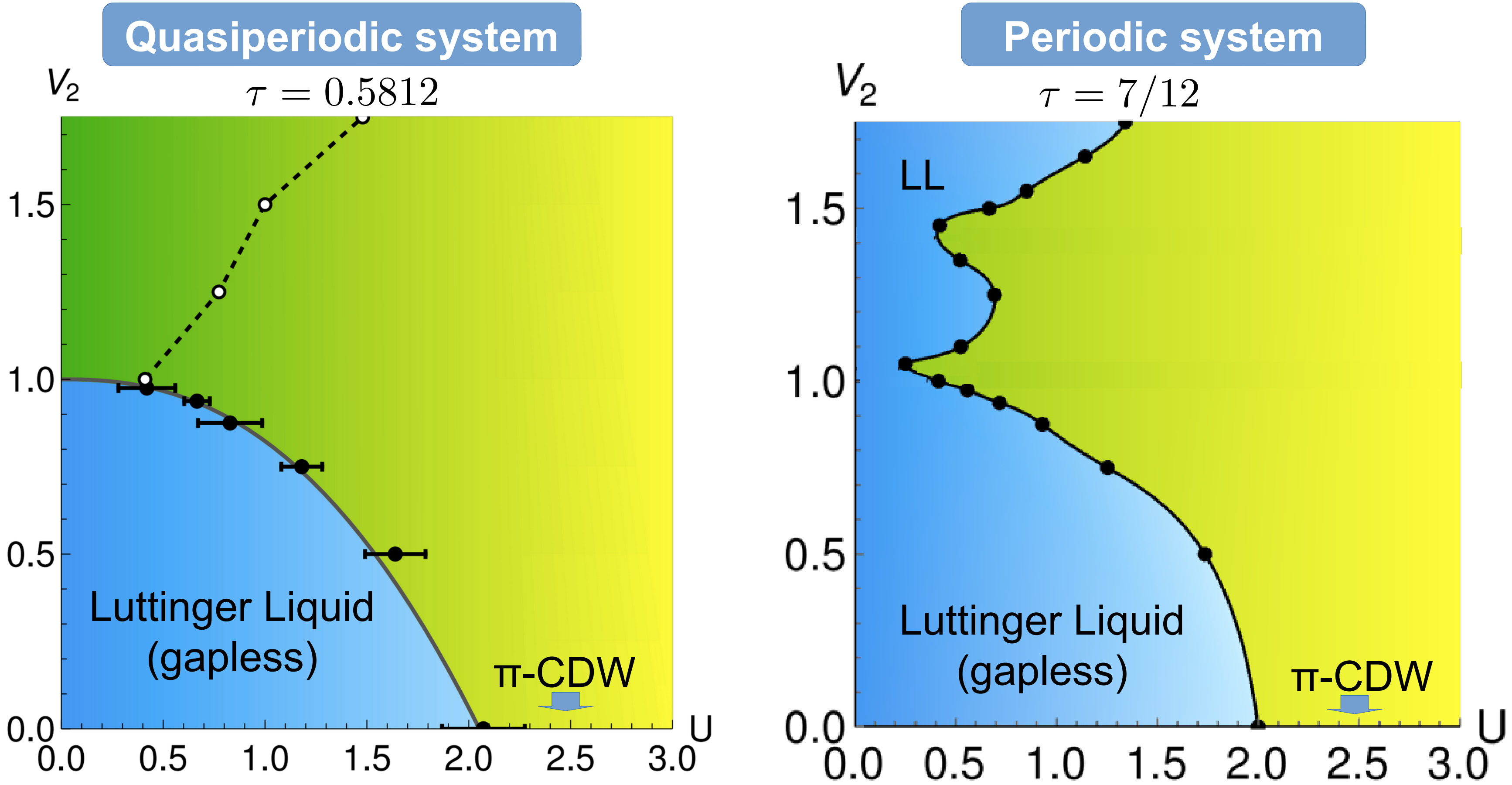

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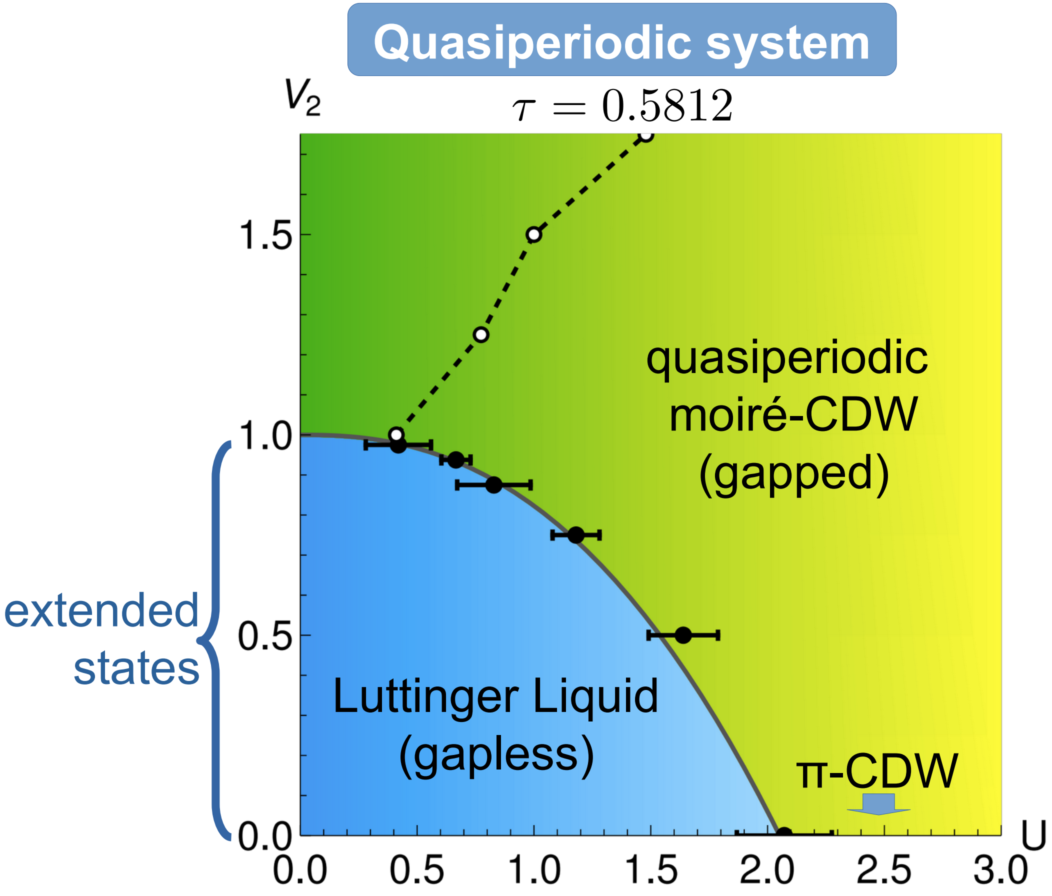

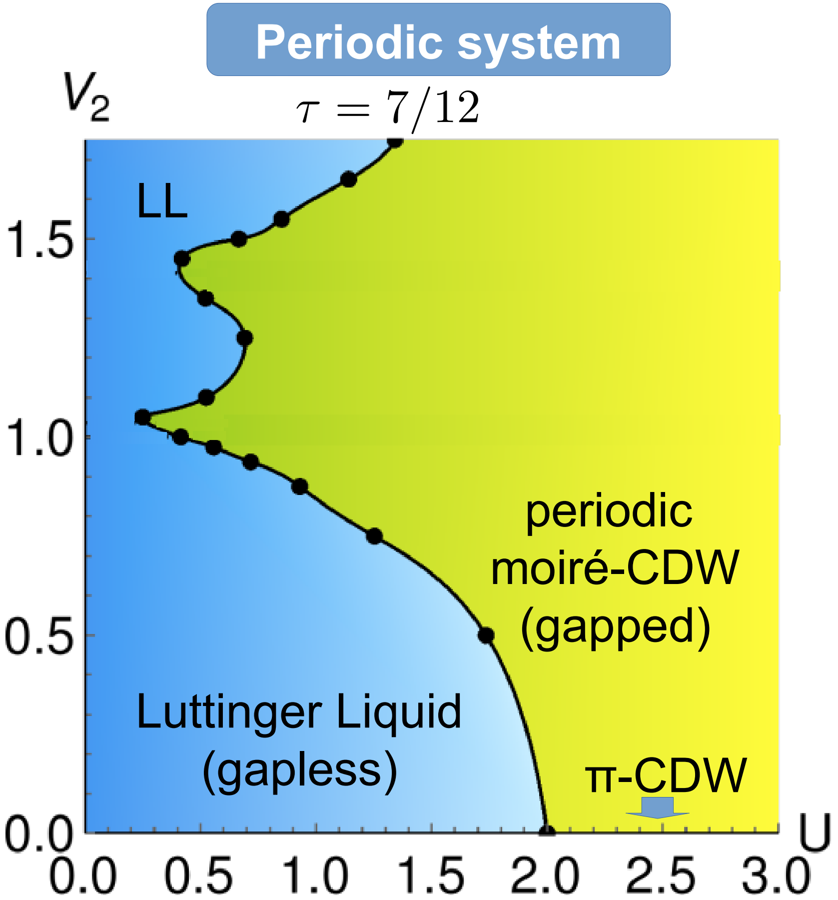

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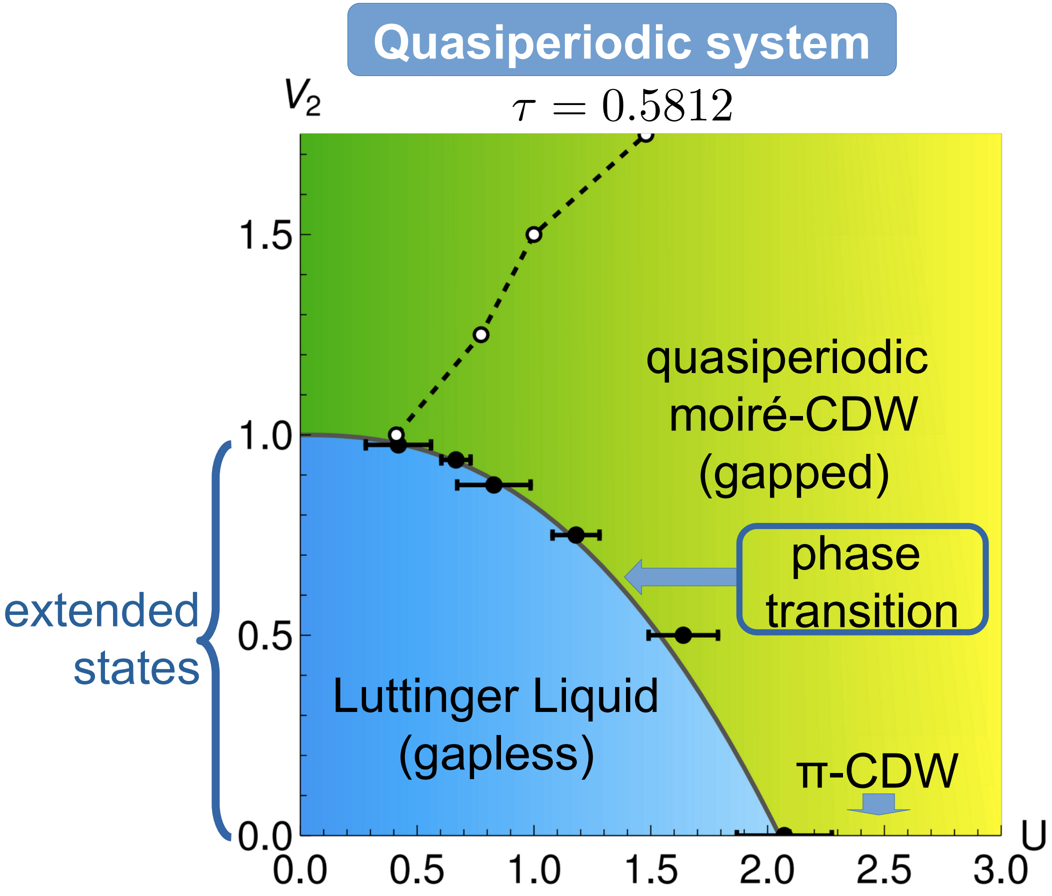

