Universal principles
of
moiré band structures

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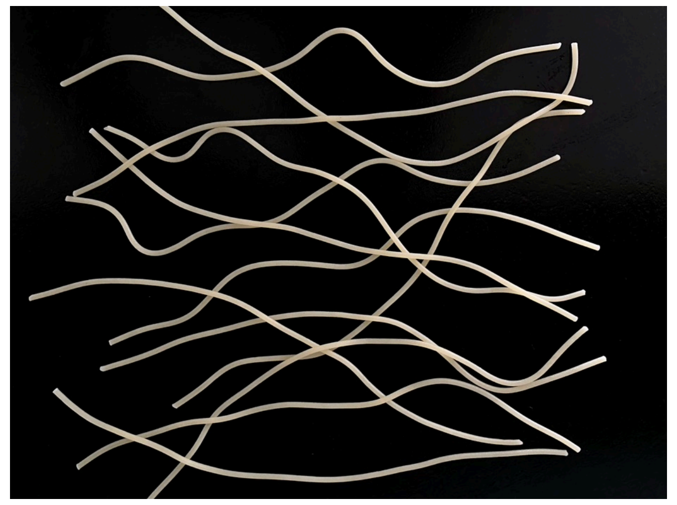
CRC 1238 Control and Dynamics of Quantum Materials

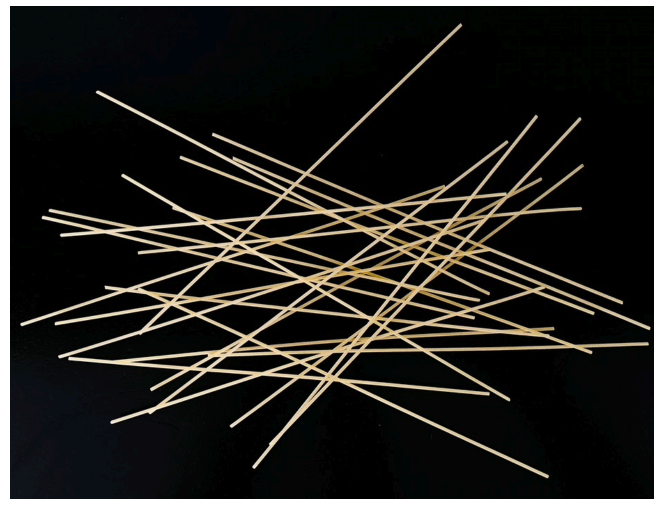
CRC 183 ENTANGLED STATES OF MATTER

why most moiré bands are **not** flat

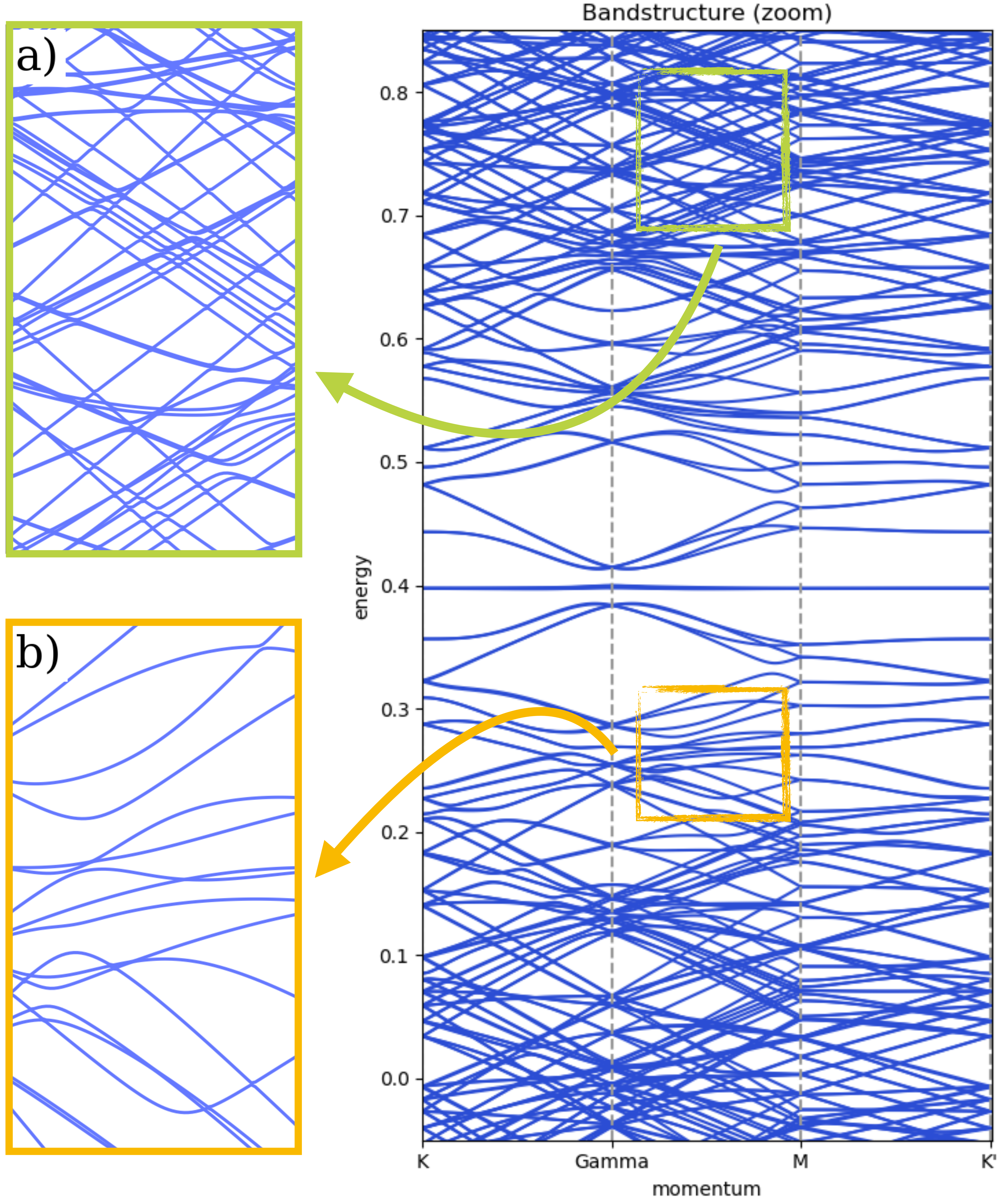
This talk

- the physics of moiré systems with **giant unit cells**
- **statistical** analysis
- **quantum chaos** versus Anderson **localization**
- **twisted bilayer graphene** and beyond





- What happens with the **spaghetti**?