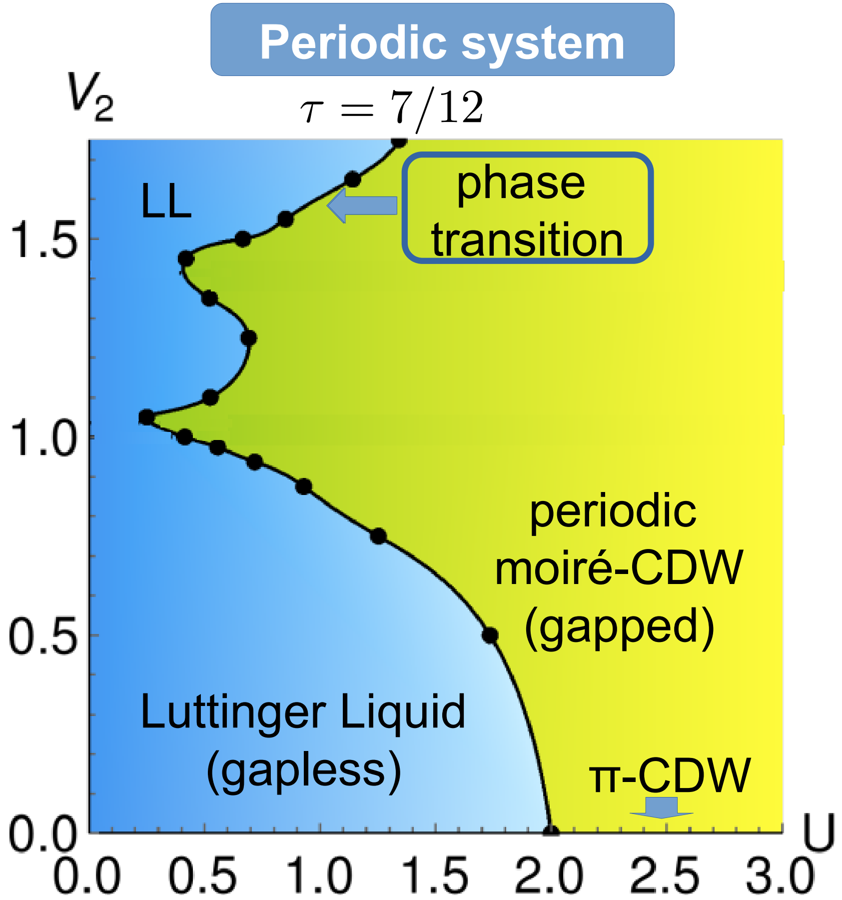

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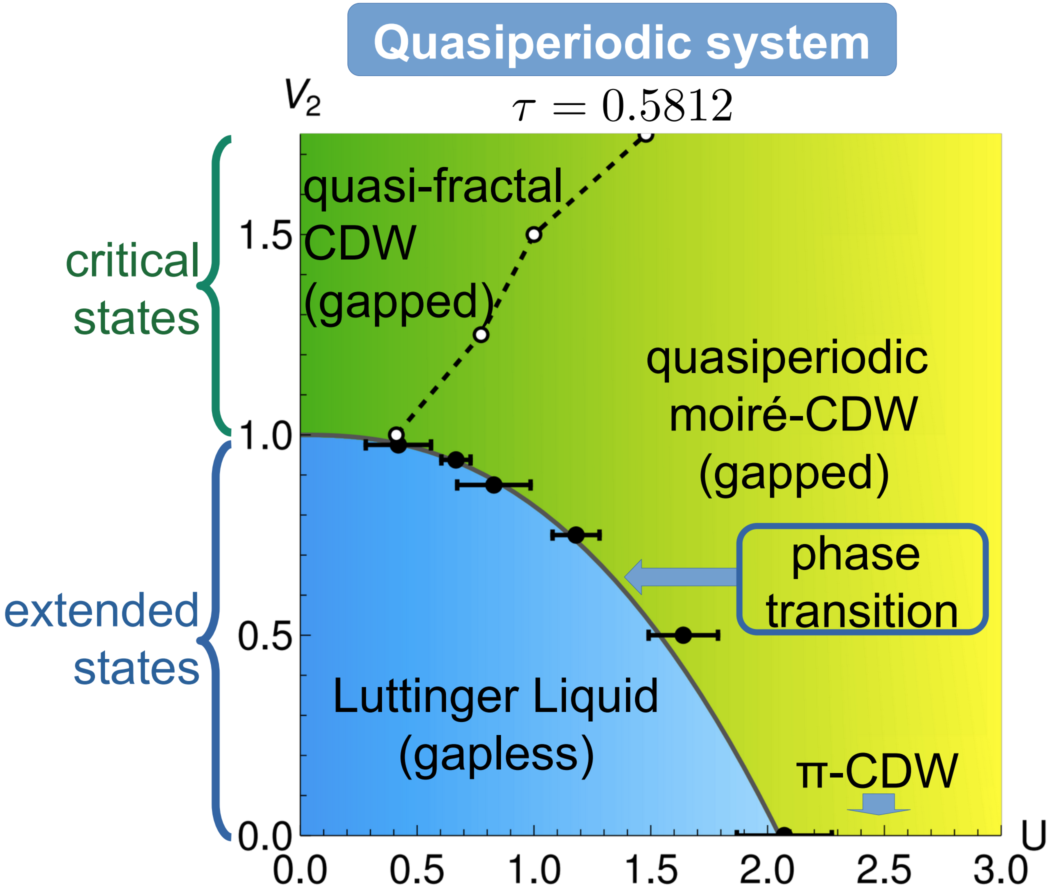

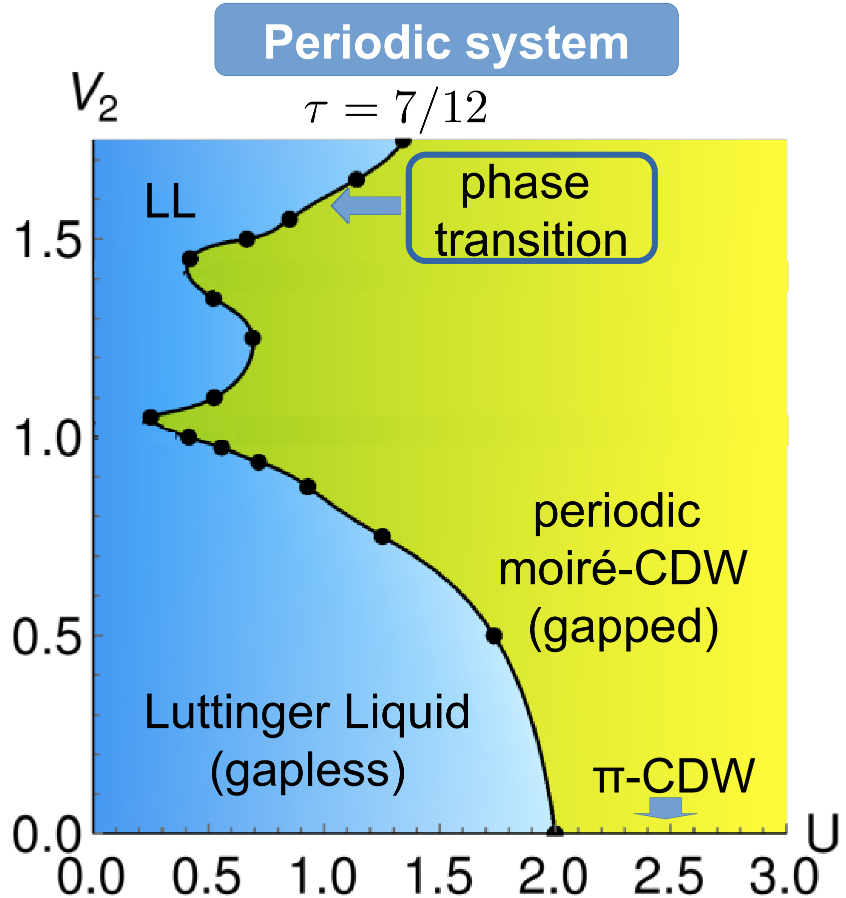

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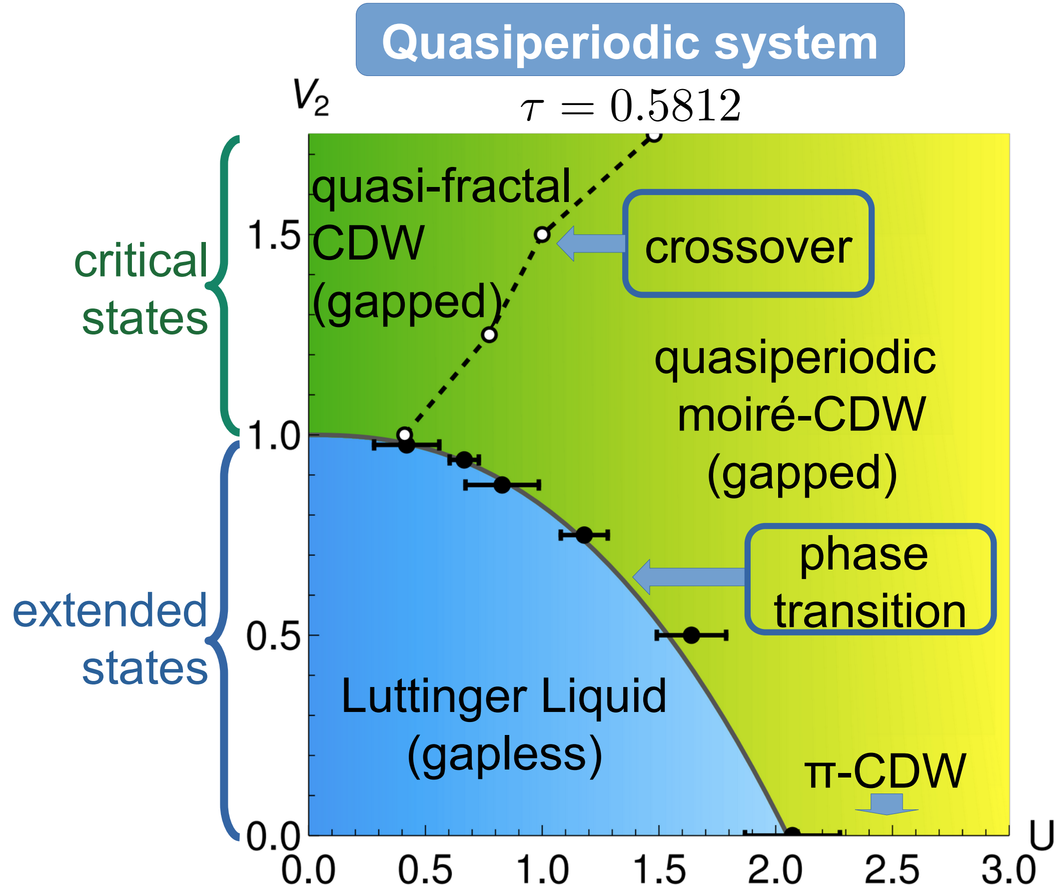

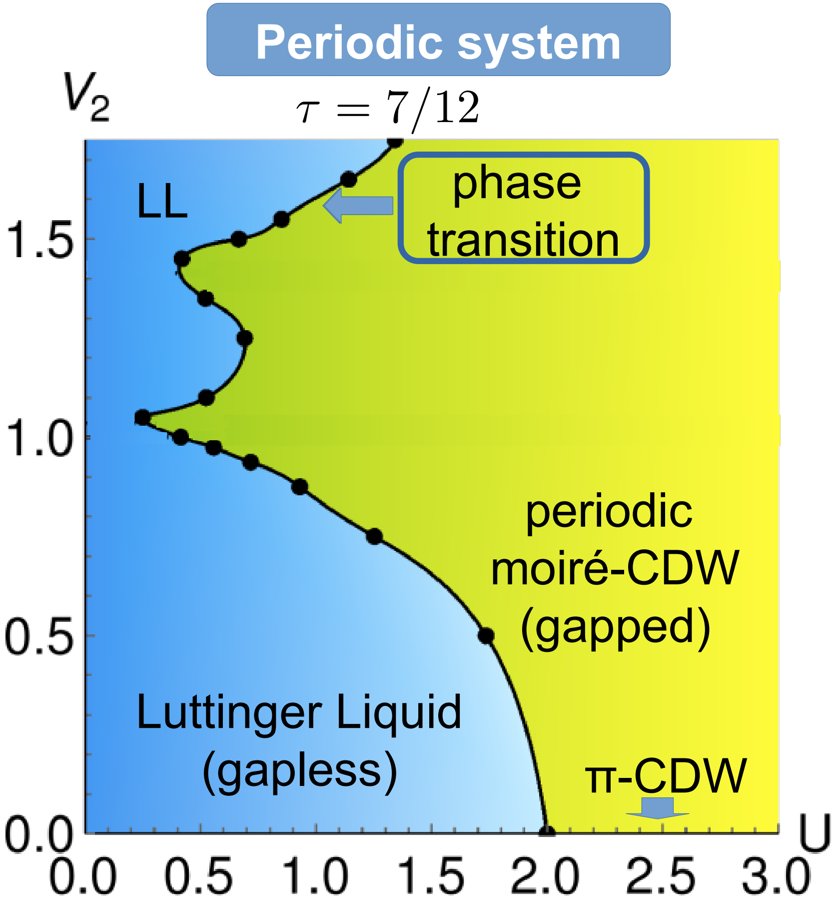

Charge modulation

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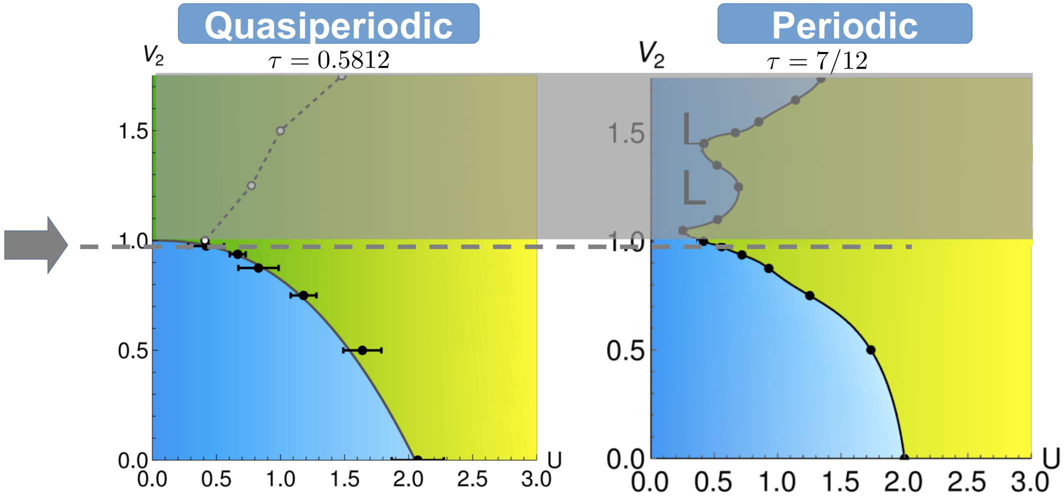