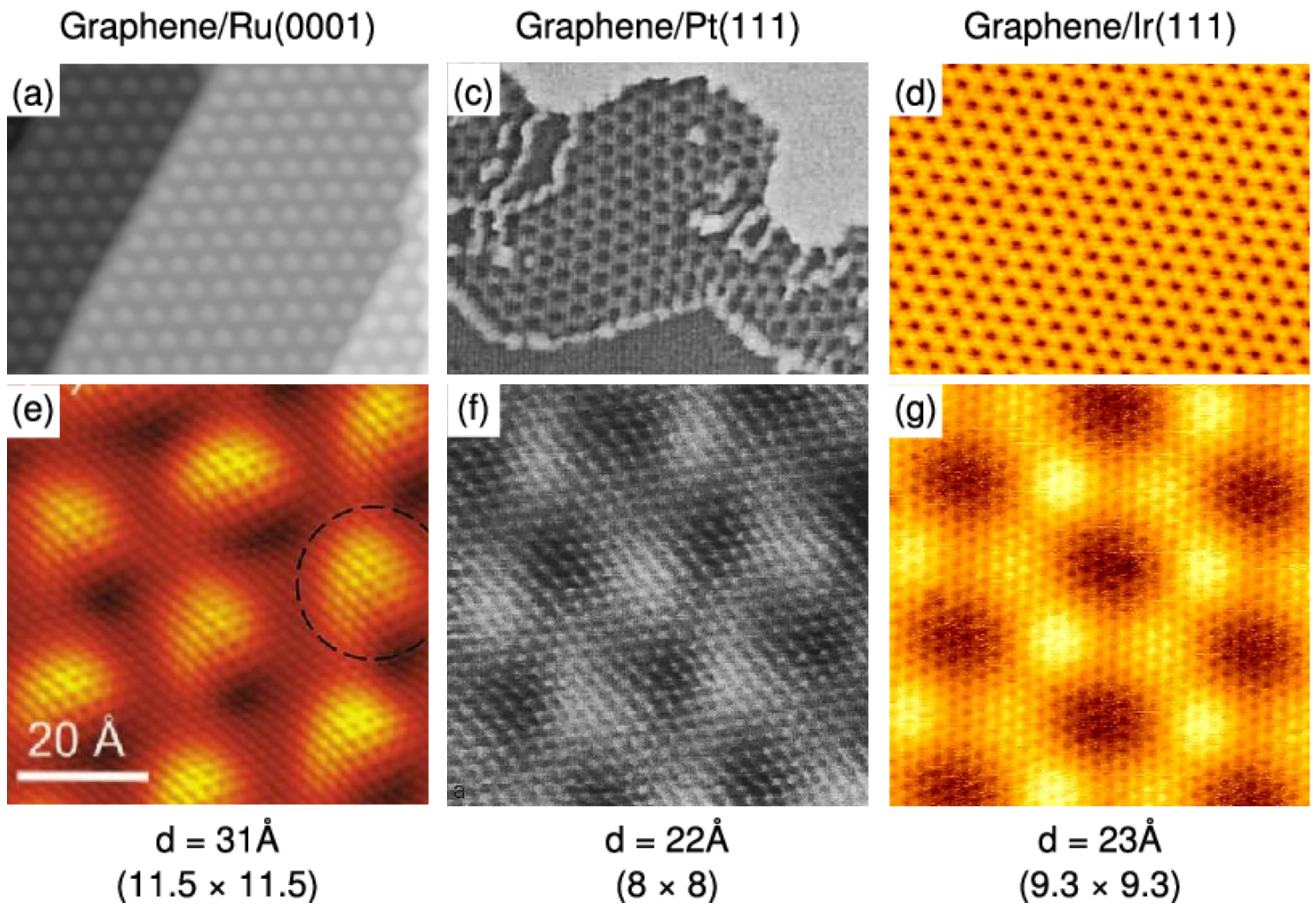


moiré materials

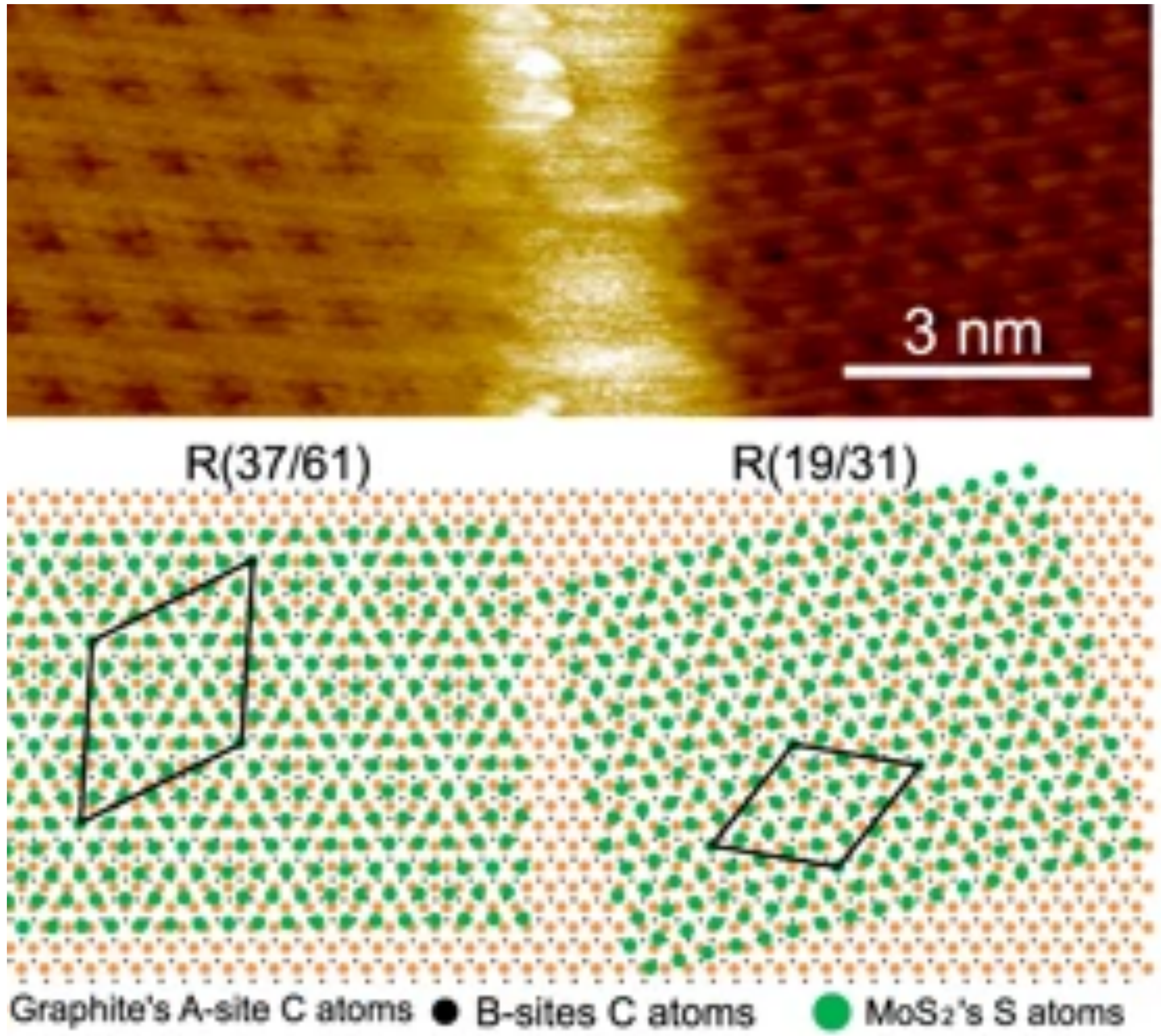
grow material 1 on material 2

if weakly coupled & **mismatch** of lattice constants

use **twisting**: “stamp“ material onto other/same material with rotation angle



Michely group, Cologne



twisted MoS_2/graphite moiré, Chun-I Lu et al. 2017

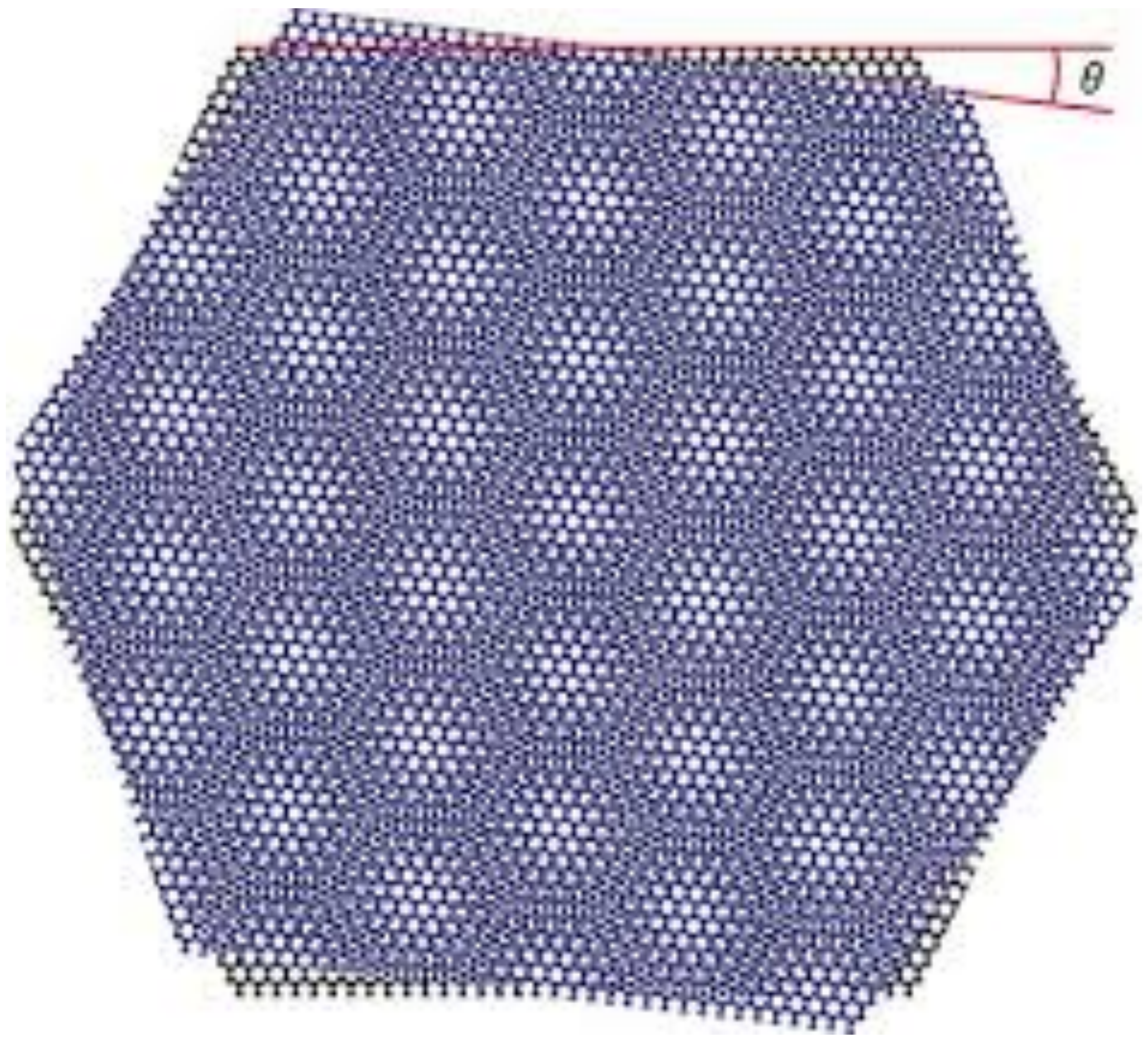
moiré materials

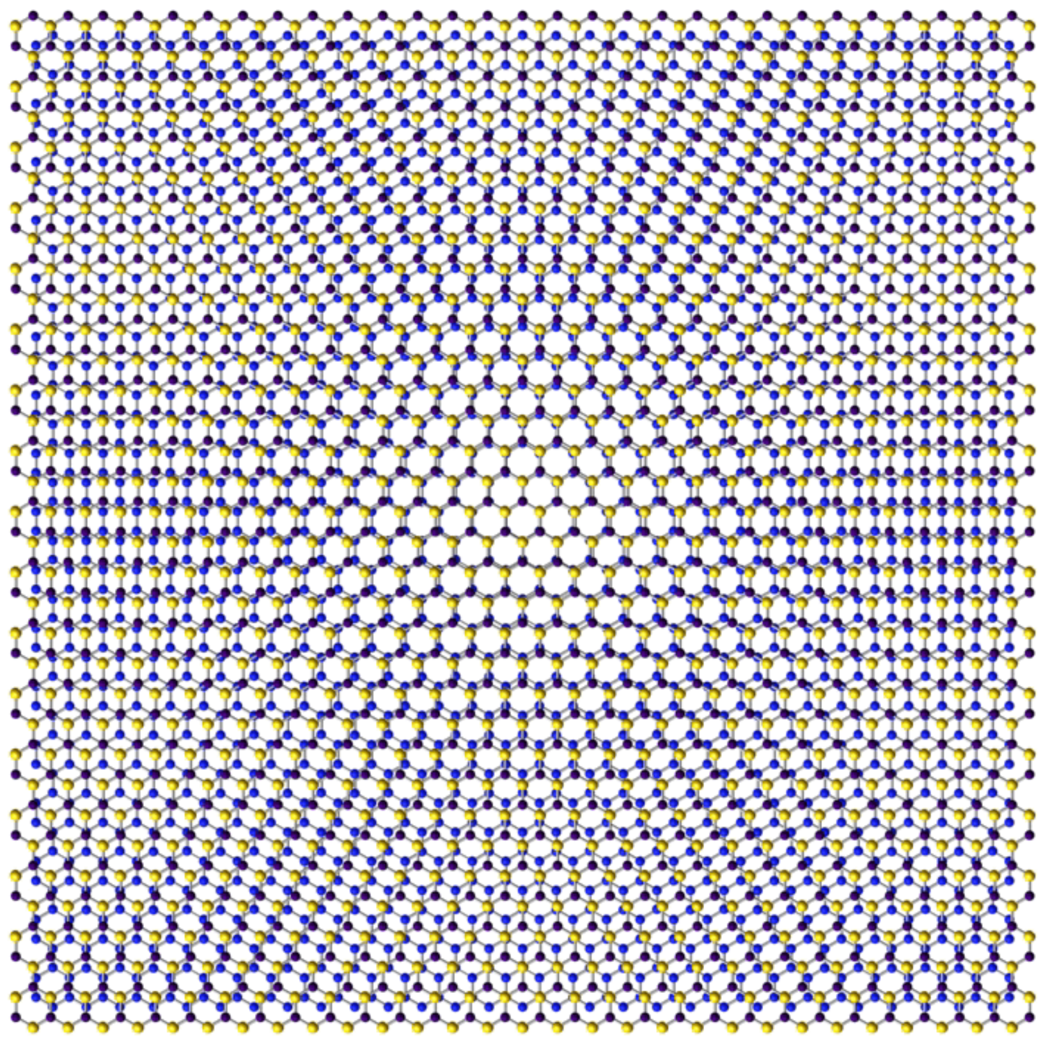
twisted bilayer graphene

- flat bands at **magic twist angle of 1.2°**

  due to interference effect

- giant unit cell of 10^4 atoms





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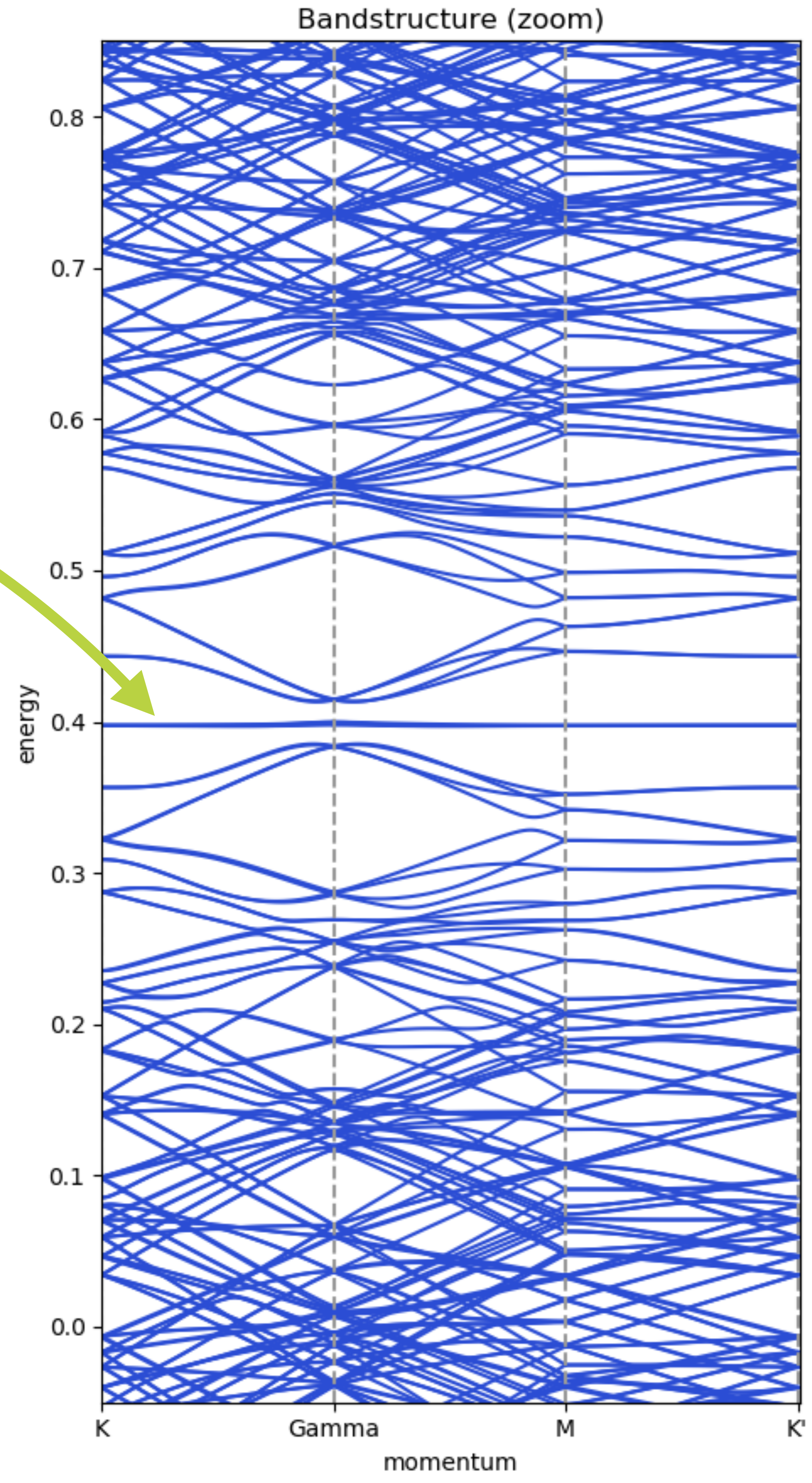


moiré materials

twisted bilayer graphene

- flat bands at **magic twist angle of 1.2º**

  due to interference effect

- tunable by gate voltage

Mott insulators

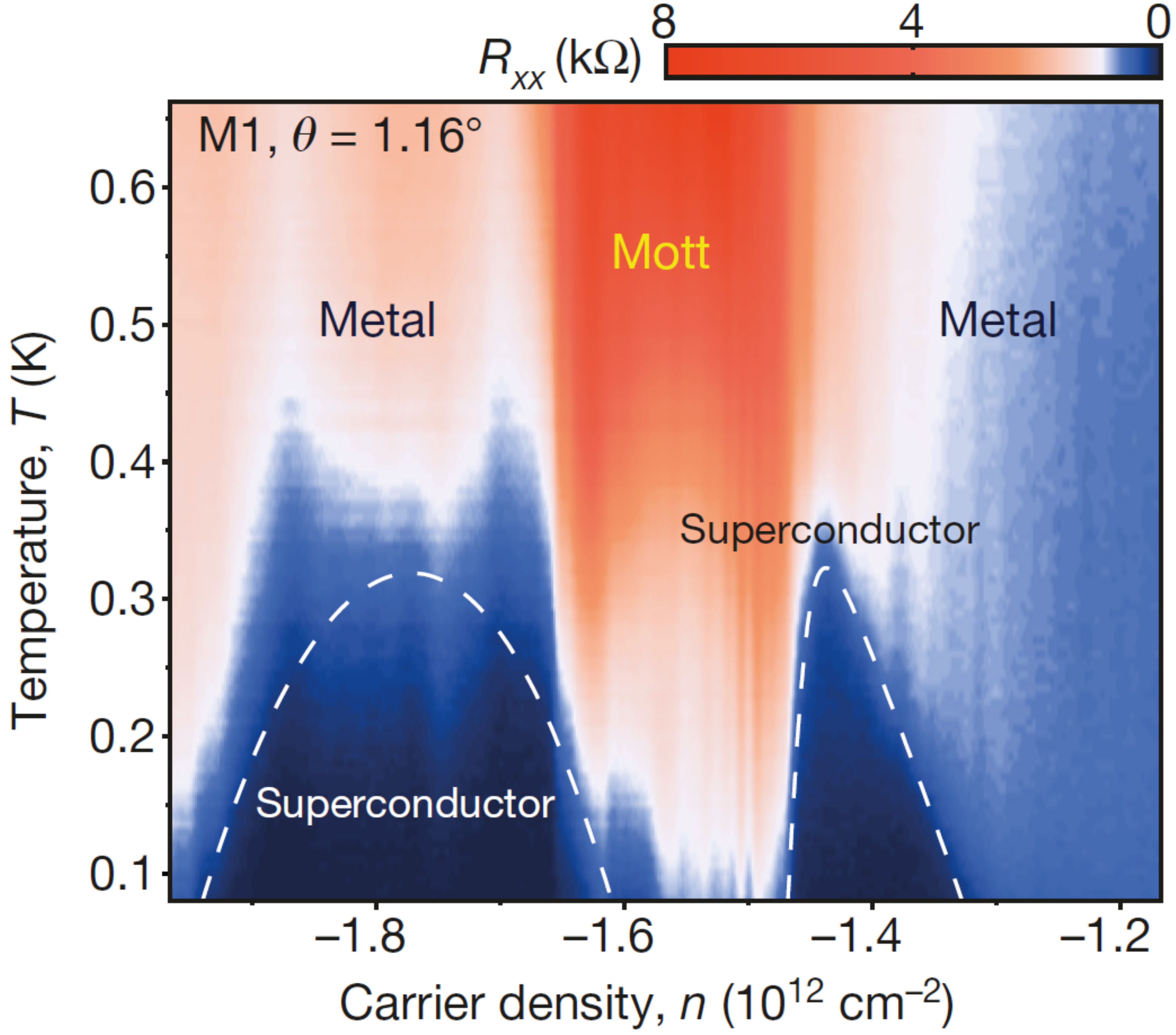
superconductors

topolgical bands & anomalous QHE

magnetic phases

nematic order

…



Cao et al., Nature (2018)

correlations & topology
in a *single* highly-tunable system

moiré materials

Why moiré systems with giant unit cells?