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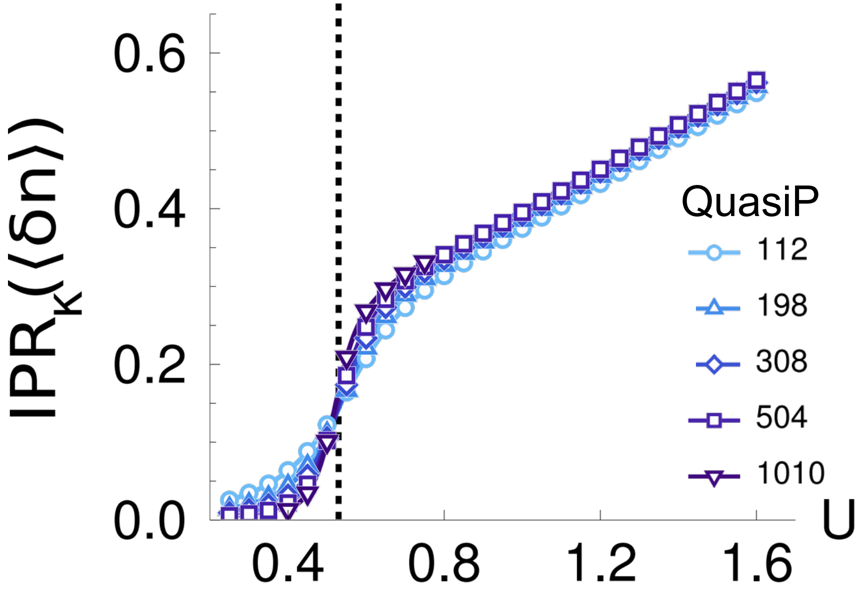

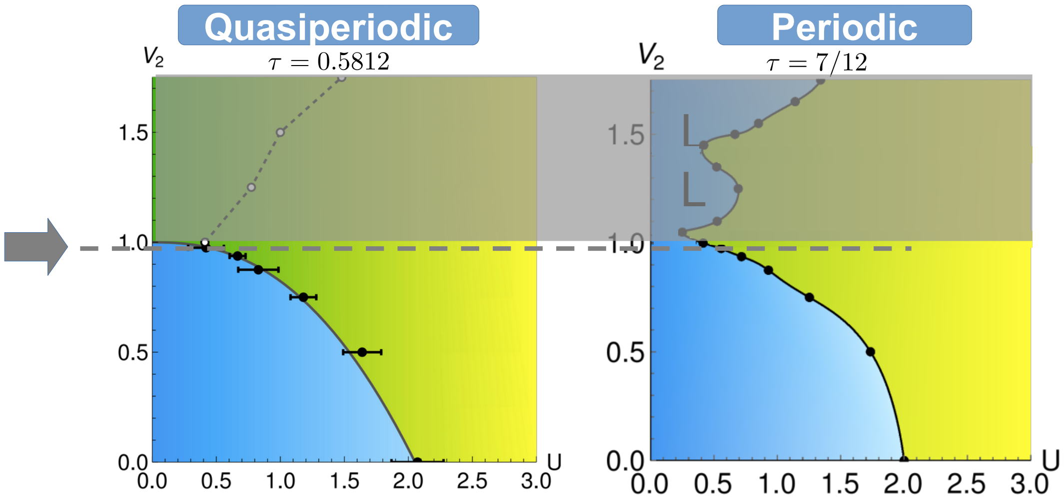

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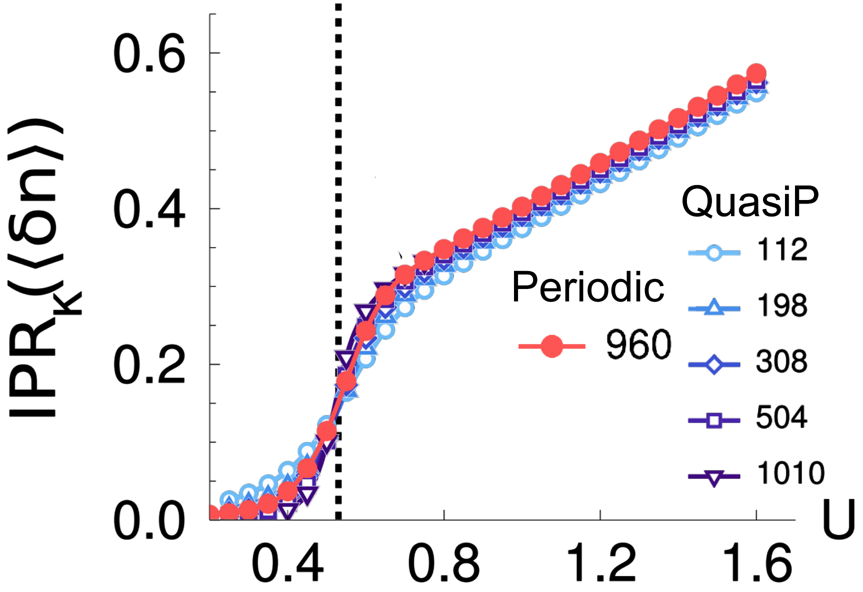

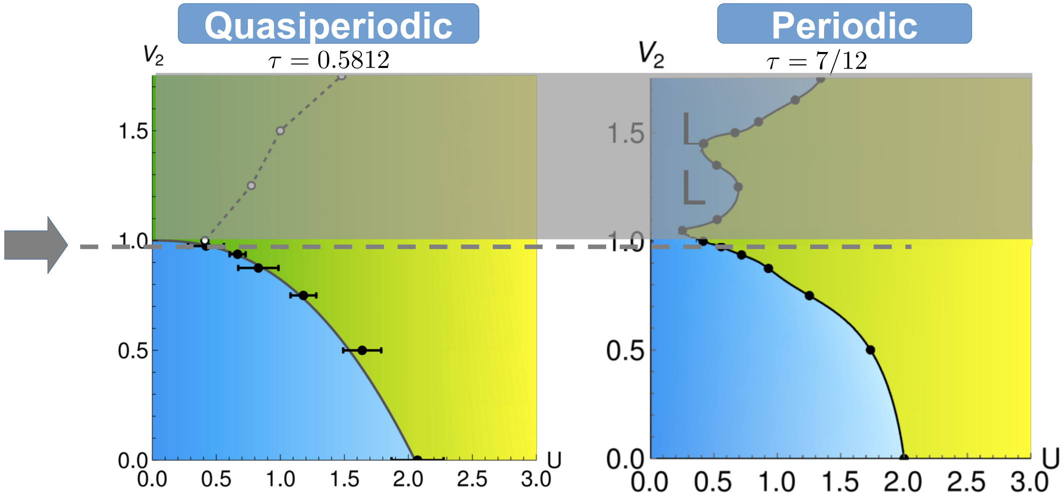

Charge modulation

Charge gap
Fidelity susceptibility

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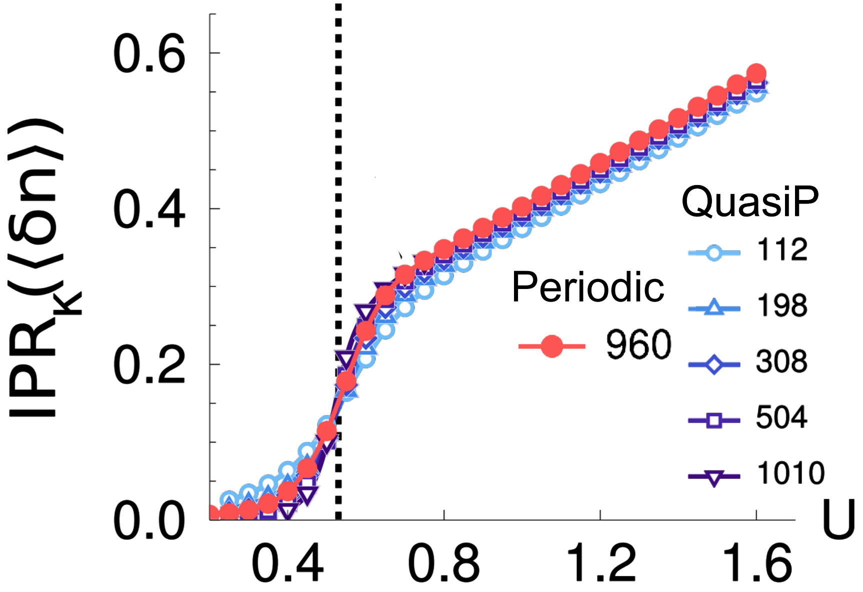

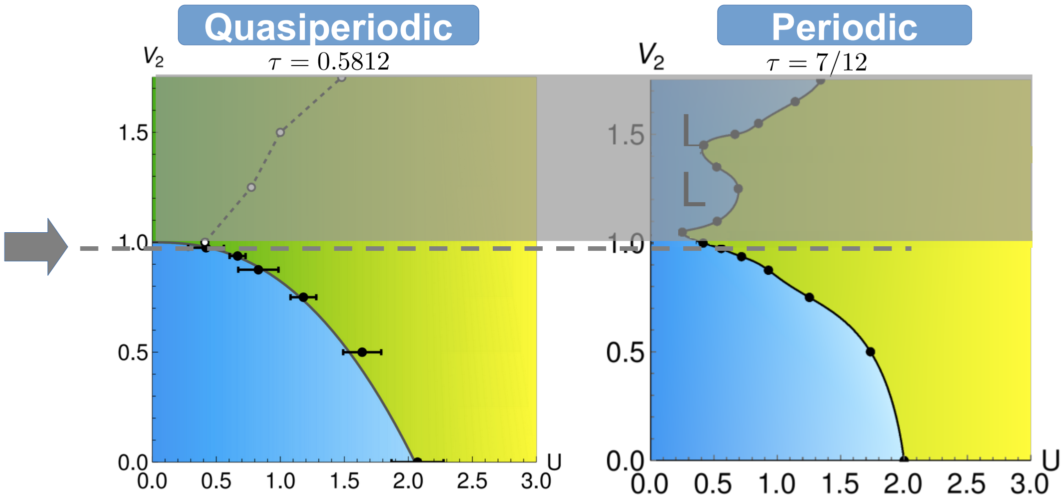

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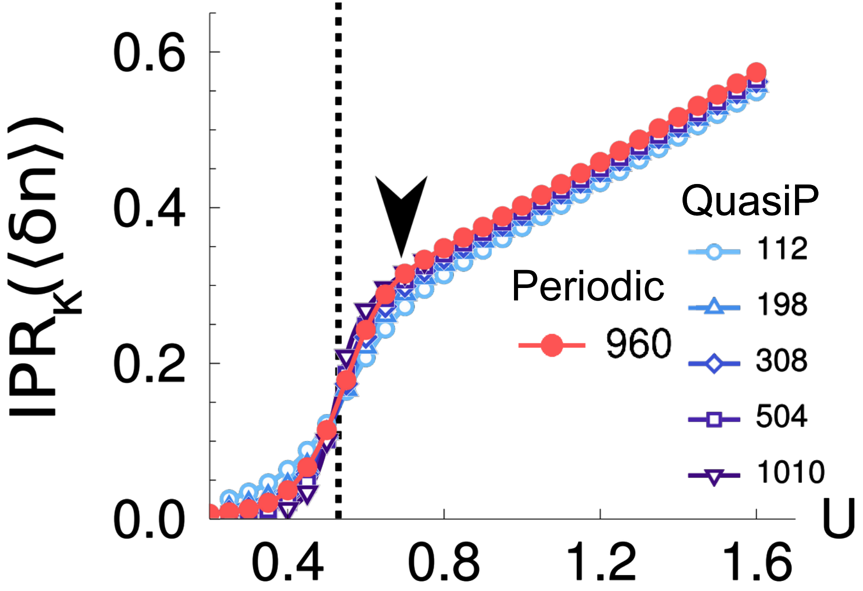
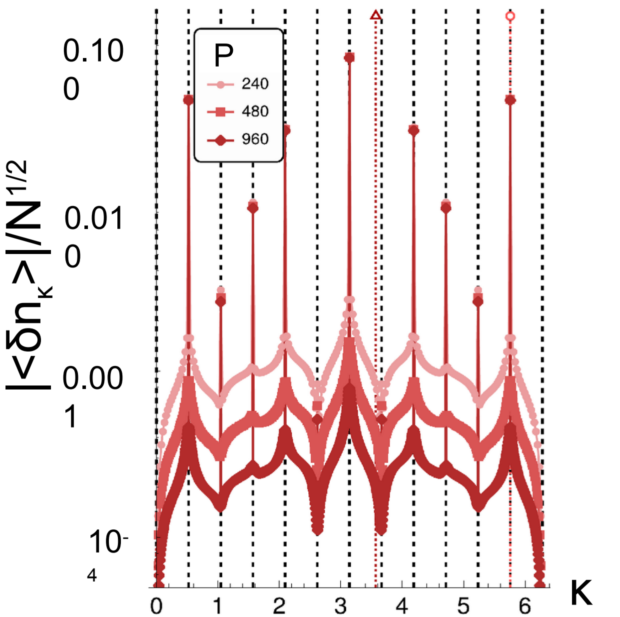
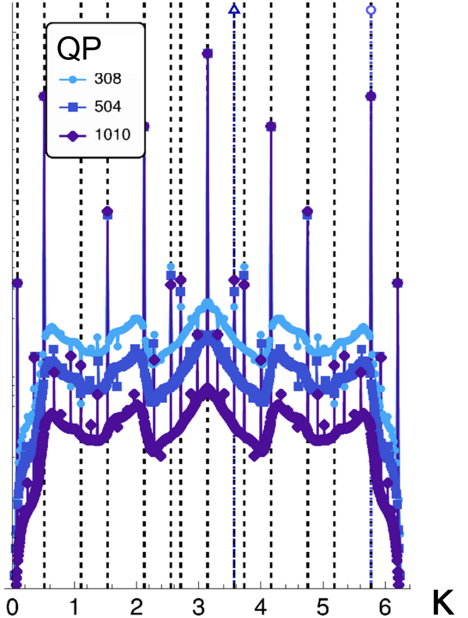


Periodic CDW



QuasiP CDW



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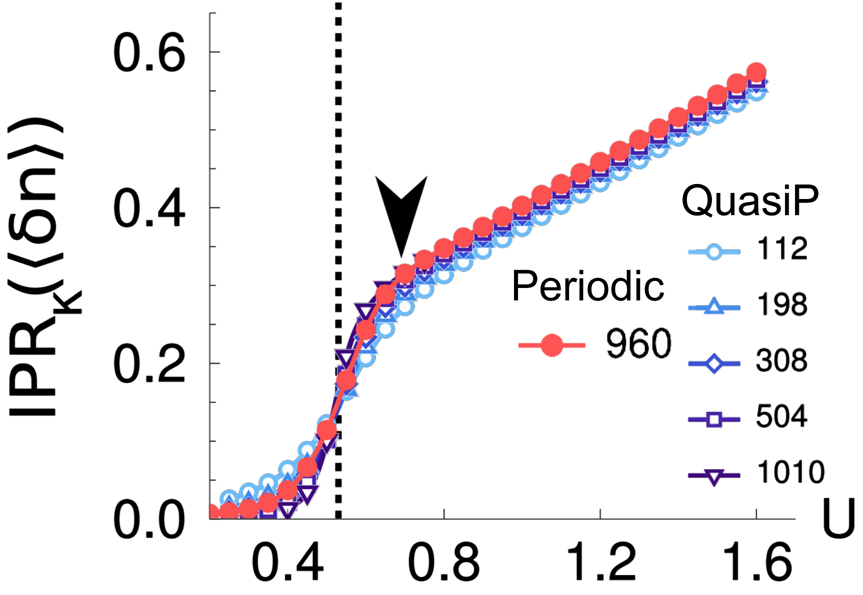
Fidelity susceptibility

FT of charge modulation: $\langle \delta n_\kappa \rangle = \frac{1}{\sqrt{N}} \sum_n e^{i\kappa m} \left(\langle n_m \rangle - \frac{1}{2} \right)$

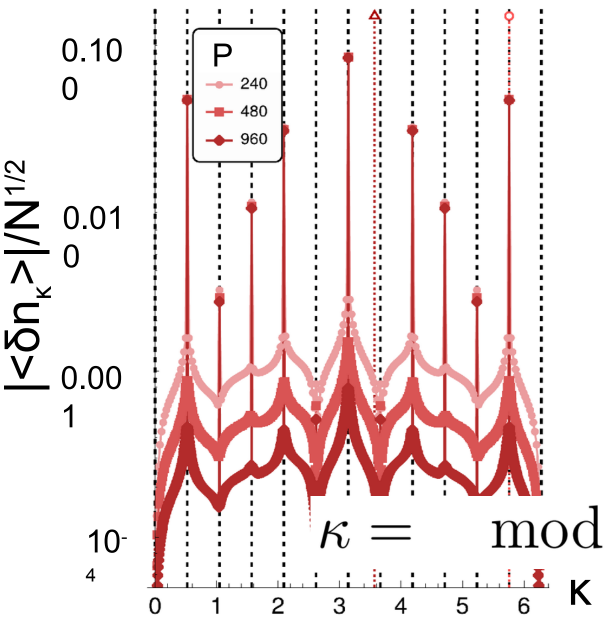
IPR of FT modulation: $\mathrm{IPR}_\kappa \left(\langle \delta \boldsymbol{n} \rangle \right) = \frac{\sum_\kappa \langle \delta n_\kappa \rangle^4}{\left(\sum_\kappa \langle \delta n_\kappa \rangle^2 \right)^2}$

- Disordered phase: $\mathrm{IPR}_\kappa \left(\langle \delta \boldsymbol{n} \rangle \right) \sim N^{-1}$
- CDW phase: $\mathrm{IPR}_\kappa \left(\langle \delta \boldsymbol{n} \rangle \right) \sim N^{0}$