- easy to add 1 electron per unit cell

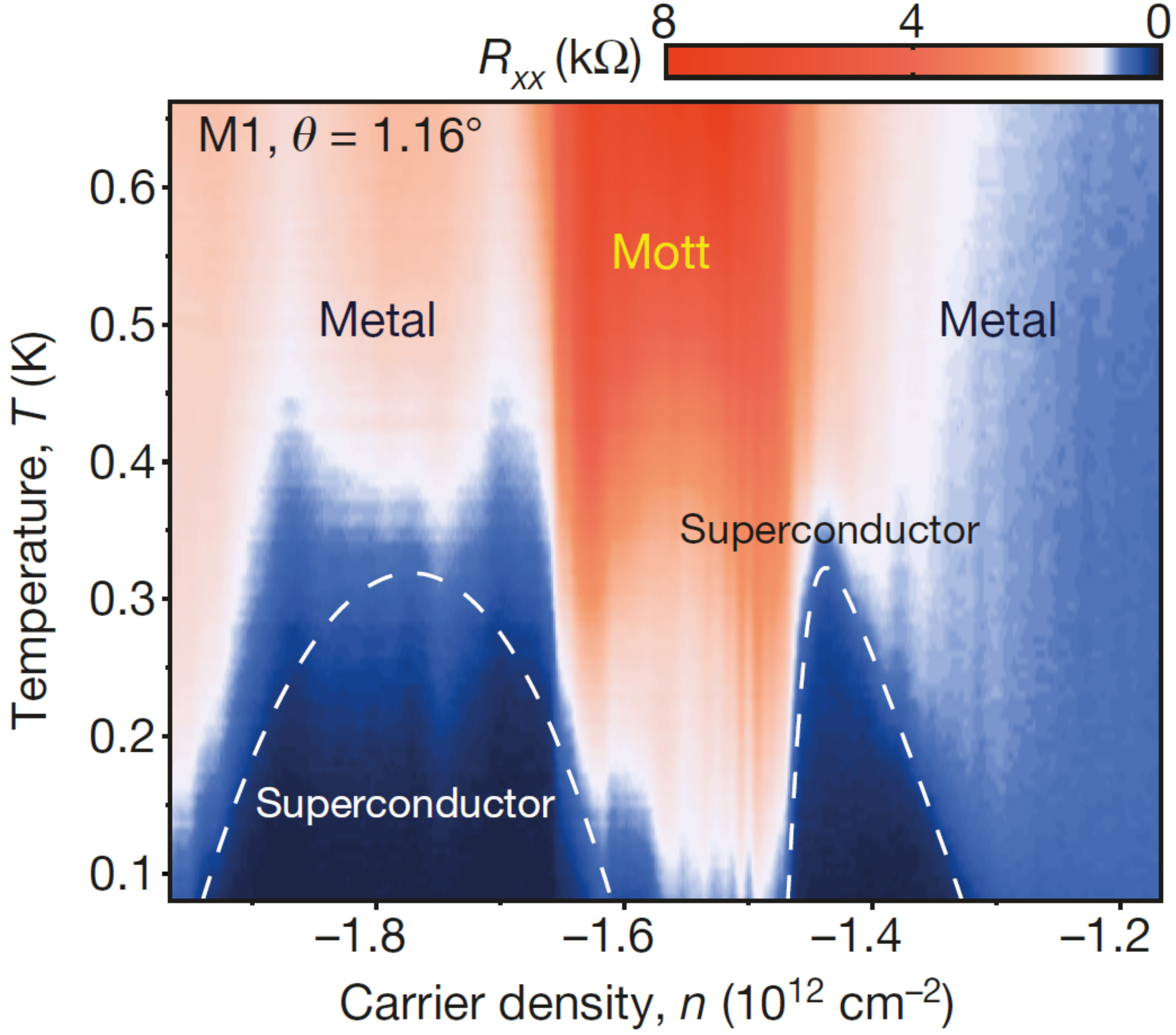
  ⇒ tunable by gate

- additional tunability from twist angle,

  chemical decoration, …

This talk

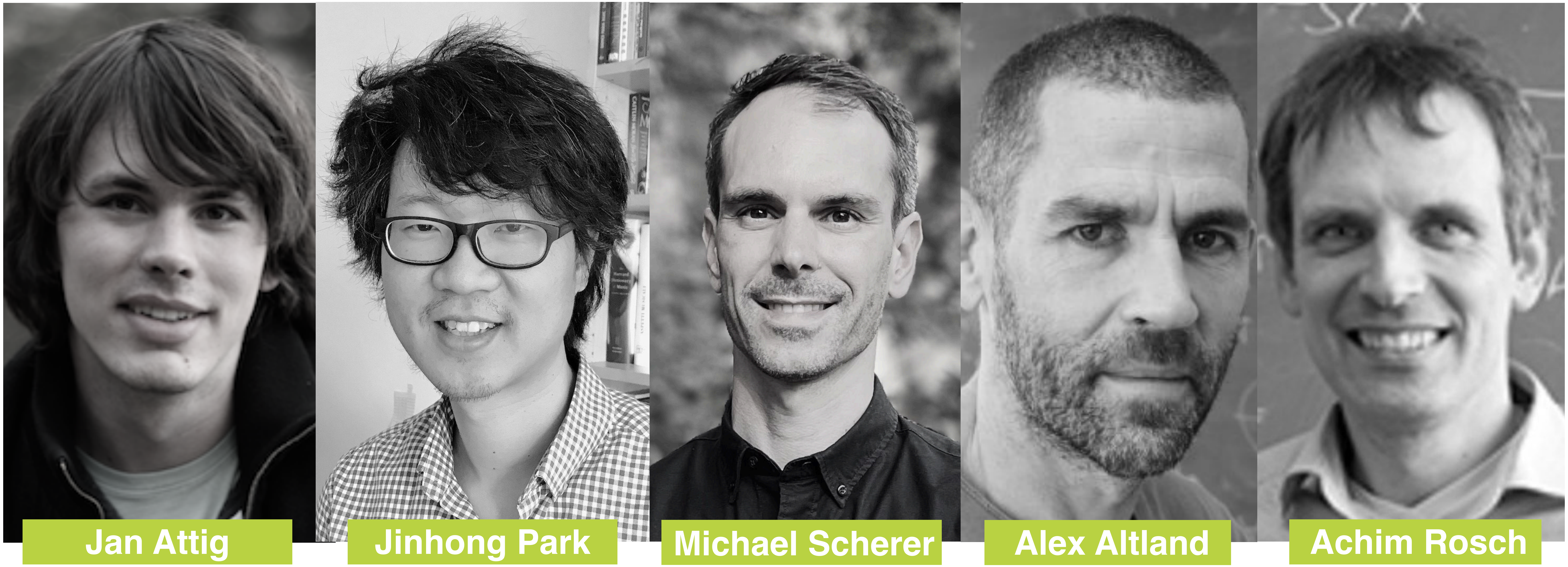
- flat bands natural or **“magic” needed ?**
- fate of all **the other 10^4 bands** ?
- what is **universally** valid ?



Cao et al., Nature (2018)

correlations & topology
in a *single* highly-tunable system

meet the team

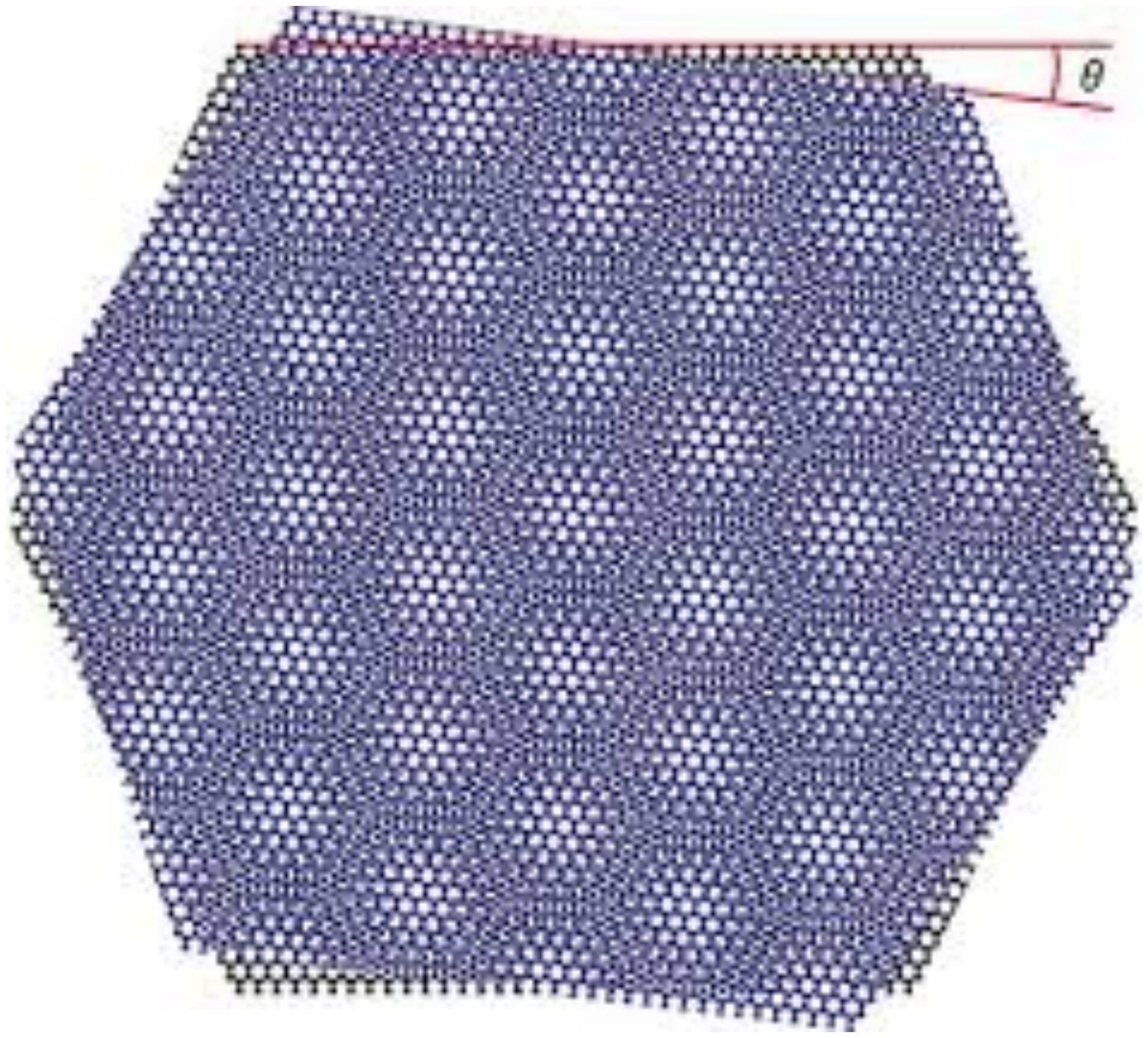


2D Materials **8**, 044007 (2021)

basic principles

lattice periodicity

- linear size of moiré unit cell $N \gg 1$
- reciprocal lattice vector $G_M \sim \dfrac{G}{N}$
- number of atoms = number of bands N^2
- moiré potential ⇒ effective **hopping in reciprocal space**



Anderson localization

- aperiodic site-to-site variations
- quantum disorder
- dimensional reduction (1D Fermi surfaces)
- **momentum space localization**

  ⇒ strong band dispersions

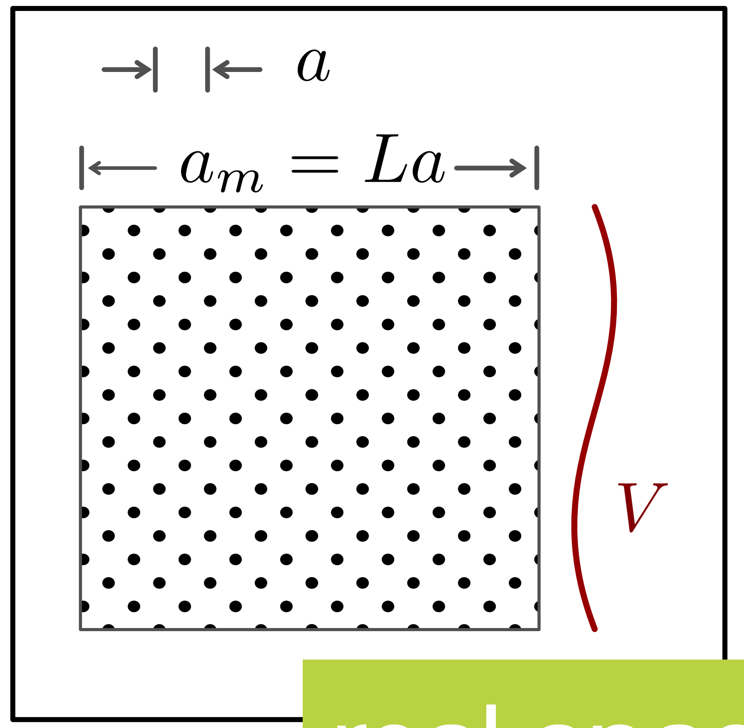
quantum chaos

- dimensional crossover 1D ⇒ quasi-2D
- **momentum space delocalization**
- ergodicity hampered

  by discrete lattice symmetries

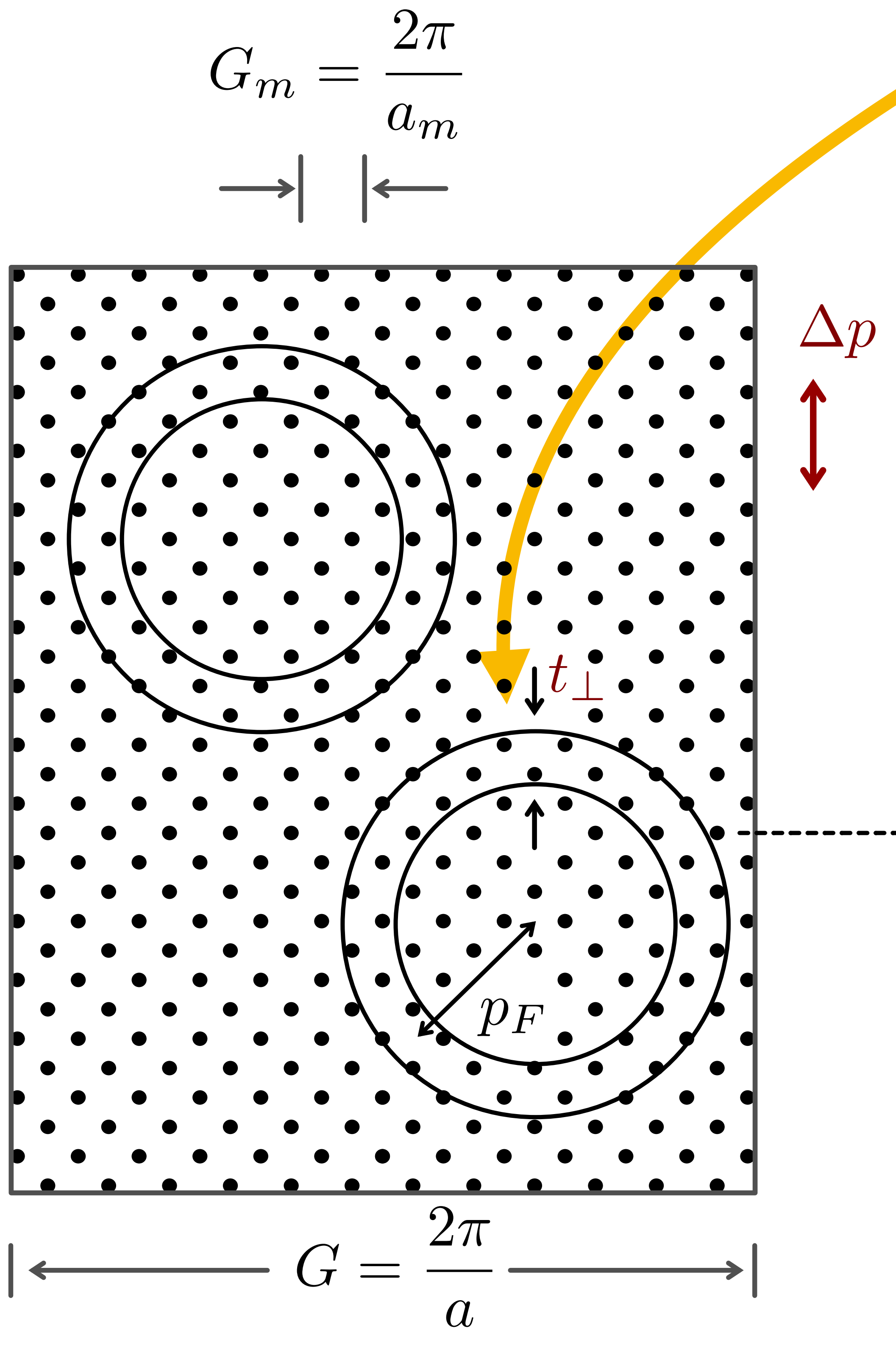
momentum space phenomenology

- 2D crystalline lattice subject to a **perturbation** *V* periodic over distances $N \gg 1$