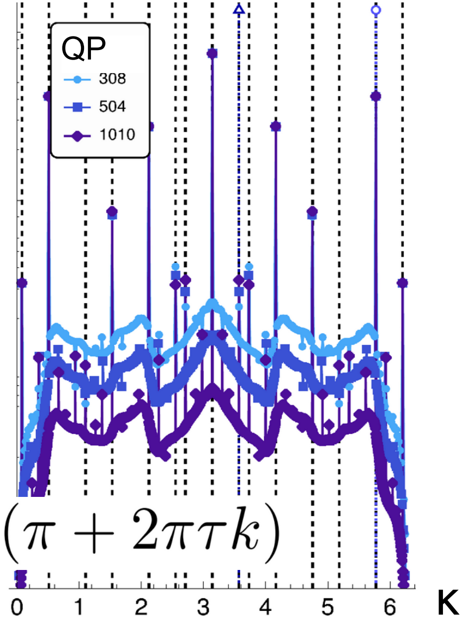
For $V_2 = 0.975 < V_c = 1$



Periodic CDW



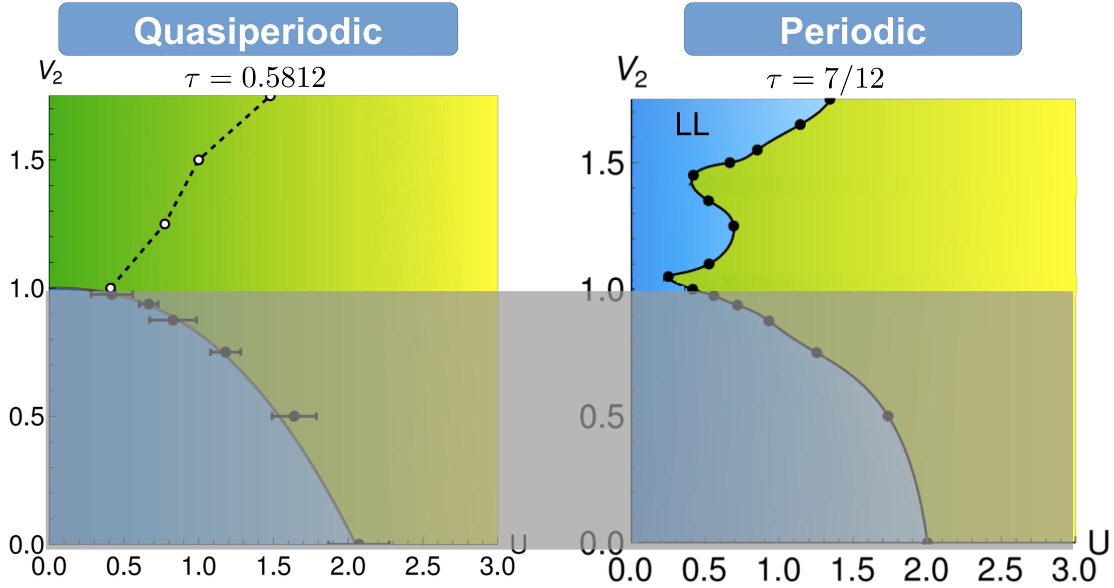
QuasiP CDW



$\kappa = \mod (\pi + 2\pi\tau k)$

Critical phase: Quasiperiodic VS Periodic

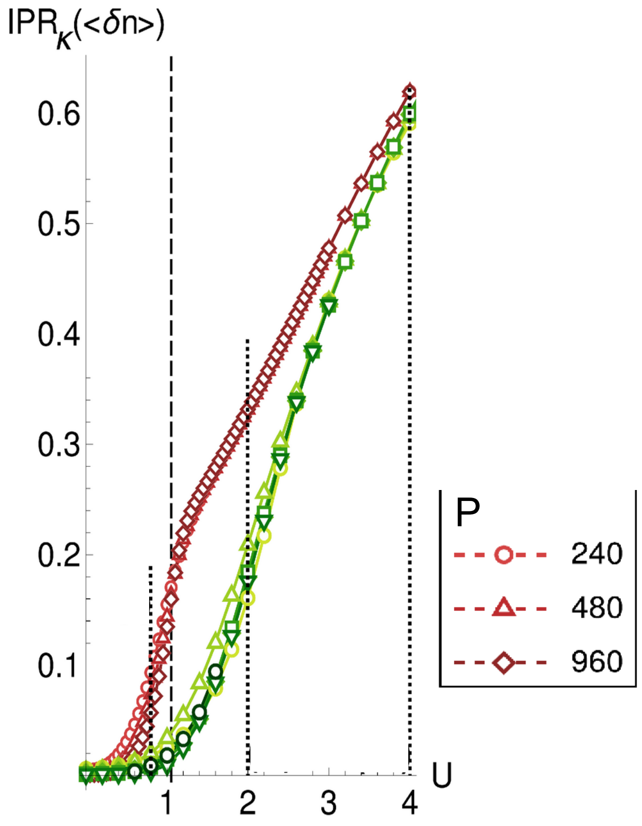
For $V_2 = 3.5 > V_c = 1$



Critical phase: Quasiperiodic VS Periodic

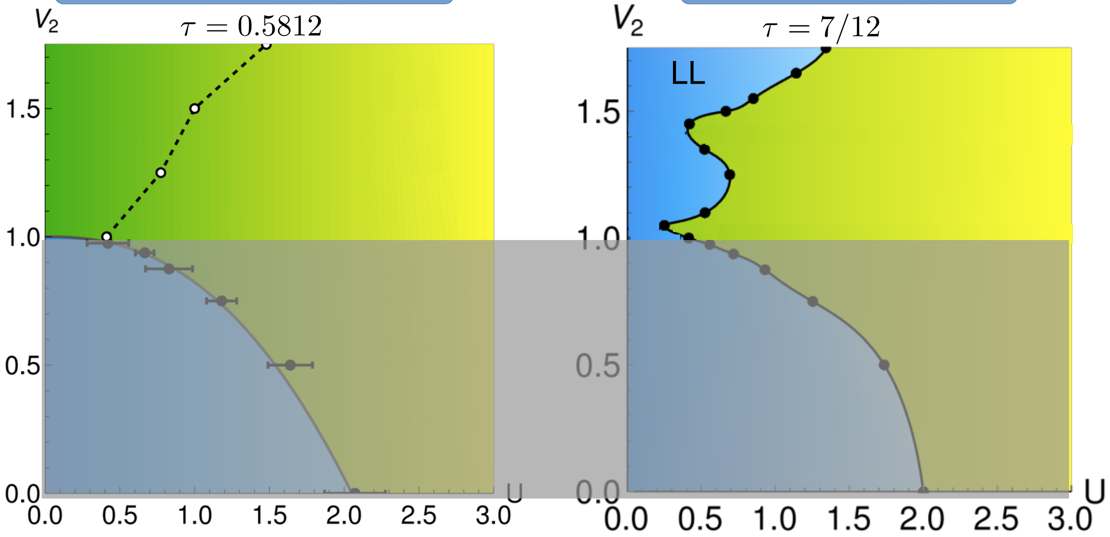
For $V_2 = 3.5 > V_c = 1$

IPR$_\kappa$



Quasiperiodic

Periodic



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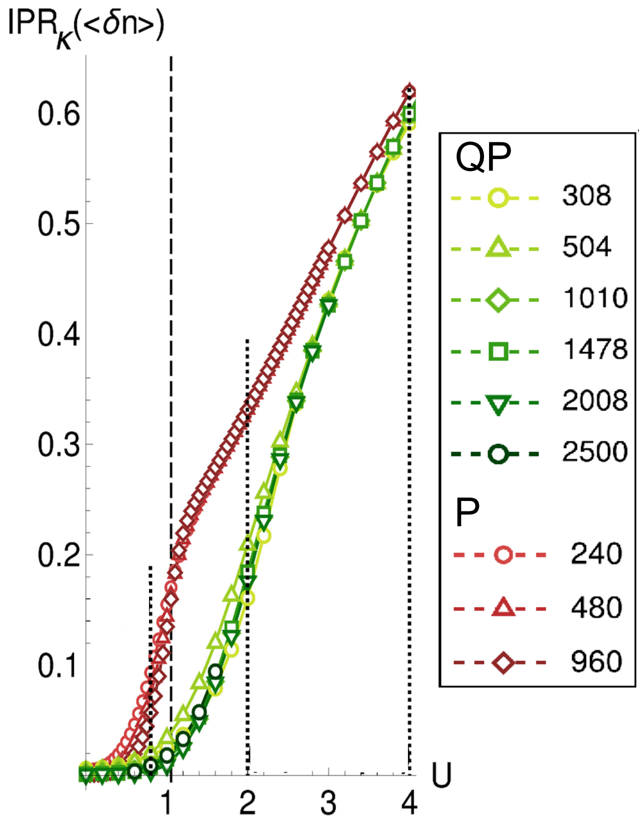
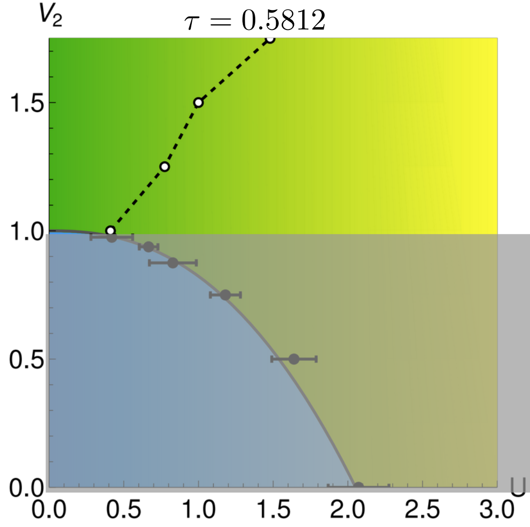
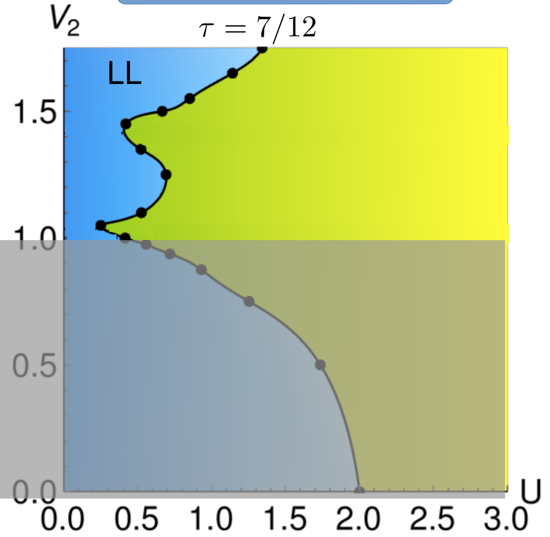