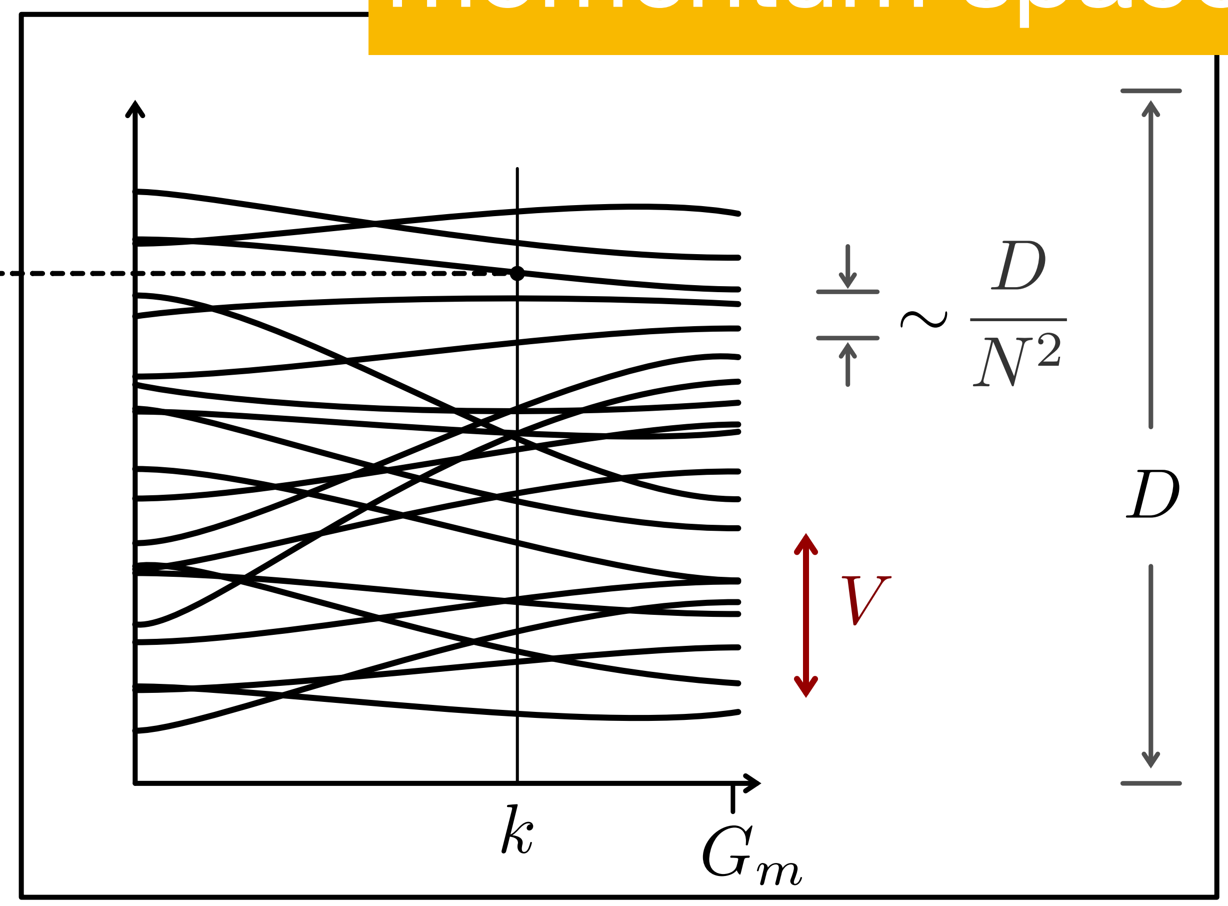
real space

- *V* defines periodic "**hopping potential**" in momentum space



- **quasi-1D Fermi surfaces** (of width $t_\perp$)
- effective **disorder**

momentum space



Anderson localization

numerical simulations

Jan Attig

real space

twisted bilayer graphene in real space
with parameters:

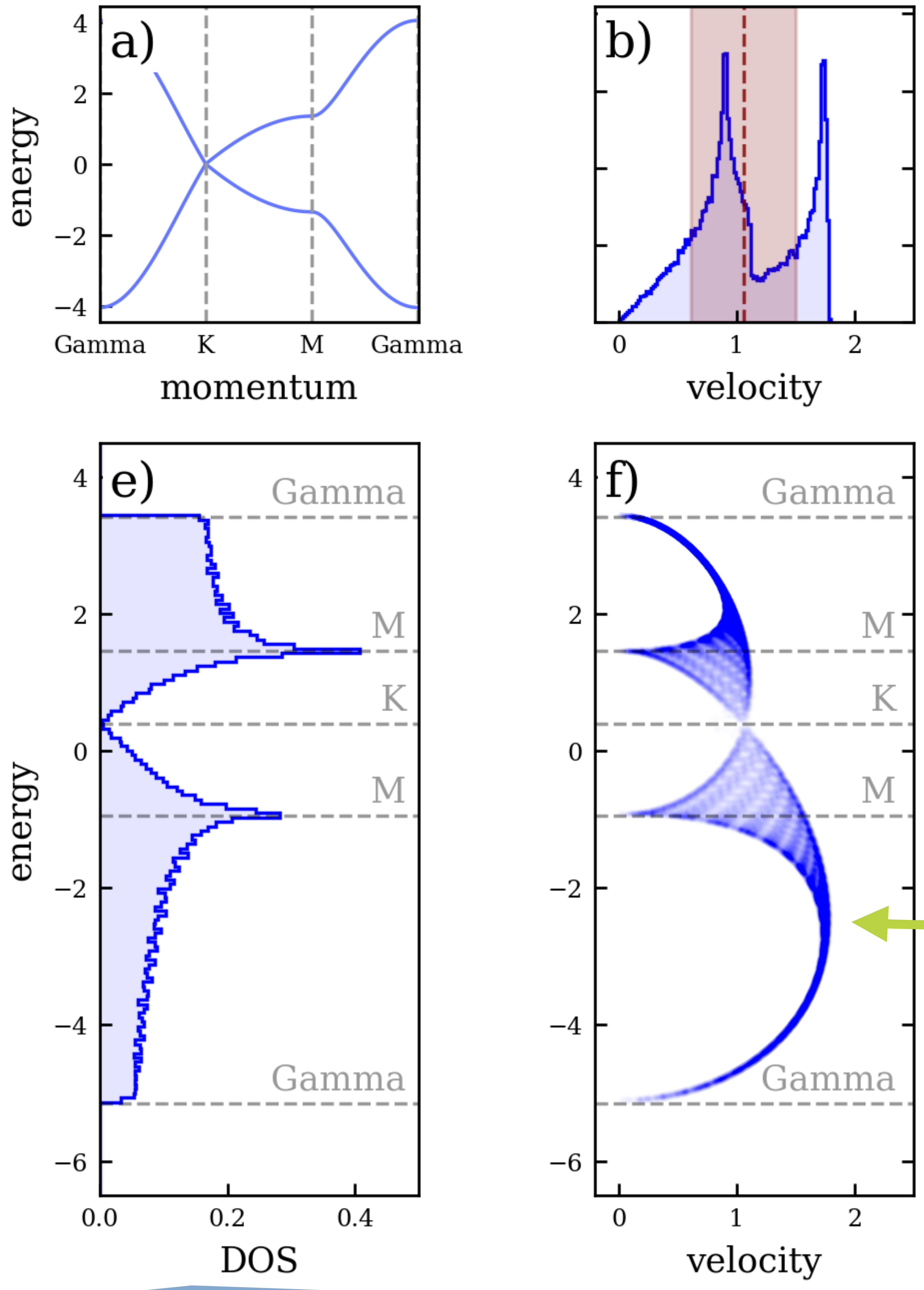
- twist angle
- distance of graphene layers
- strength of corrugation

momentum space

momentum space code
based on
continuum model

Jinhong Park

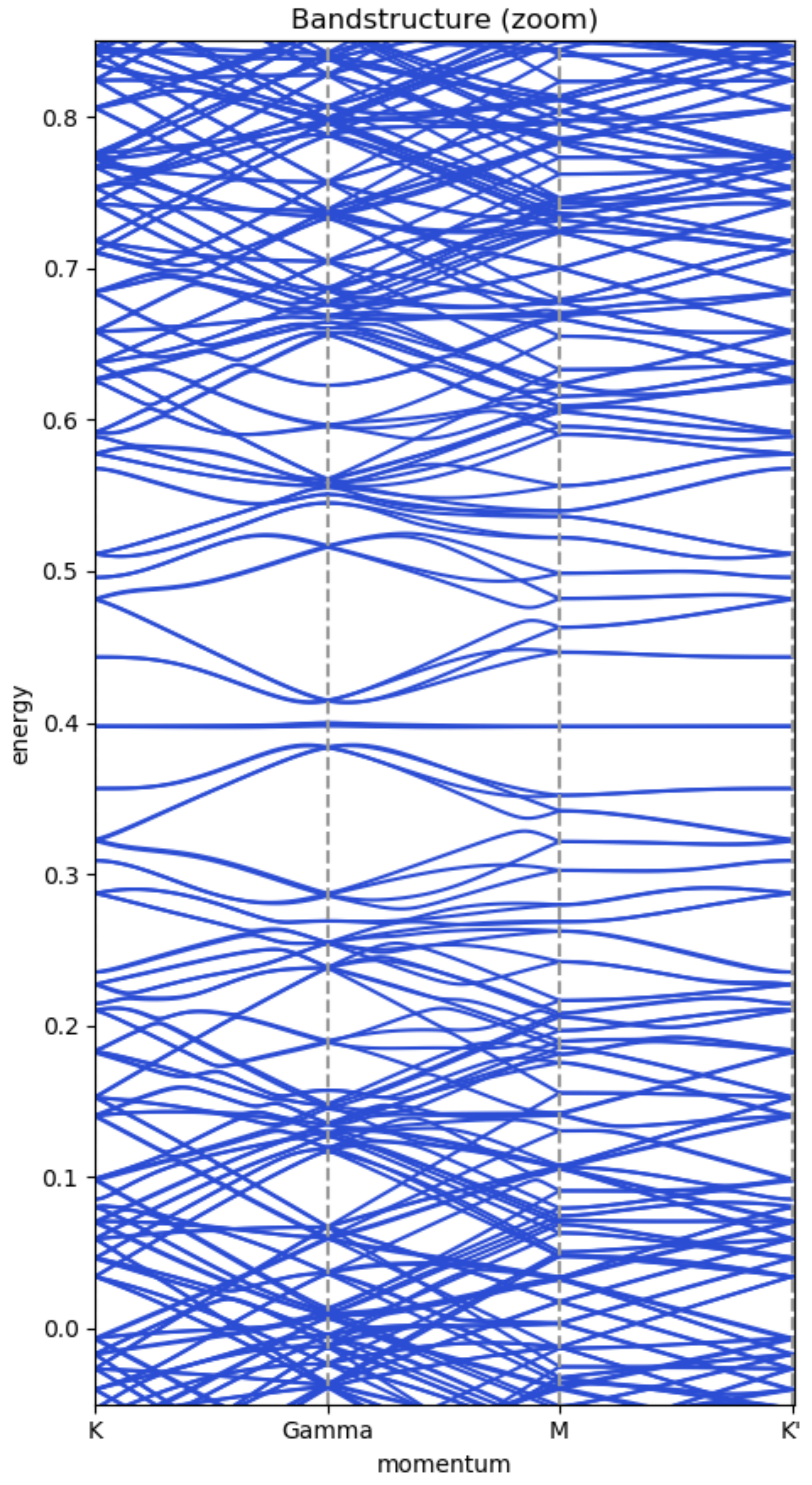
real-space numerical simulations



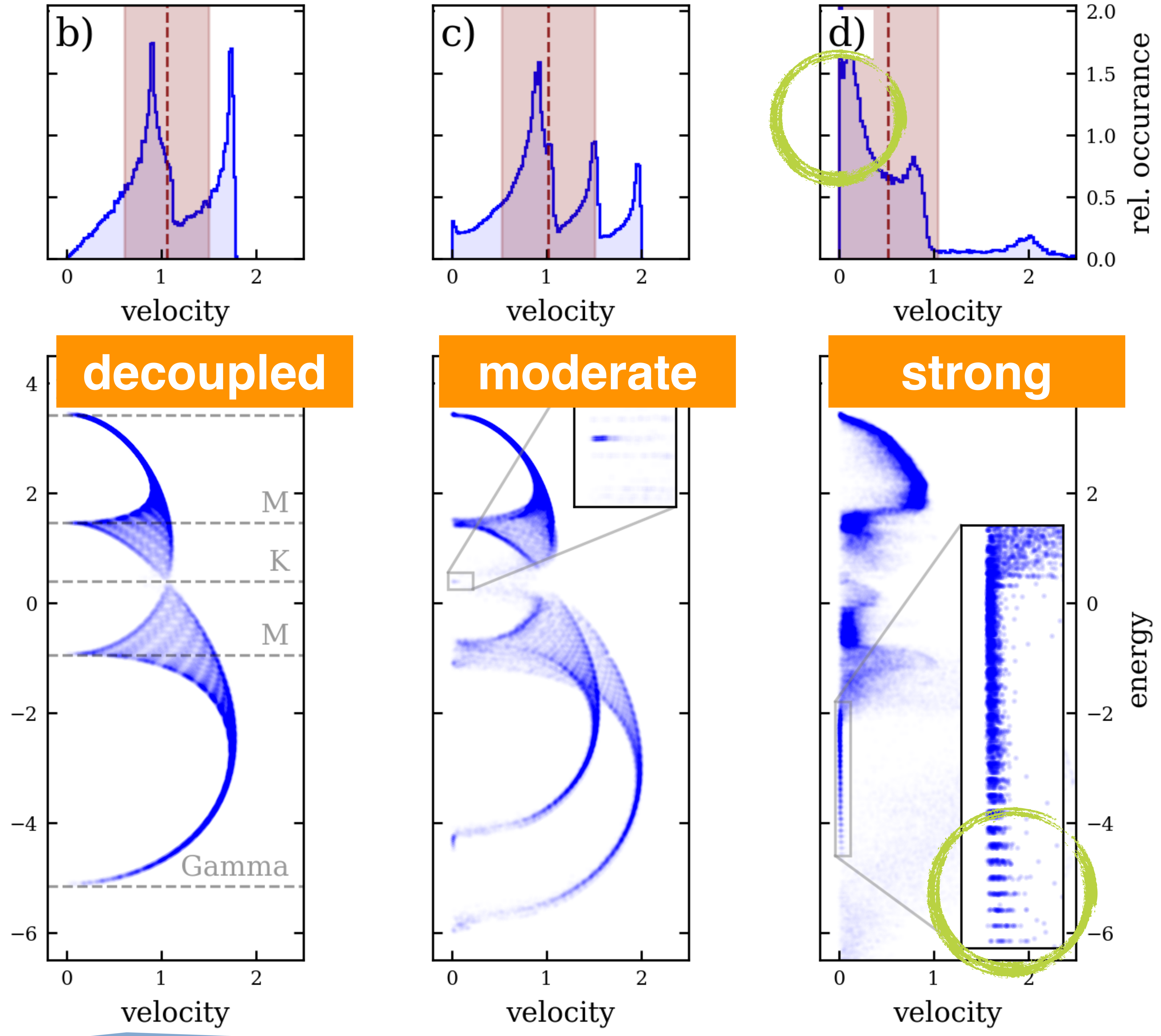
distribution of **velocities**

decoupled layers

“waterfall” plots

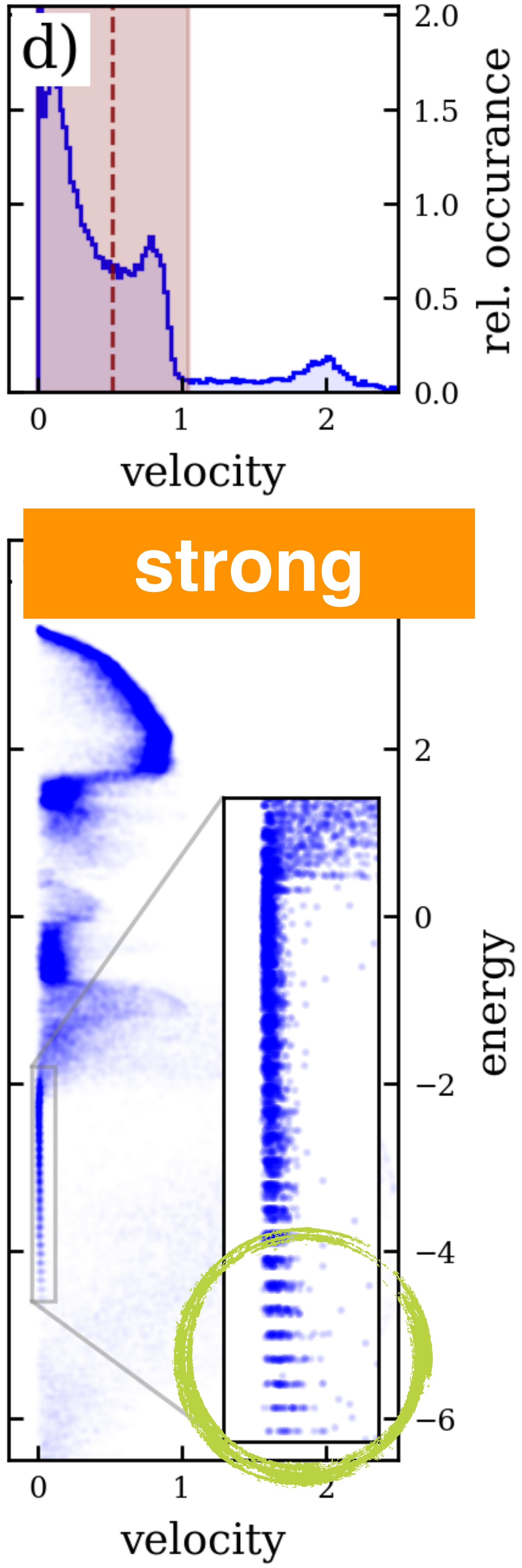


real-space numerical simulations

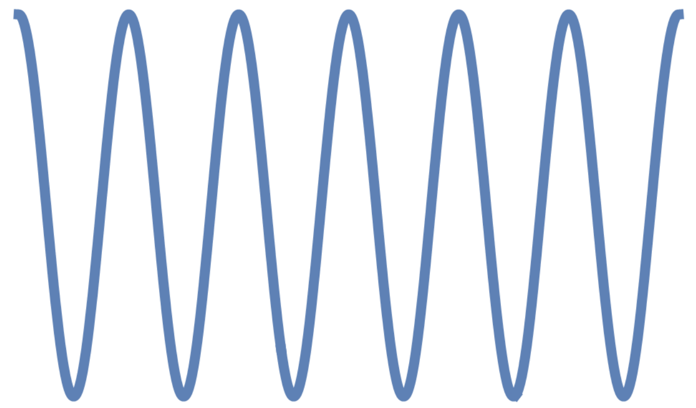


- **typical** velocities of **O(1)**, not O(1/*N*)
- **enhanced** probability for small v ?
- why are some regions unaffected ?
- **equally spaced**, very flat bands ?

real-space numerical simulations



- close to minimum/maximum of graphene band, map to tunnelling in a potential $t_\perp \cos(Q_M x)$



- potential is large

$$t_\perp \sim \frac{1}{\boldsymbol{N}} \gg \frac{Q_M^2}{2m} \sim \frac{1}{\boldsymbol{N}^2}$$

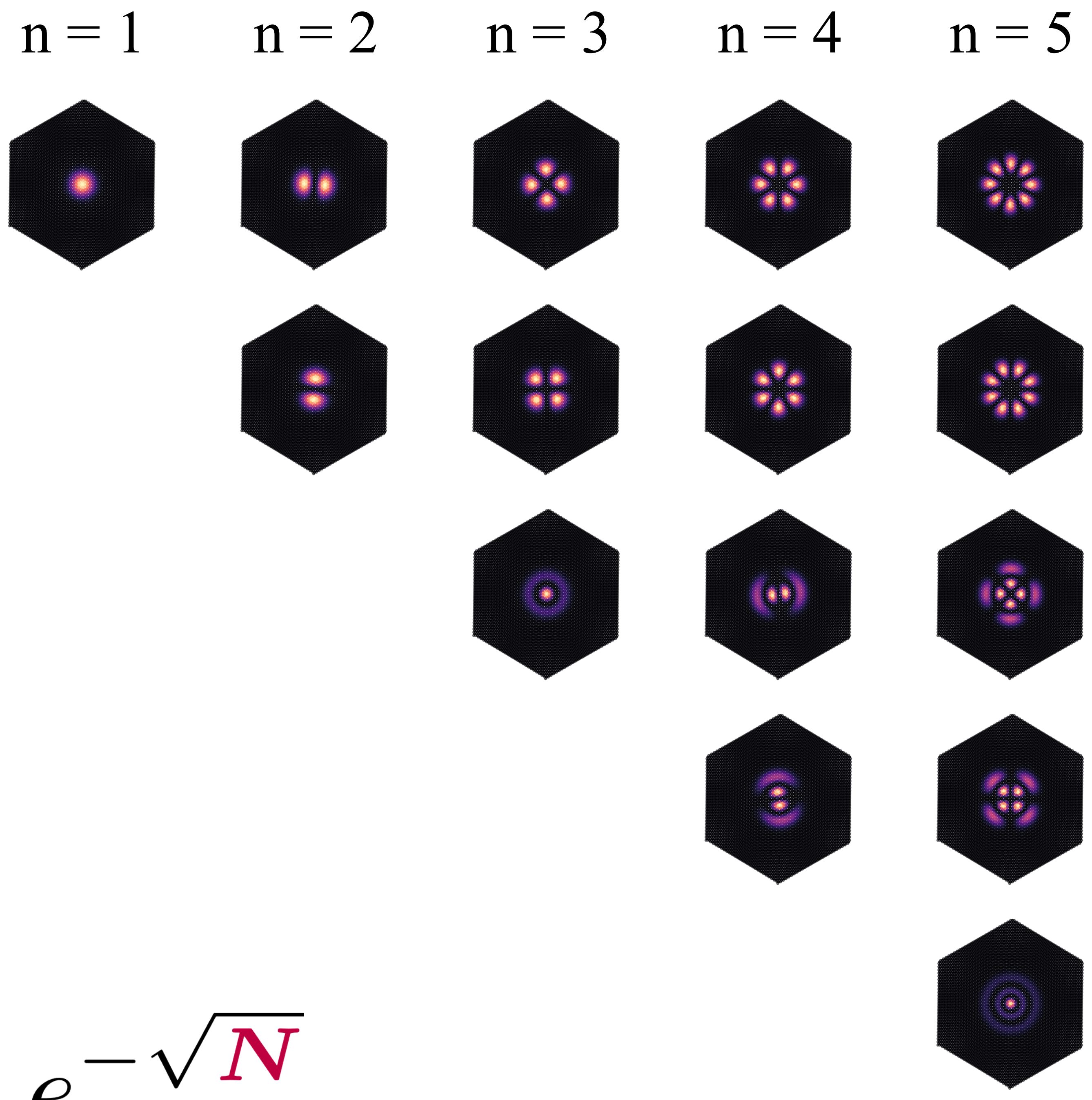
- harmonic oscillator spacing

$$\sqrt{\frac{t_\perp Q_M^2}{m}} \sim \frac{1}{\boldsymbol{N}^{3/2}} \gg \frac{1}{\boldsymbol{N}^2}$$

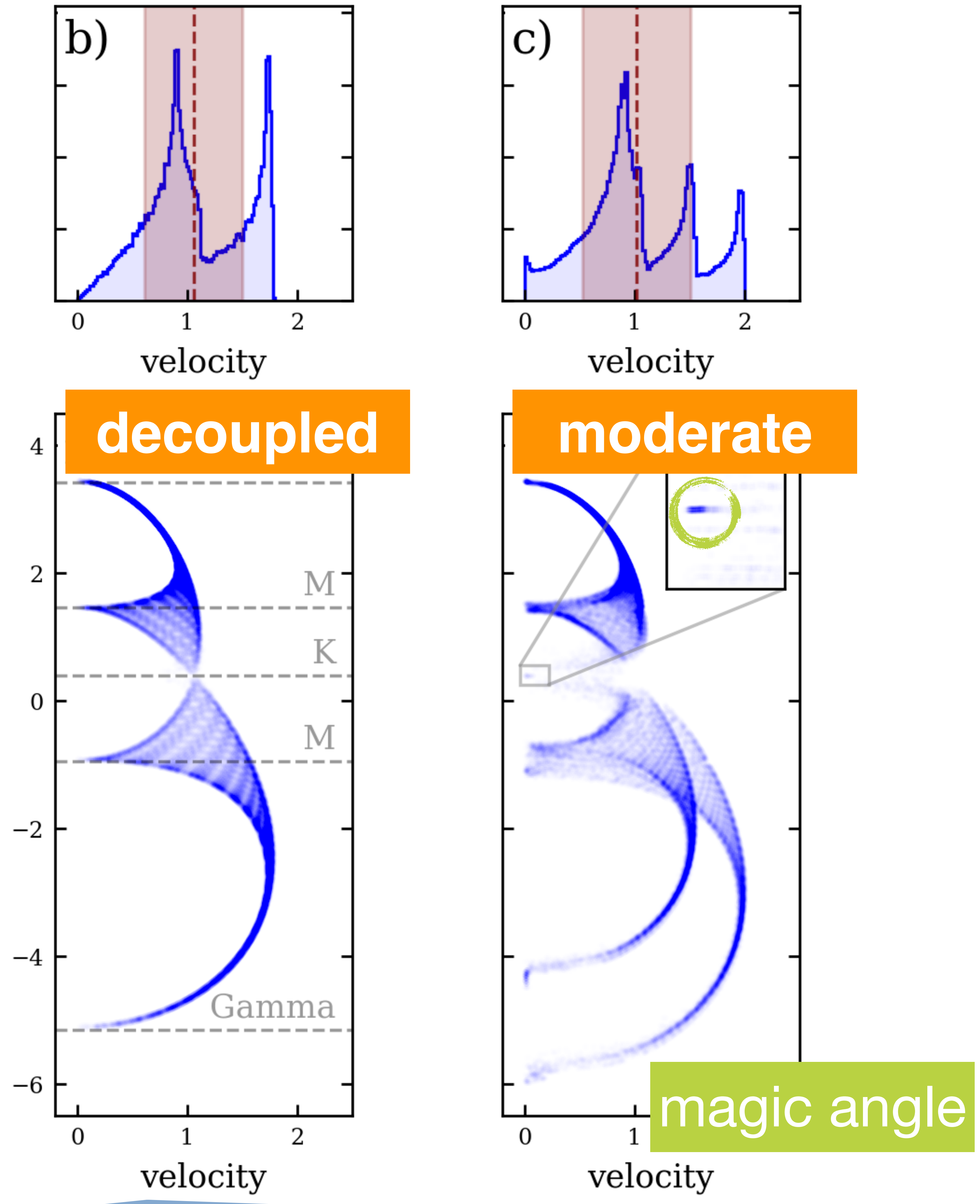
- exponentially small bandwidth

$$e^{-\sqrt{m t_\perp} Q_M} \sim e^{-\sqrt{\boldsymbol{N}}}$$

harmonic oscillator states



real-space numerical simulations



- Why is there **almost no effect** of tunnelling for most energies ?

momentum space localization

momentum-space dynamics

- **dynamics in momentum space:** lattice points spanned by reciprocal moiré lattice

- **tunnelling** between graphene layers
  or **scattering** from moiré potential