Quasiperiodic



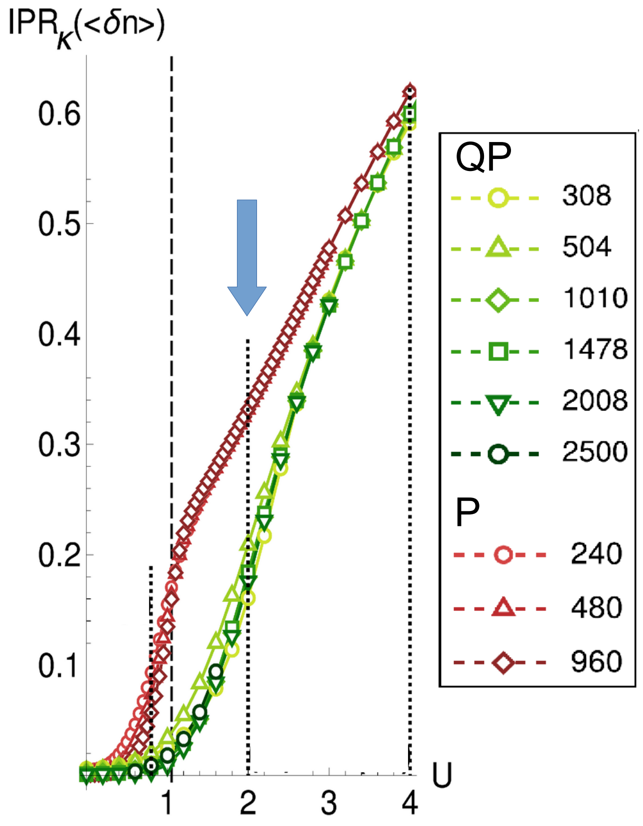
Periodic



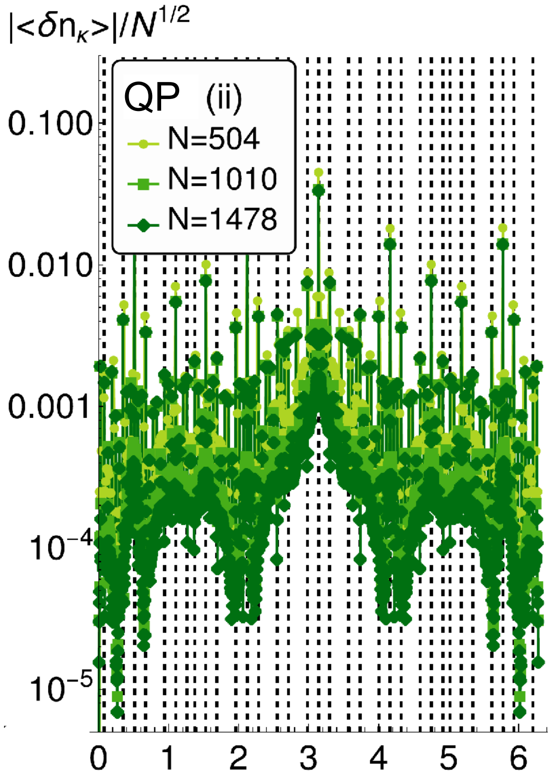
Critical phase: Quasi-fractal CDW

For $V_2 = 3.5 > V_c = 1$

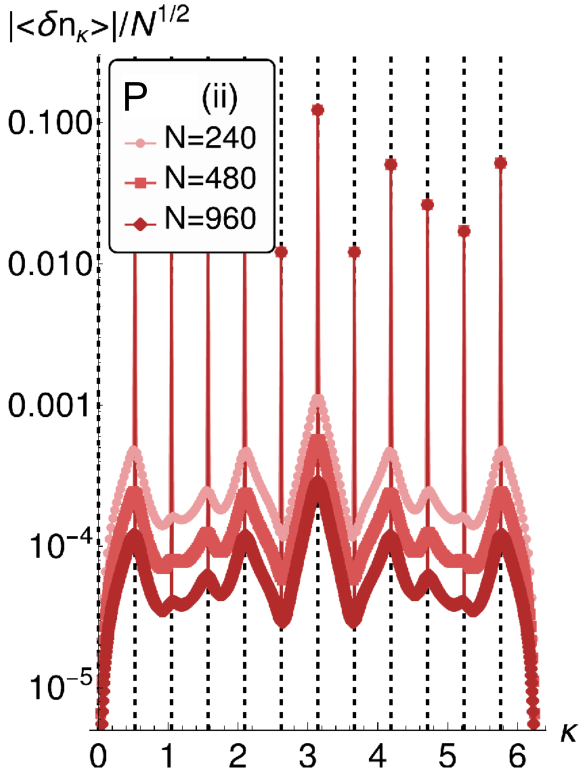
IPR_κ



QuasiP: quasi-fractal CDW



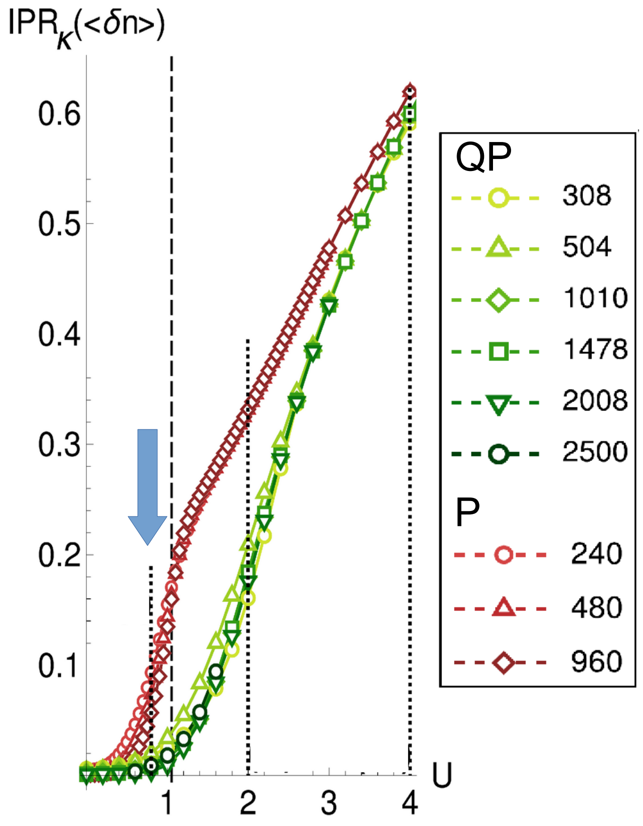
Periodic: moiré CDW



Critical phase: Quasi-fractal CDW

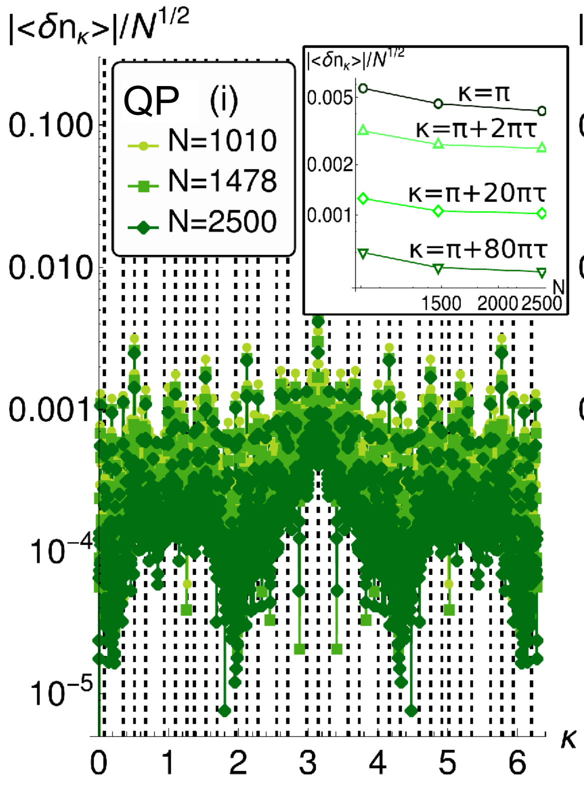
For $V_2 = 3.5 > V_c = 1$

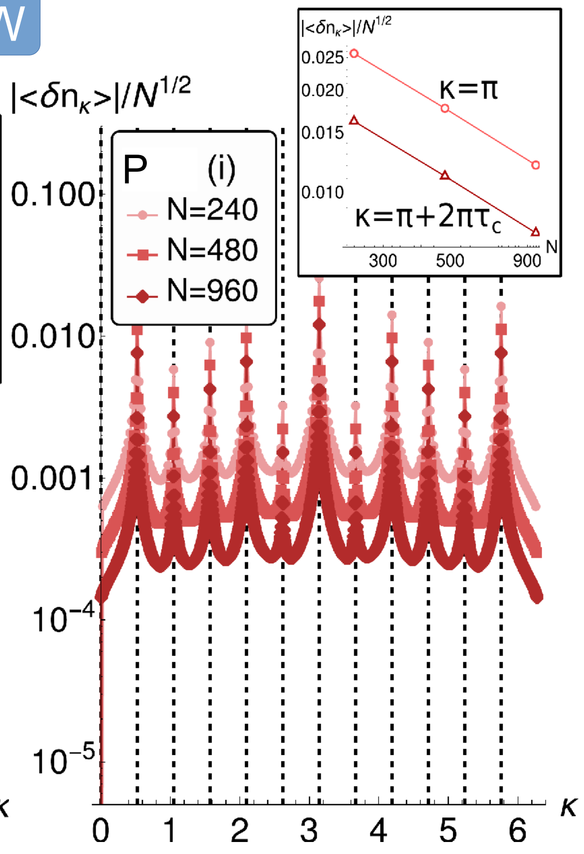
IPR_κ



Periodic: moiré CDW

QuasiP: quasi-fractal CDW





Mean Field analysis

Nearest-neighbour repulsion:
(half-filling, spinless electrons)

$$H = H_0 + U \sum_j n_j n_{j+1} \longrightarrow H_0 + \sum_i \epsilon_i c_i^\dagger c_i + \sum_i \Delta_i c_i^\dagger c_{i+1} + h.c.$$

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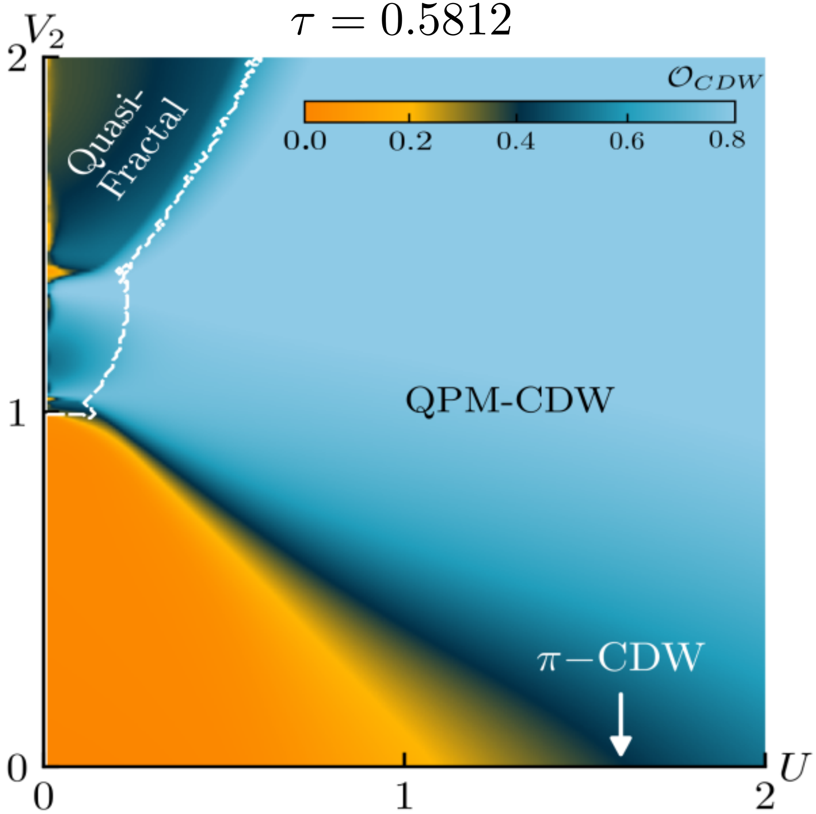
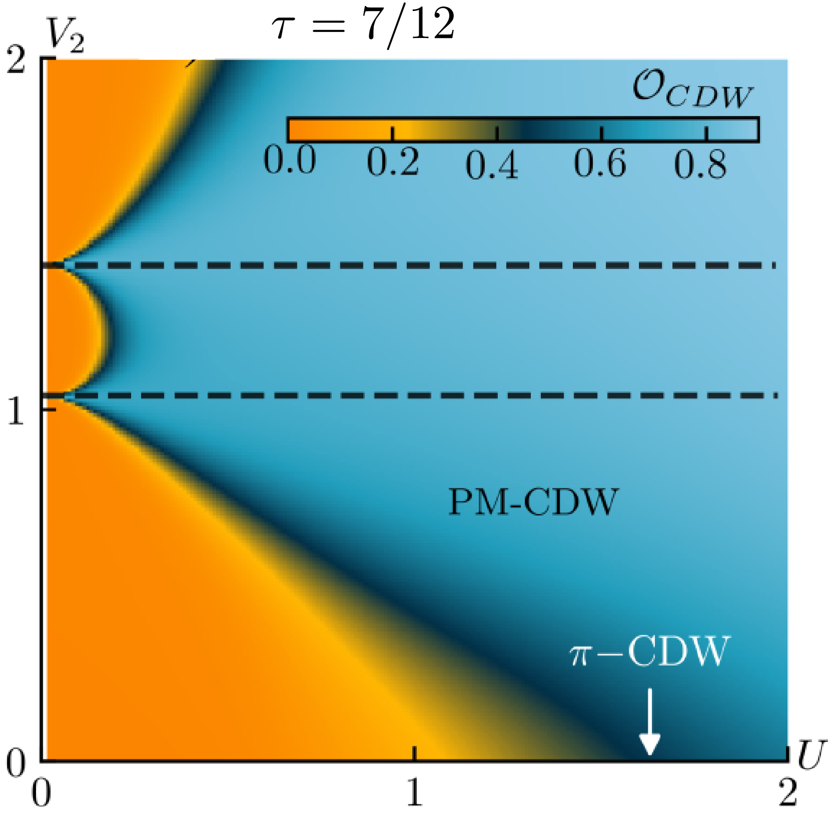
Quasiperiodic system

$\tau = 0.5812$



Periodic system

$\tau = 7/12$



Mean Field analysis

[N. Sobrosa (*to appear*)]

$$\mathcal{O}_{CDW} = \max \langle n_i \rangle - \min \langle n_i \rangle$$

Nearest-neighbour repulsion:
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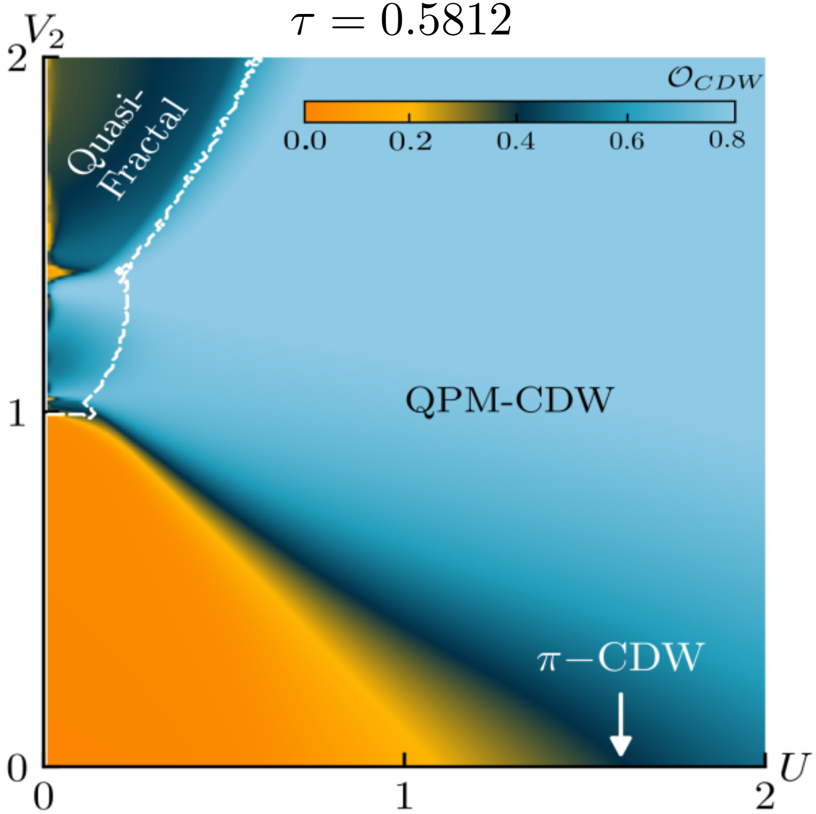
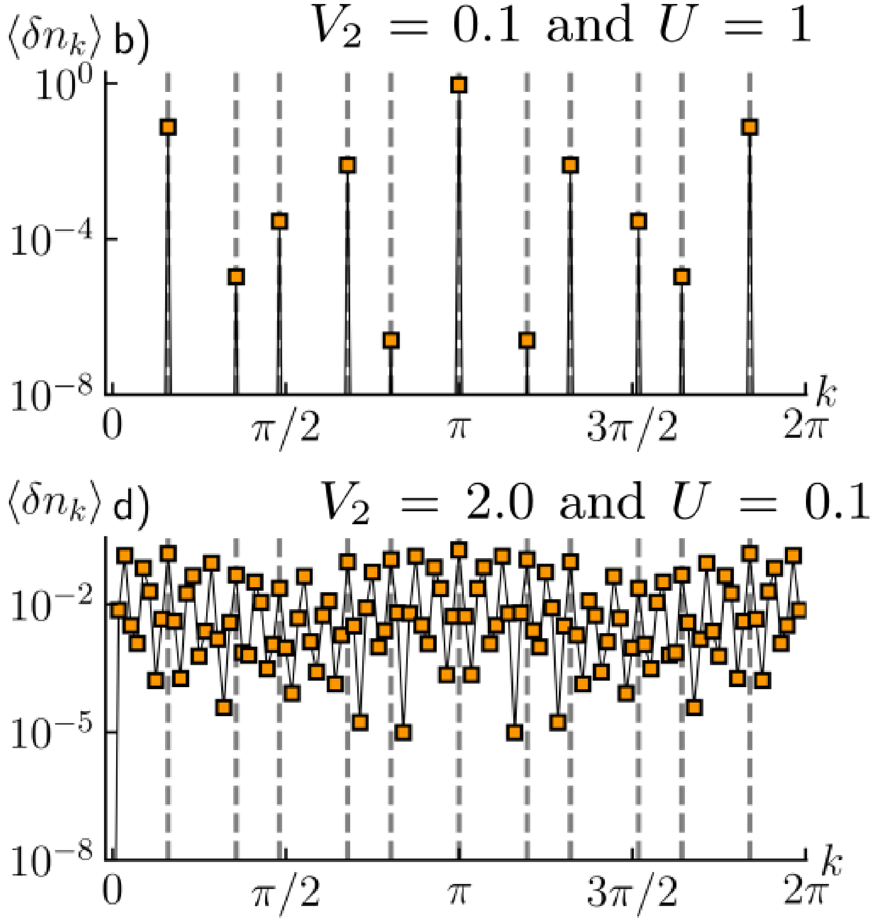
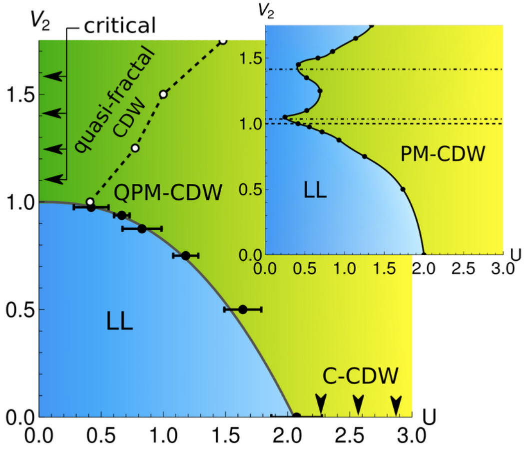