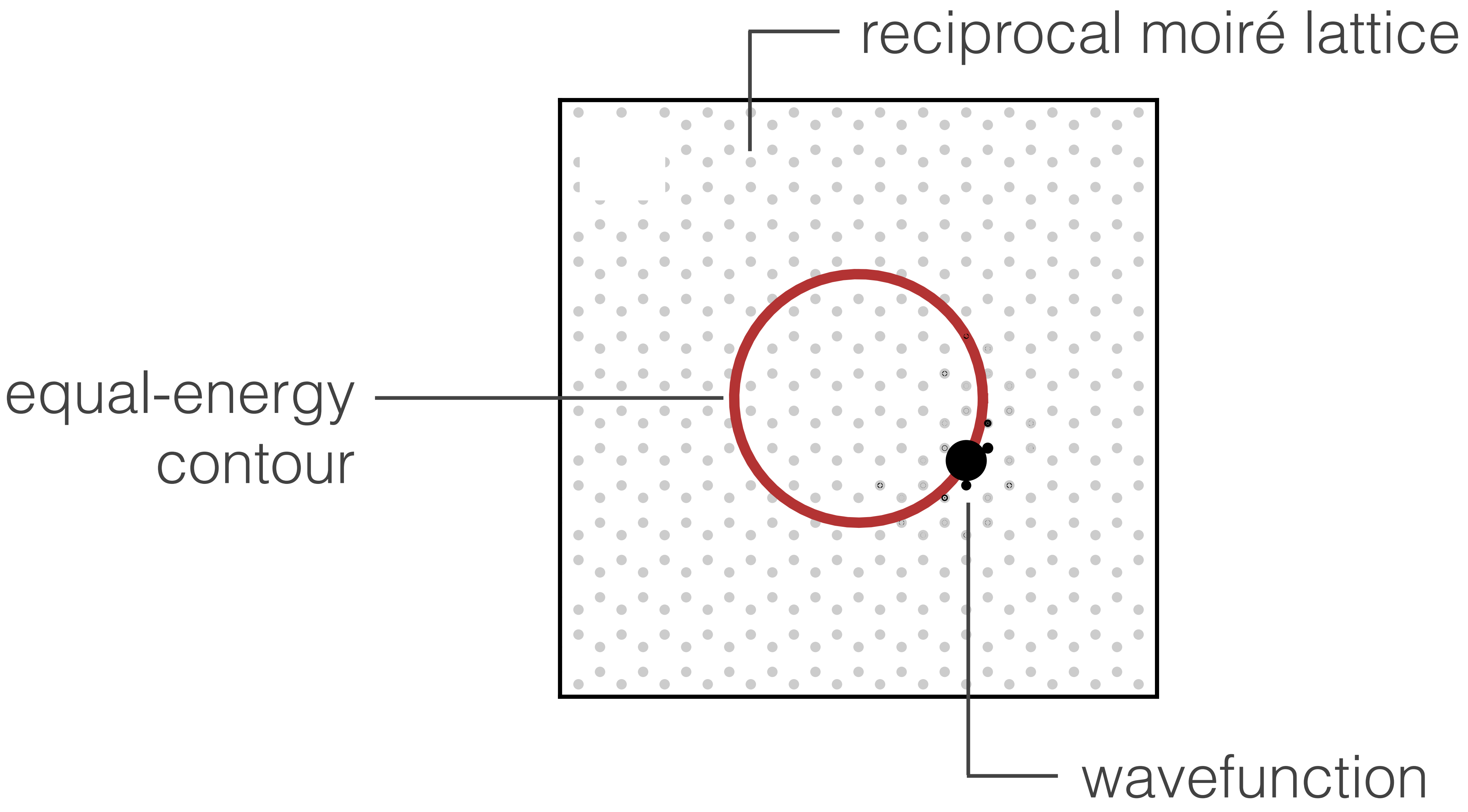
  hopping in reciprocal space

- graphene **band structure**

  potential term in k-space

- tunnelling along **equal-energy contours** (circles)

$$v_F|k| = E \pm t_\perp$$



momentum-space localization

Anderson localization

- **localization** by “effective disorder”

- localization **in 1D** highly efficient

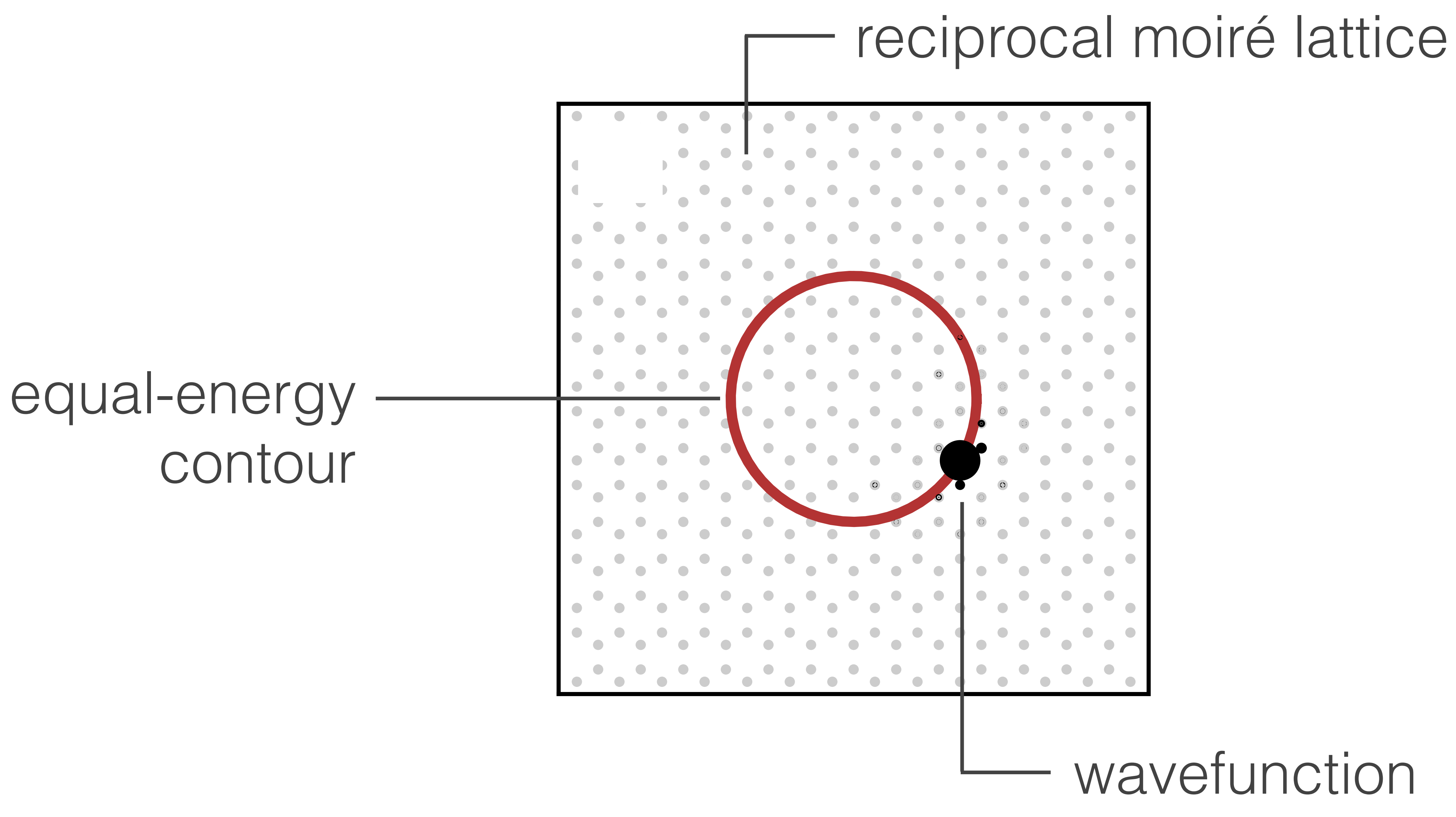
  why 1D?
  hopping along Fermi surface
  (equal-energy contour)

- localization **length**

  = mean-free path times # of channels

- **velocity**

  = weighted average of underlying Fermi velocities



localization in k-space

⇒ no level repulsion
high velocity

momentum-space localization

Anderson localization

- **localization** by “effective disorder”

- localization **in 1D** highly efficient

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  hopping along Fermi surface
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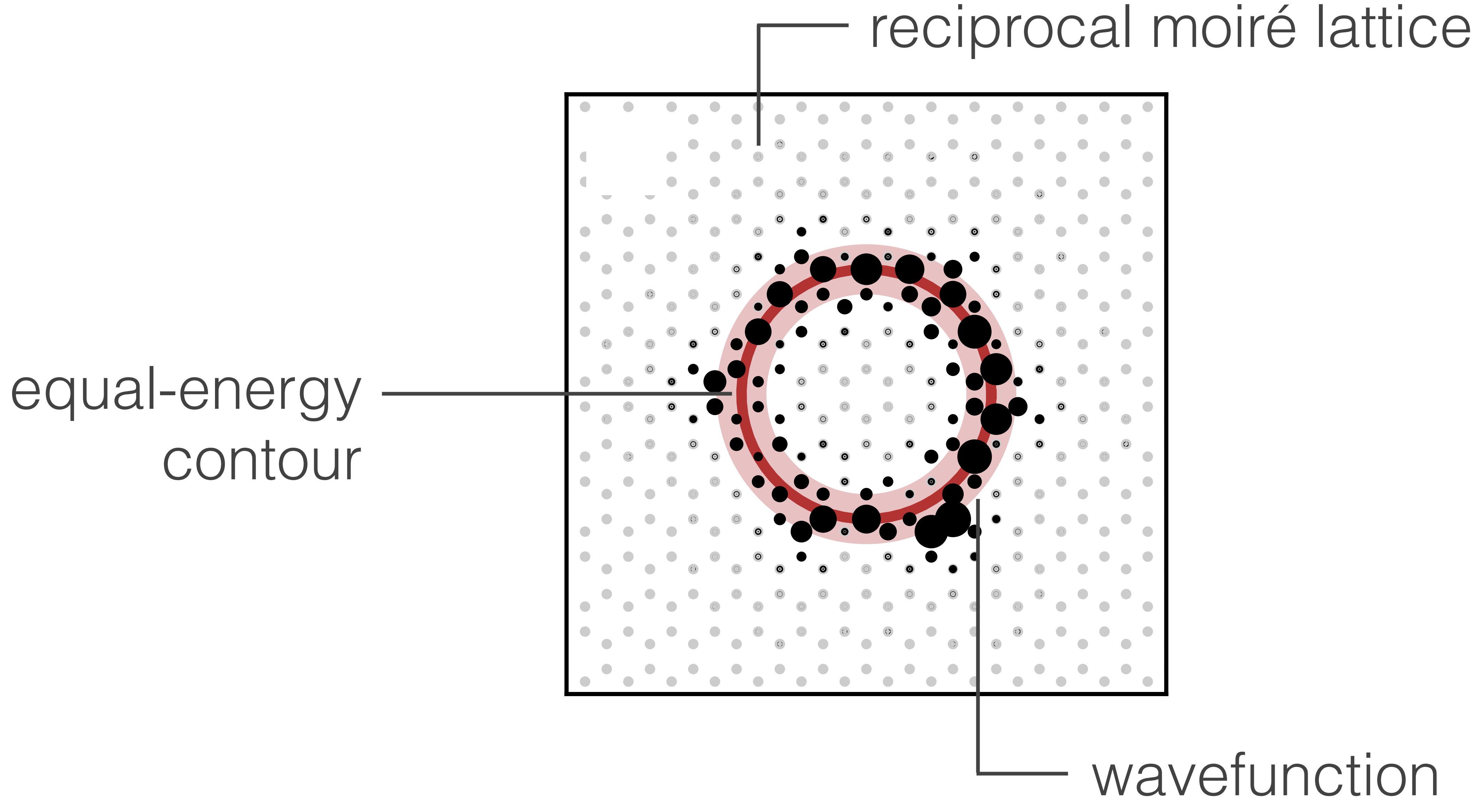
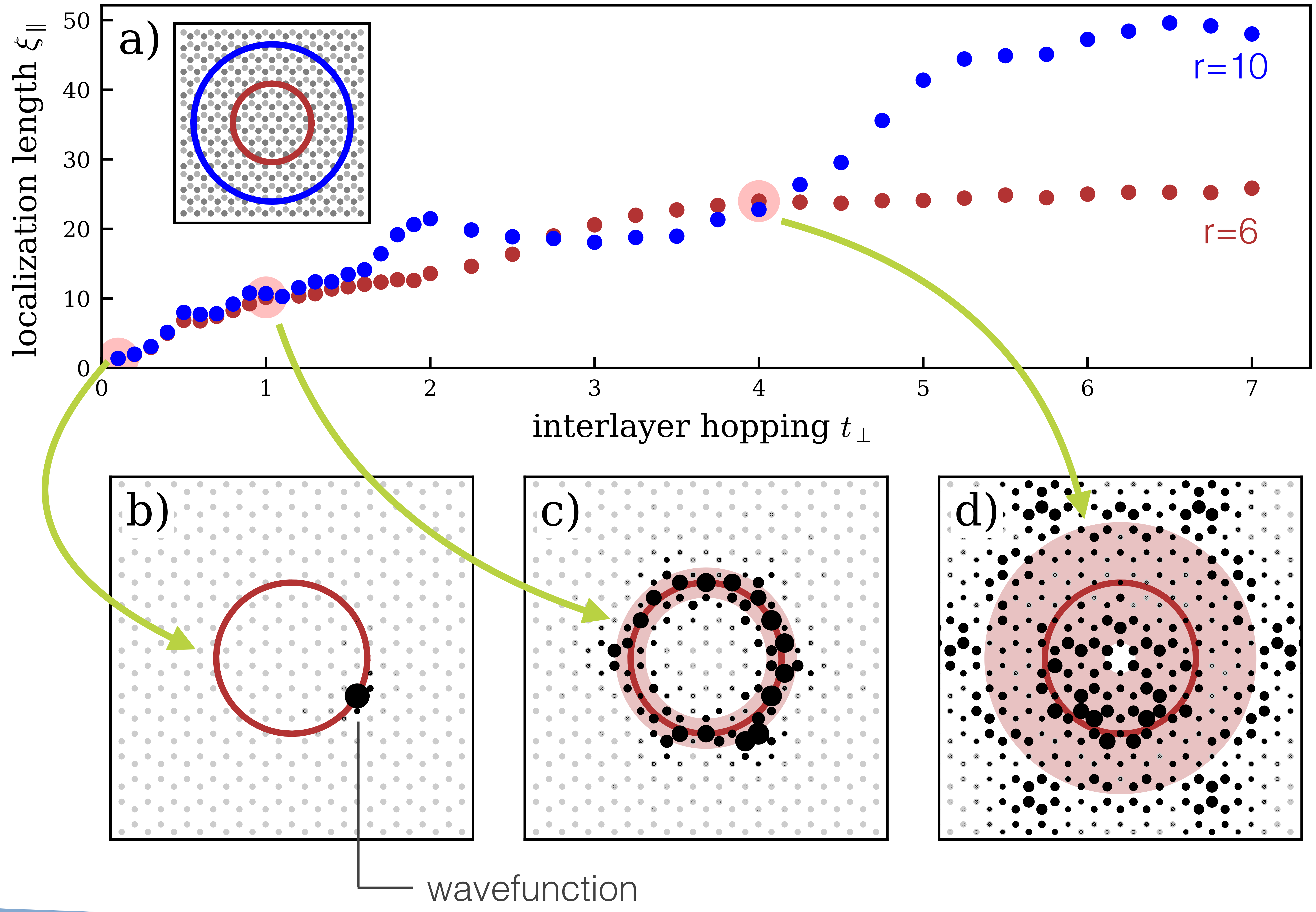