Conclusions

- *Quasiperiodicity in interacting 1D moiré systems*
  - narrow band enhances interactions both for periodic and quasiperiodic structures
  - only in the quasiperiodic case, for the critical phase regime, the ordered phase extends down to infinitesimal interactions
  - critical phase unstable to a quasi-factal ordered state with infinitely many contributing wave vectors



Nat. Phys. **20**, 1933–1940 (2024)

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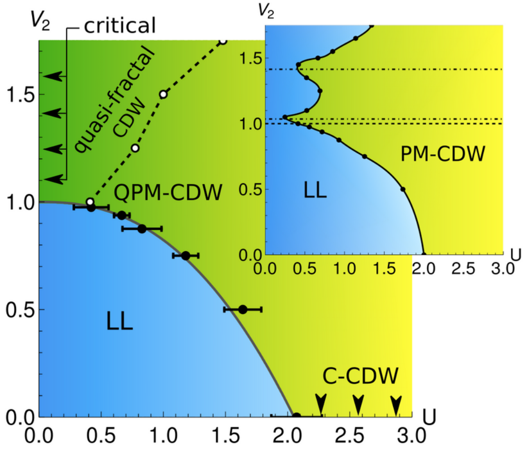

Nat. Phys. **20**, 1933–1940 (2024)

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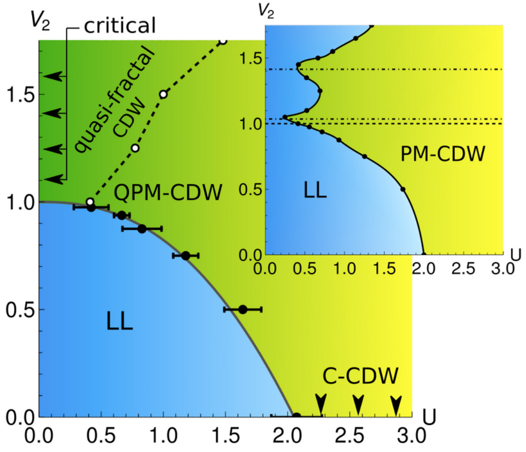
    – We are confident that mean field should work



Nat. Phys. **20**, 1933–1940 (2024)

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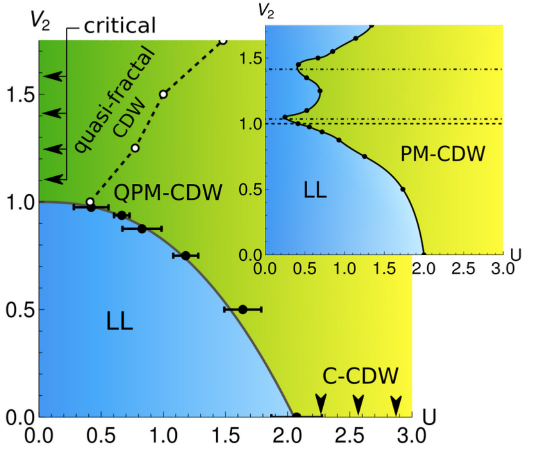

Nat. Phys. **20**, 1933–1940 (2024)

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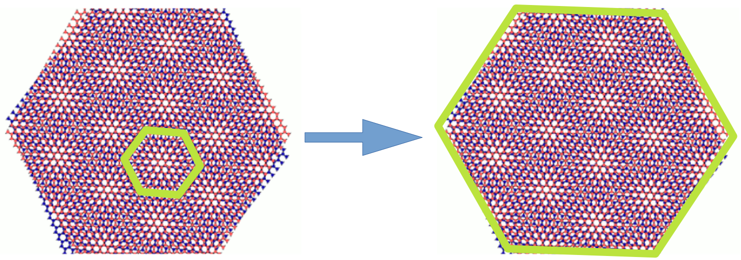
Thank you all for your attention

Appendix

Model

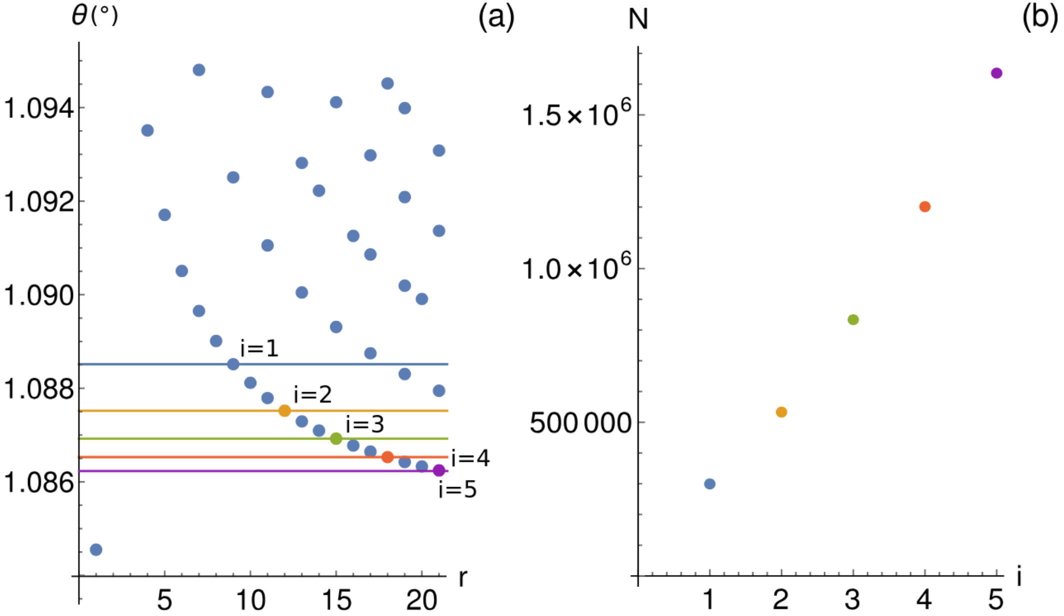


To capture quasiperiodicity:

- Real-space tight-binding Hamiltonian for tBLG
- Sequence of approximants: pairs (m_i, r_i), twist angle $\theta_i = \theta_c(m_i, r_i)$

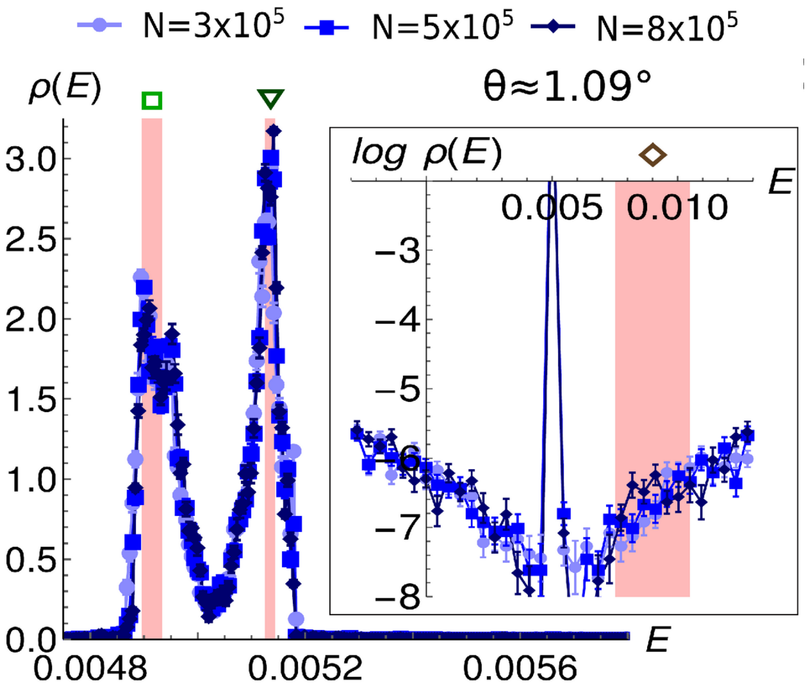
- $|\theta_{i+1} - \theta_i|$ decreases
- N_i increases

$$\cos\theta_{m,r} = \frac{3m^2 + 3mr + r^2/2}{3m^2 + 3mr + r^2}$$



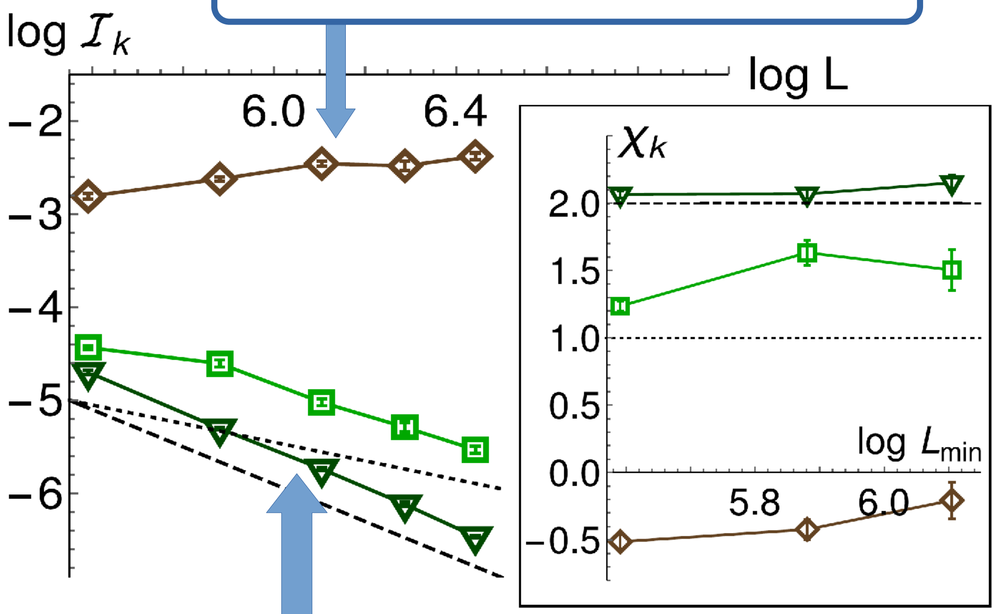
Sub-ballistic behavior: flatband vs the rest

DoS at the flatband



IPR-k scalling

Outside flatband: usual behaviour



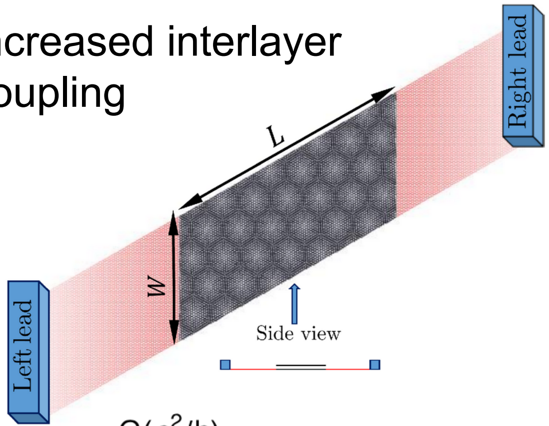
Momentum space delocalization in the flatband!

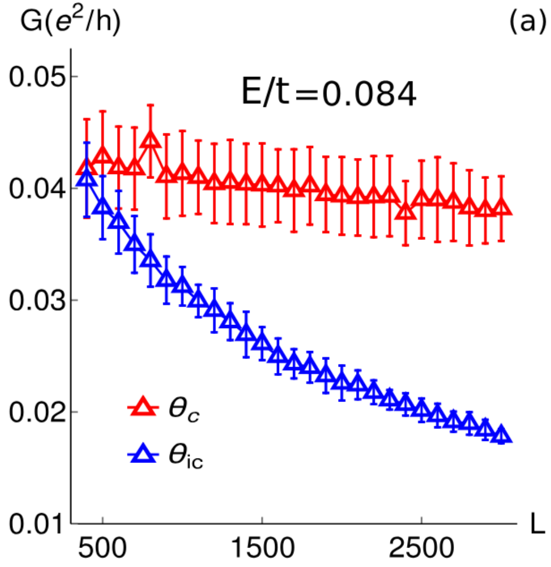
tBLG belongs to the class of “magic angle semimetals”

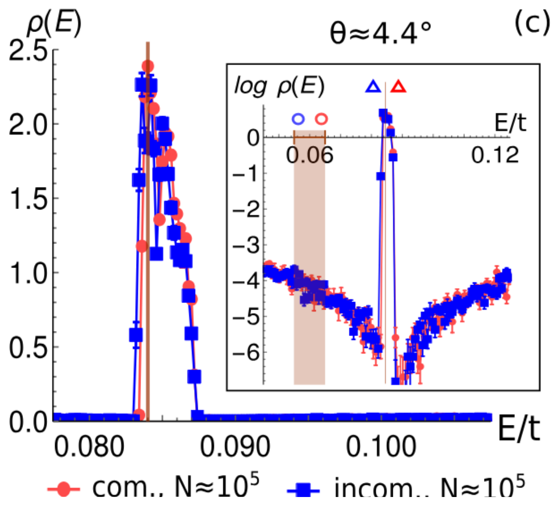
Fu, König, Wilson, Chou & Pixley npj Quantum Mater. **5**, 71 (2020)

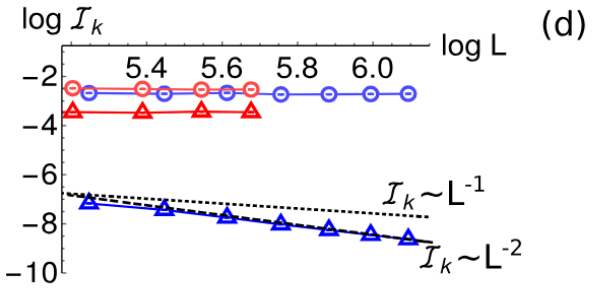
Sub-ballistic behavior and Landauer transport

Increased interlayer coupling

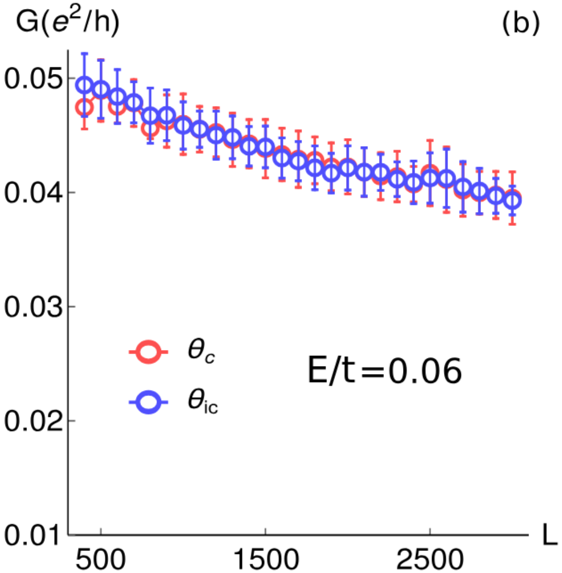








In agreement with IPR-k scalling



Sub-balisttic transport at the flatband for QuasiP. system

Disorder

RG theory of localization through periodic approximants

- At fixed energy, the contours of E(φ,κ) flow to effective single-band models corresponding to:
  - Extended fixed-point: only renormalized hopping survives yielding a $t_R \cos(\kappa)$ contribution;
  - Localized fixed-point: only renormalized potential survives yielding a $V_R \cos(\varphi)$ contribution;
  - Critical fixed-point: both renormalized hoppings and potential survive at any scale.

$$
\begin{aligned}
\mathcal{P}^{(n)}(E,\varphi,\kappa) &\equiv \det[H^{(n)}(\varphi,\kappa) - E] \\
&\rightarrow t_R^{(n)}(E)\cos(\kappa) + V_R^{(n)}(E)\cos(\varphi) \\
&+C_R^{(n)}(E)\cos(\kappa)\cos(\varphi) + T_R^{(n)}(E)
\end{aligned}
$$

RG theory of localization through periodic approximants

More generic models

Extended

Localized

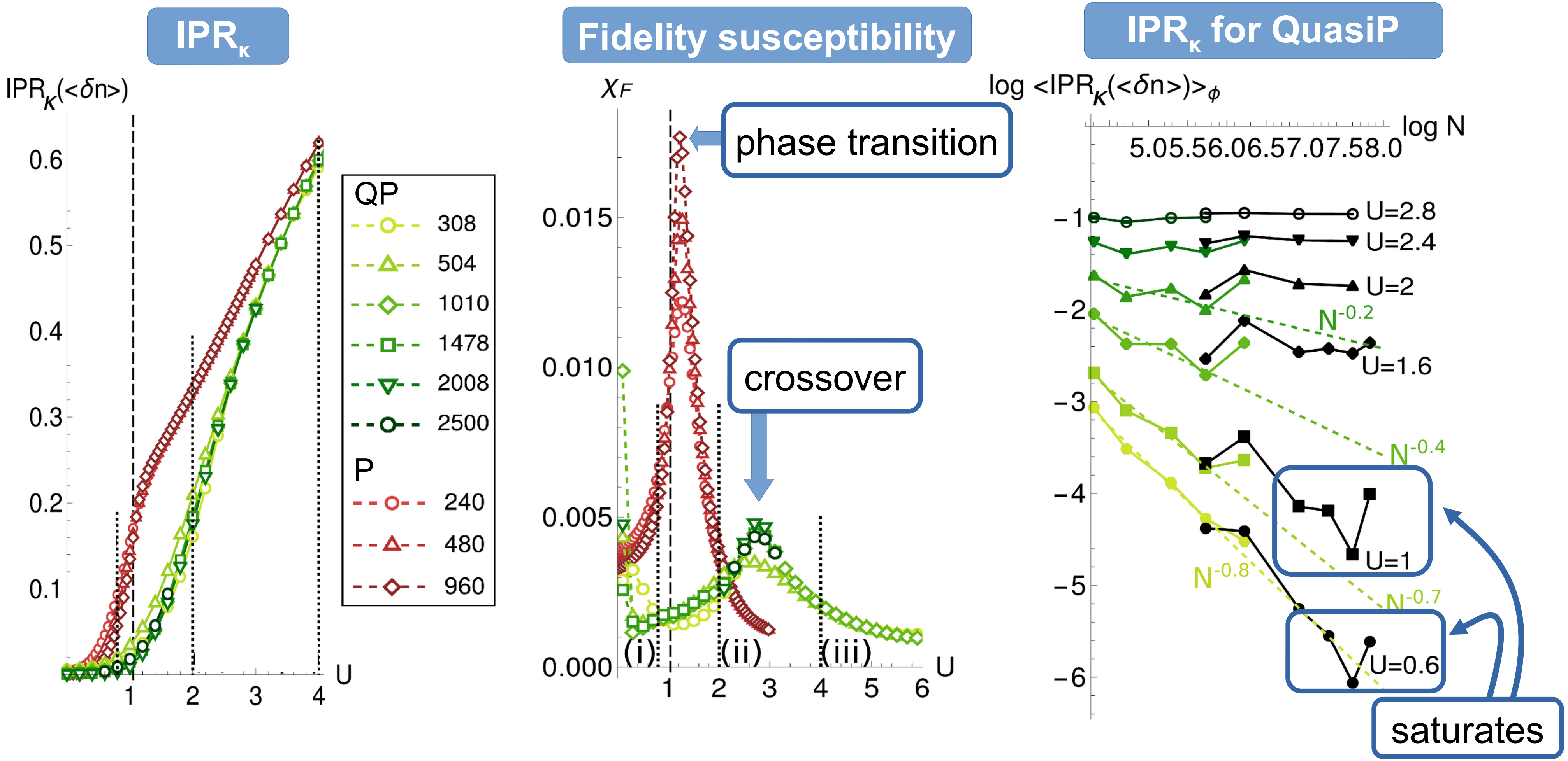
$$
\begin{aligned}
H = & -t\sum_j (c_j^\dagger c_{j+1} + \text{h.c.}) + V\sum_j \cos(2\pi\tau j + \phi) c_j^\dagger c_j \\
& - t_2 \sum_j (c_j^\dagger c_{j+2} + \text{h.c.}) + V_2 \sum_j \cos[2(2\pi\tau j + \phi)] c_j^\dagger c_j \\
& - t_3 \sum_j (c_j^\dagger c_{j+3} + \text{h.c.}) + V_3 \sum_j \cos[3(2\pi\tau j + \phi)] c_j^\dagger c_j
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{P}^{(n)}(E,\varphi,\kappa) \equiv & \; t_R^{(n)}(E)\cos(\kappa) + V_R^{(n)}(E)\cos(\varphi) \\
& + t_{2R}^{(n)}(E)\cos(2\kappa) + V_{2R}^{(n)}(E)\cos(2\varphi) + \cdots
\end{aligned}
$$

Irrelevant

Critical phase: Quasiperiodic VS Periodic

For $V_2 = 3.5 > V_c = 1$



Critical phase: Quasi-fractal CDW

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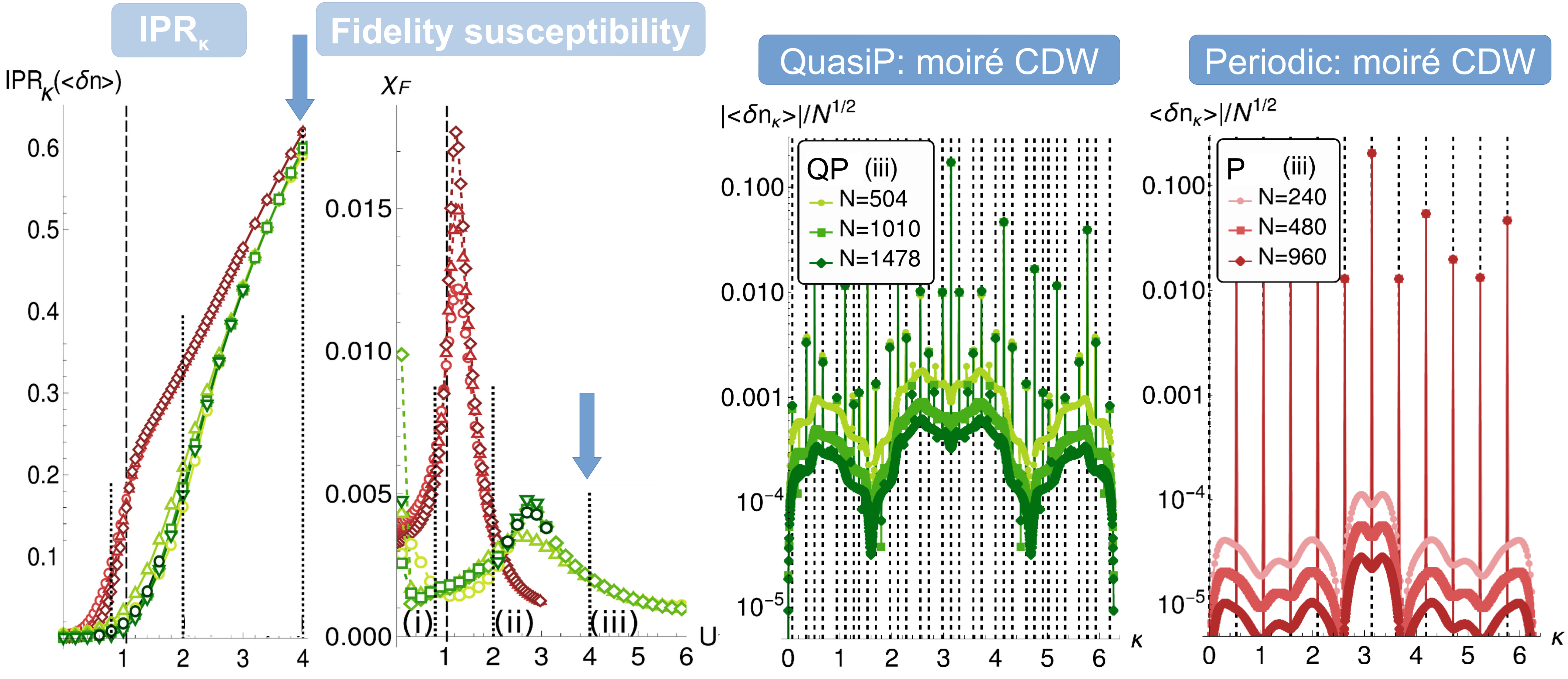

Relevance of short range interactions from generalized Chalker scaling

$$H = \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha - \sum_{\alpha,\beta,\gamma,\delta} \bar{V}_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

$$\bar{V}_{\alpha\beta\gamma\delta} = \Big(V_{\alpha\beta\gamma\delta} - V_{\beta\alpha\gamma\delta} + V_{\beta\alpha\delta\gamma} - V_{\alpha\beta\delta\gamma}\Big)/4$$

$$V_{\alpha\beta\gamma\delta} = U \sum_r \langle\alpha\,|r\rangle\,\langle\beta\,|r+1\rangle\,\langle r\,|\gamma\rangle\,\langle r+1\,|\delta\rangle$$

Miguel Gonçalves et al., Phys. Rev. B **109**, 014211 (2024)

- $\bar{V}_{0\alpha0\alpha}$ dominates at low energies
- Collapse for different sizes and energies

$$\epsilon_\alpha \to N^z \epsilon_\alpha$$

$$\bar{V}_{0\alpha0\alpha} \to N^{D_{\bar{V}}} \bar{V}_{0\alpha0\alpha}$$

- Interaction scaling dimension:

$$D_U = z - D_{\bar{V}}$$

- Aubry-André $D_{\bar{V}} = 2z - 1 \Rightarrow D_U = 1 - z,\ \ z > 1$