partial localization in k-space

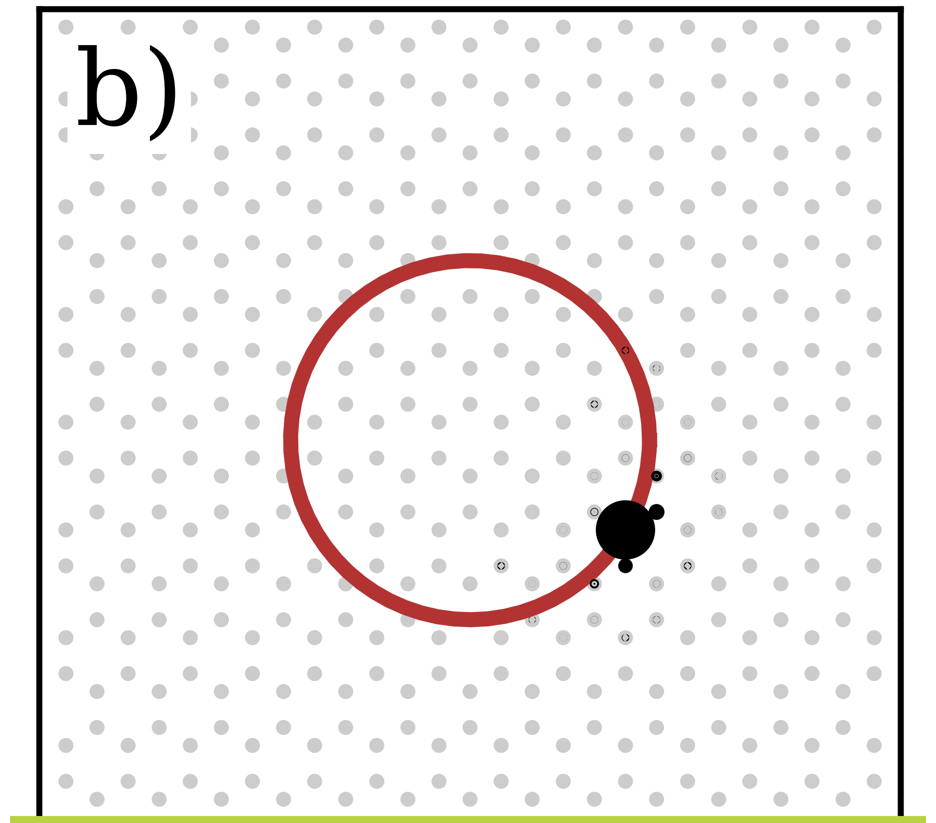
⇒ level repulsion
reduced velocity

momentum-space localization

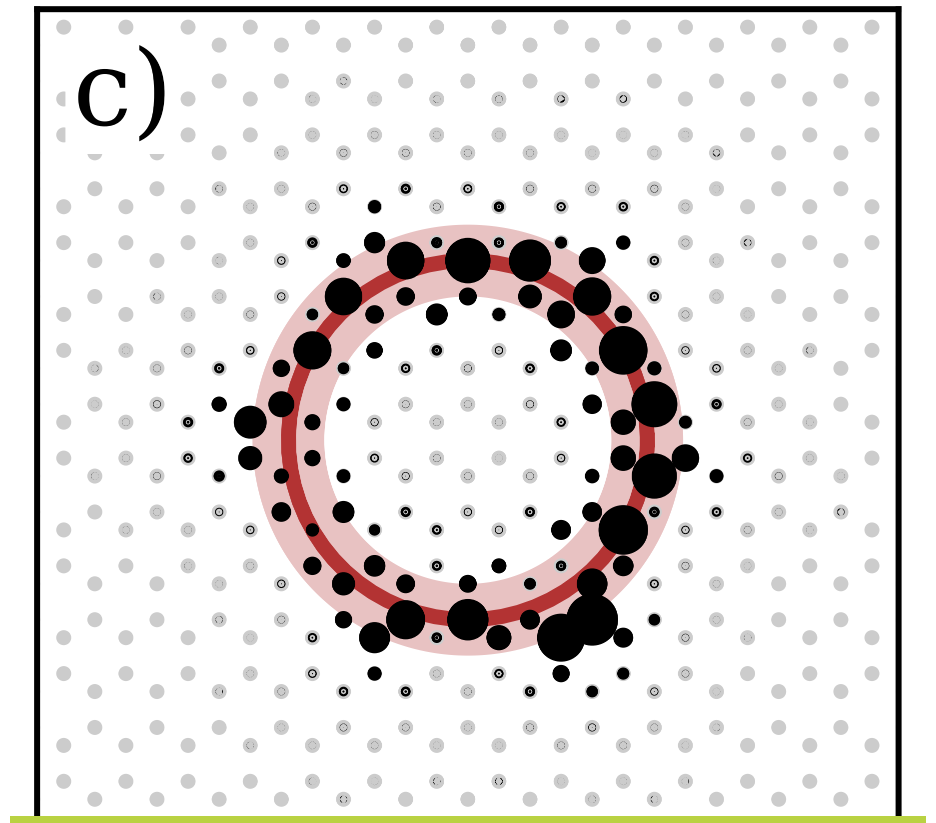


localization driven by **interlayer hopping**

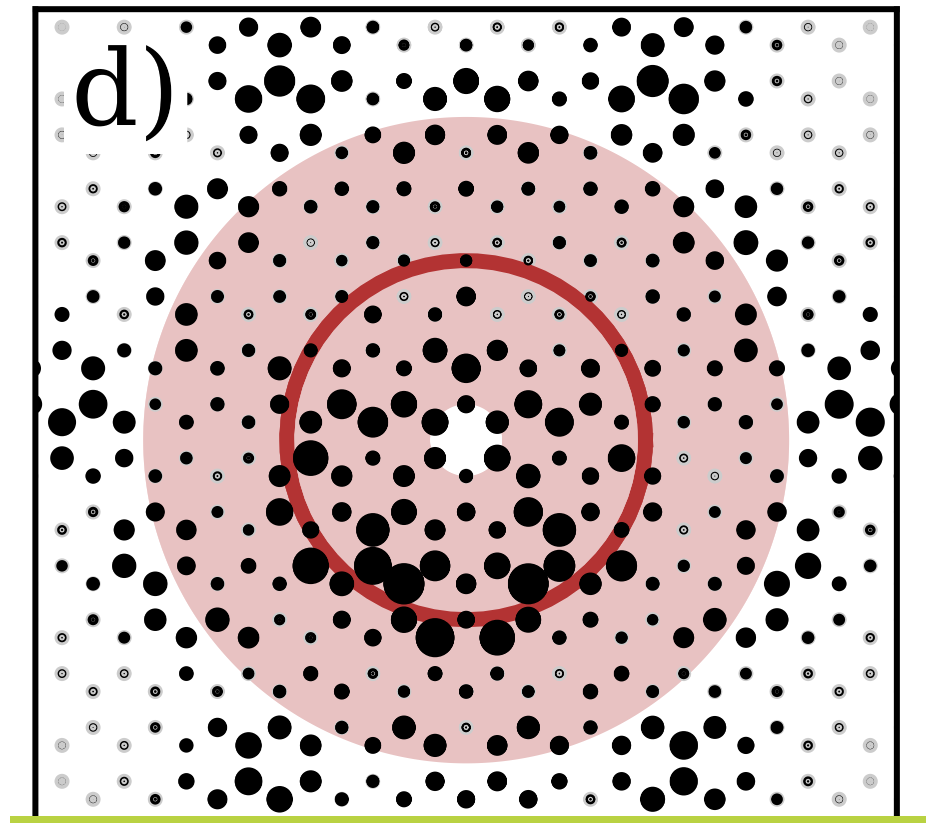
three localization regimes



deep localization

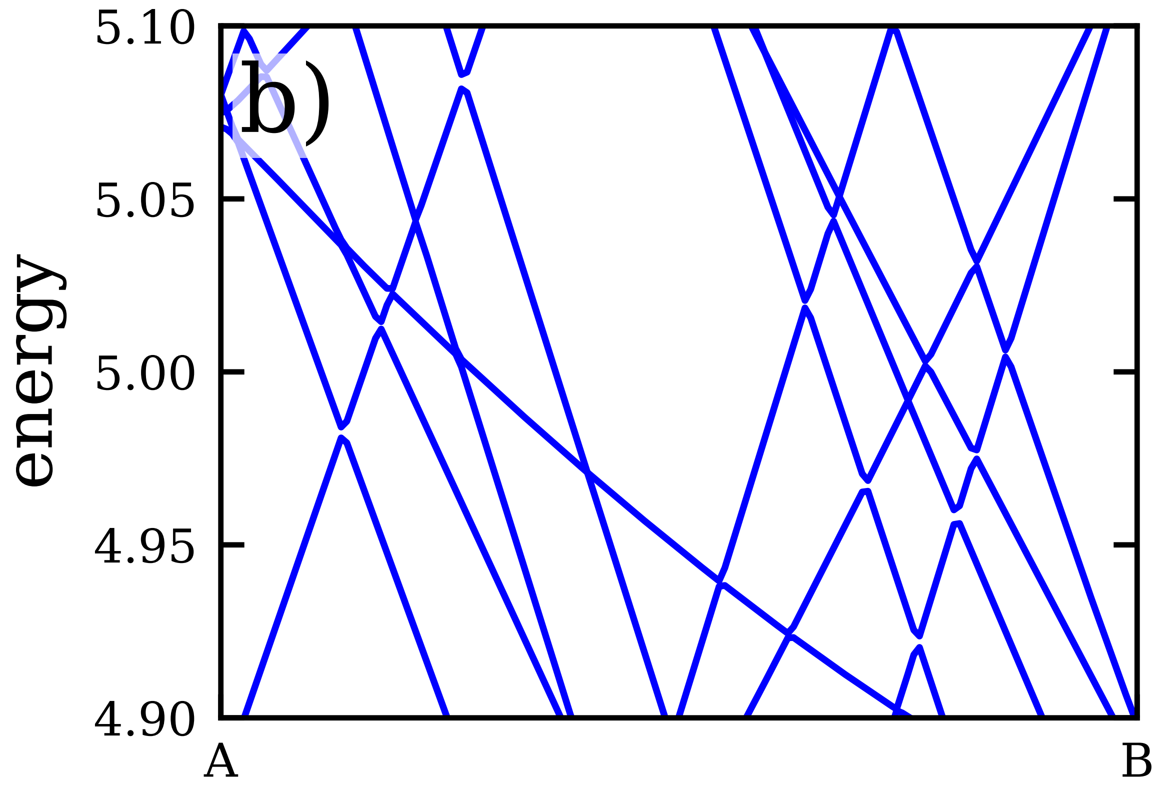


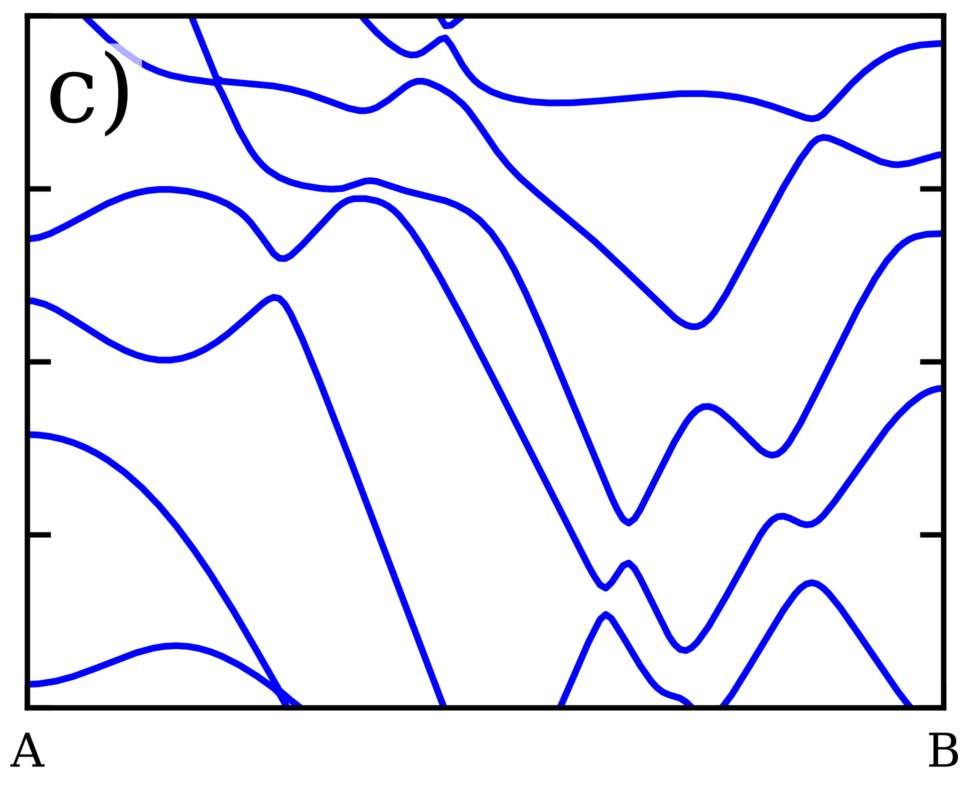
1D delocalization

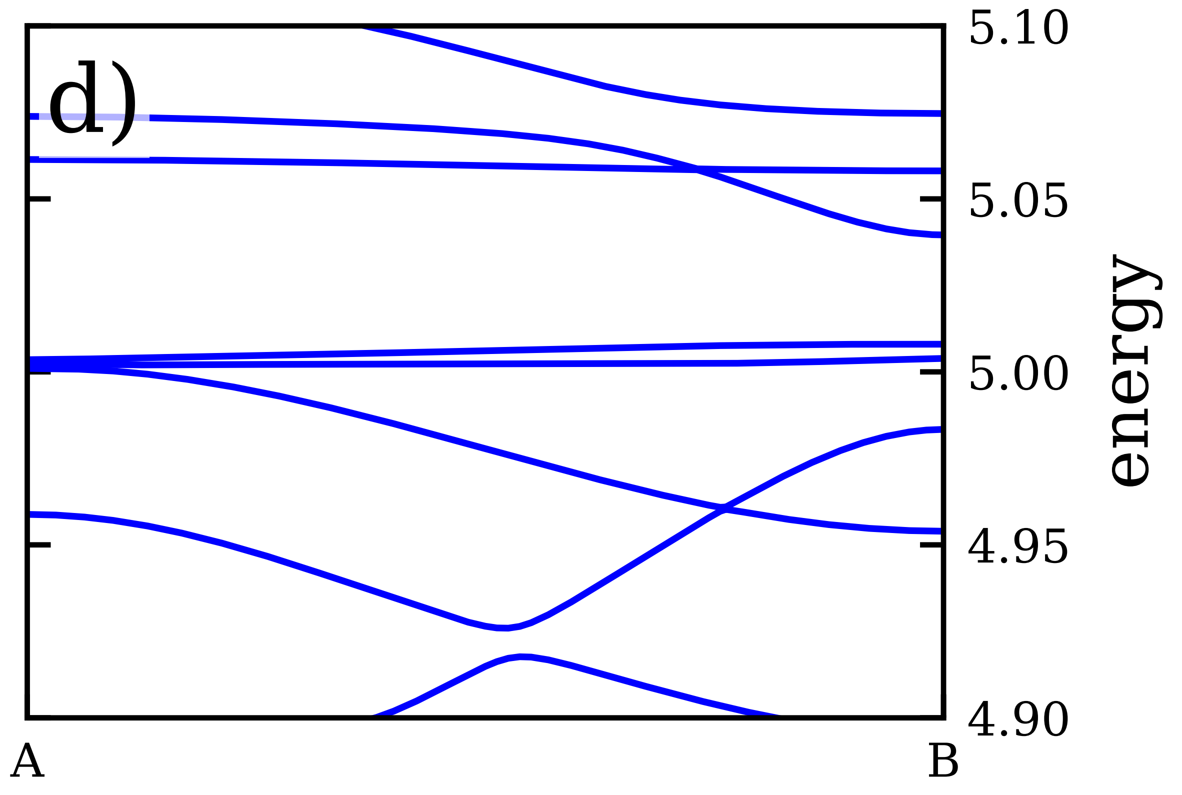


not ergodic!

strong coupling





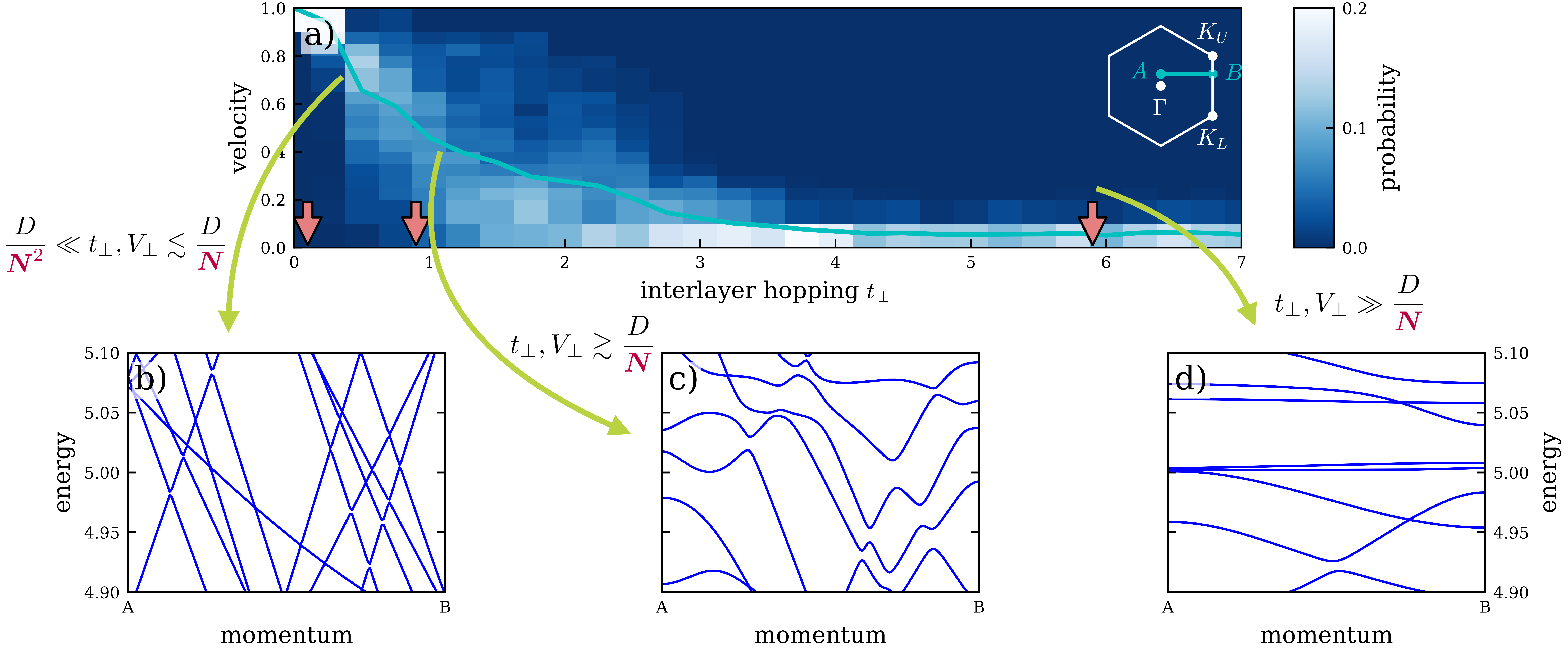


- **localization** in momentum space for incommensurate angles
- level repulsion exponentially small

- **delocalized** along circumference
- level repulsion substantial
- regions of high velocity prevails

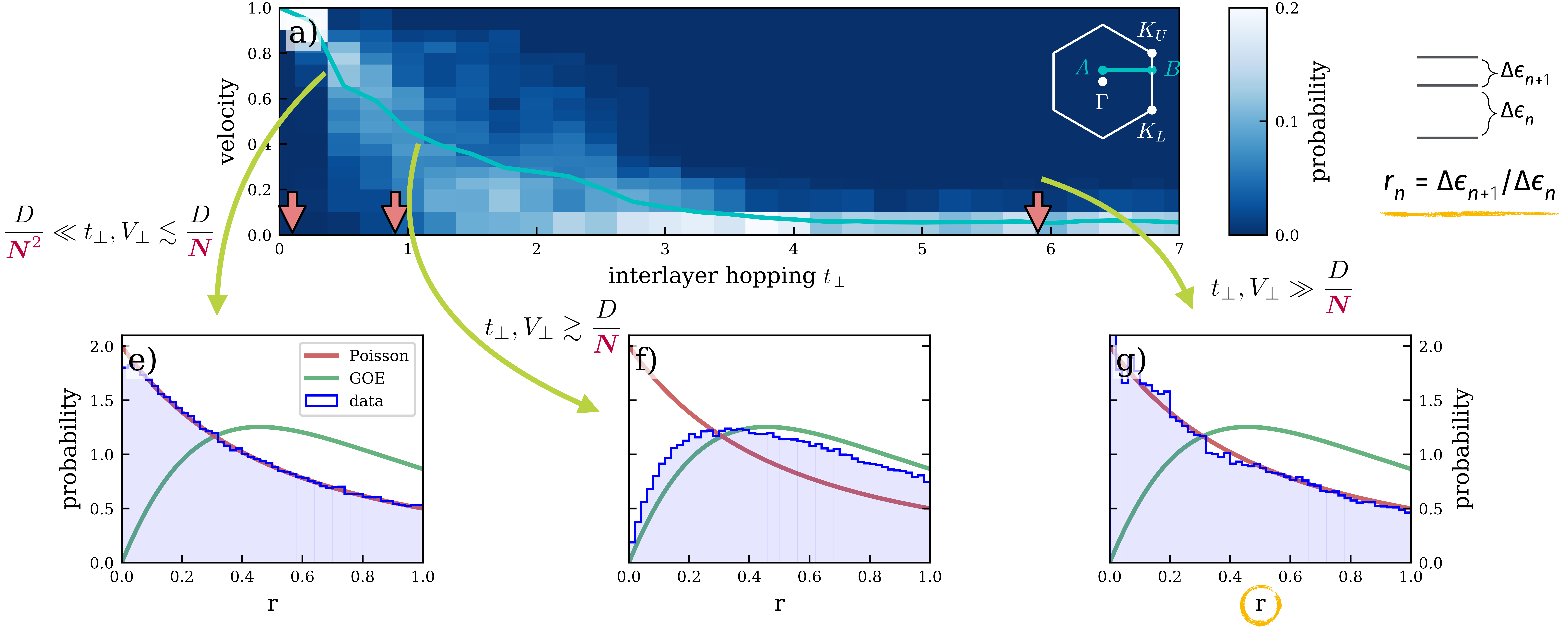
- **dimensional crossover**
- discrete symmetries become relevant
- small velocities prevail

spectral statistics



uncooked spaghetti **semi-cooked spaghetti** **cooked spaghetti**

spectral statistics



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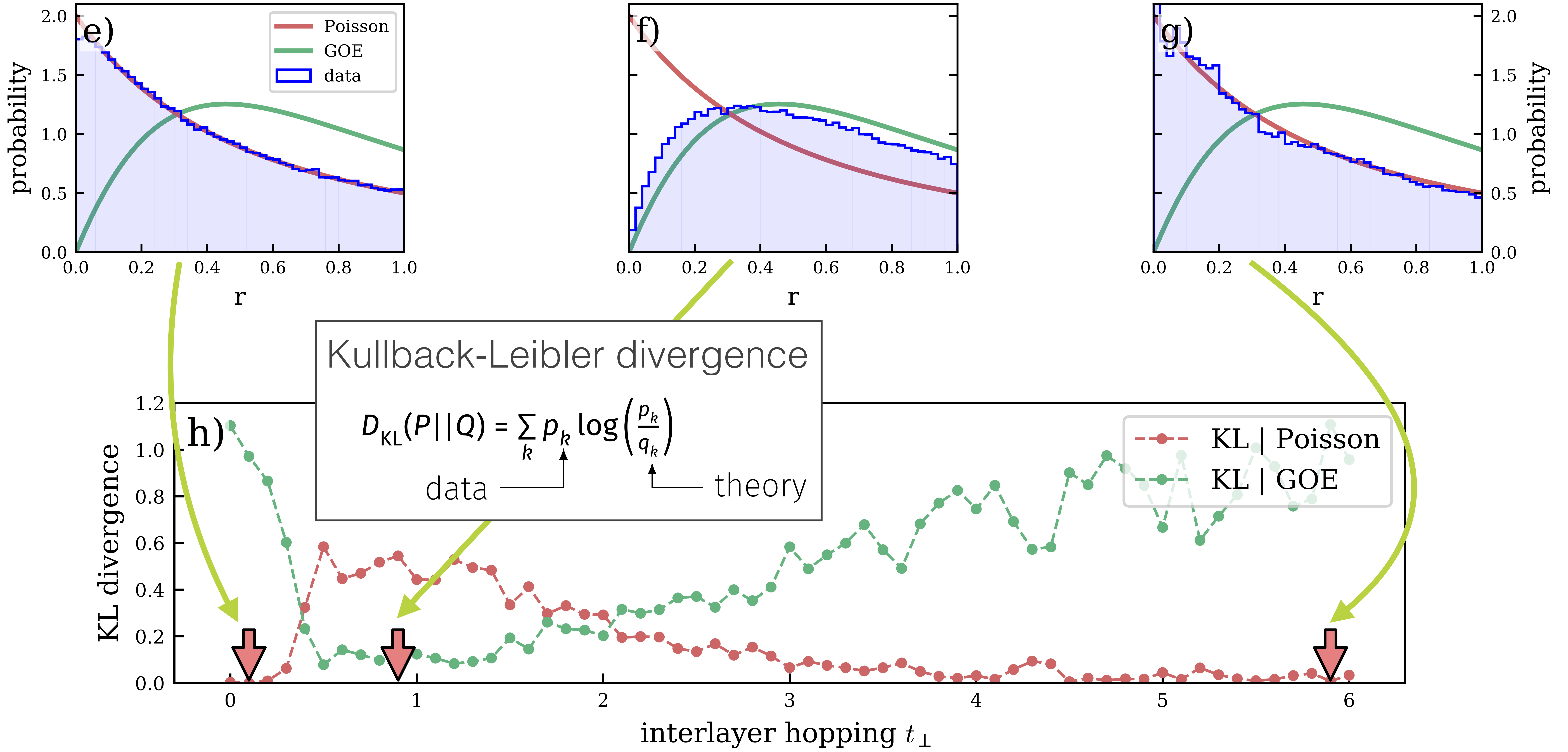


Kullback-Leibler divergence

$$D_{\mathrm{KL}}(P||Q) = \sum_k p_k \log\left(\frac{p_k}{q_k}\right)$$

data

theory

Where to go from here?

summary

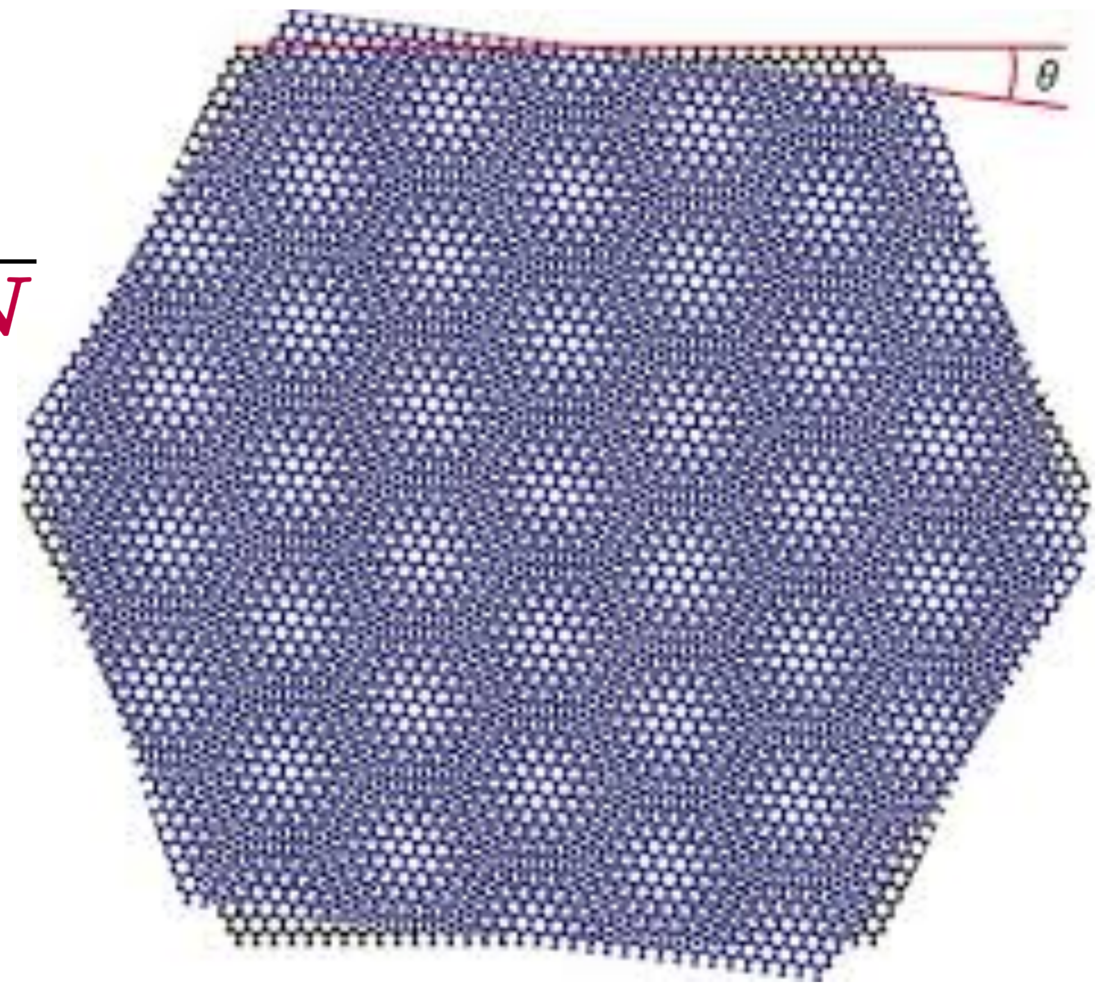
2D Materials **8**, 044007 (2021)

Take-away messages

- **typical band** in generic moiré system: **not flat**, but velocities of O(1)
- reason – **localization in momentum space** along **1D** Fermi surface

three localization regimes:
deep localization, 1D delocalization, strong coupling

- **exceptions** to the rule:
  - close to **minima/maxima** of unperturbed bands expect bandwidth $e^{-\sqrt{N}}$
  - at **magic points** (derived from Dirac points of graphene)



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