

Tight-Binding Models and continuous Schrödinger operators in magnetic fields

mSPACE

Bocconi University, Milan



Simon Becker (Bocconi University)

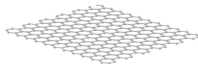
March 16, 2026

Motivation: Graphene and bilayer graphene

graphite



graphene



MacGyver in the physics lab



Scotch tape



piece of graphite



Nobel prize
2010

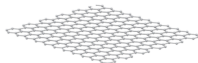
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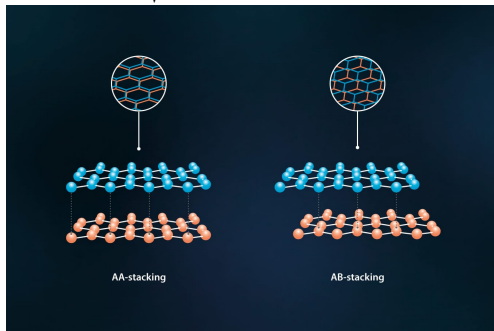
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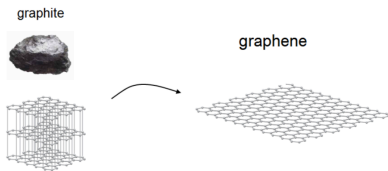
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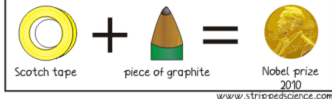
$$\updownarrow 3.4\text{\AA} \leftrightarrow 1.86\text{\AA}$$



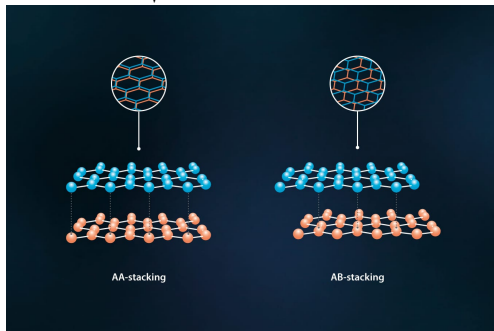
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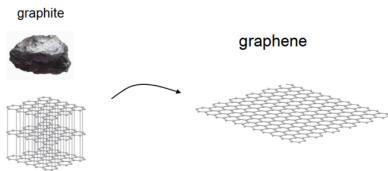


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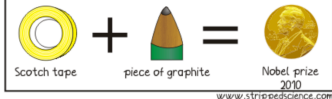


BE:11.5 vs.17.7 meV; Mostaani et al (2015).

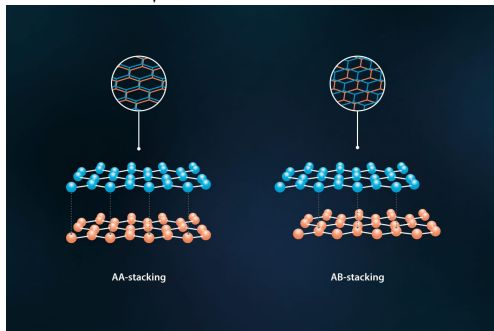
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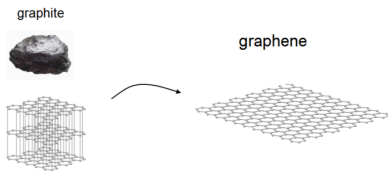


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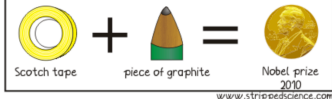


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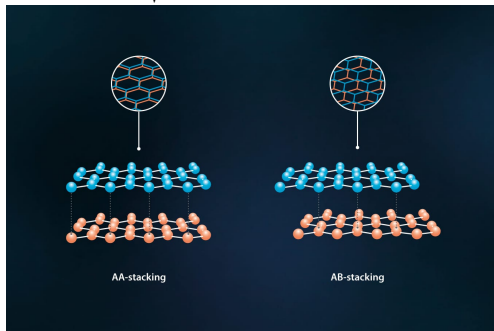
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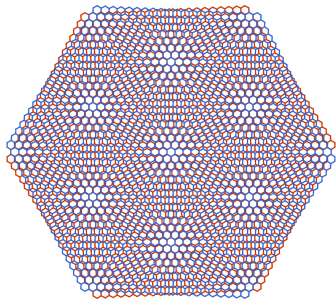


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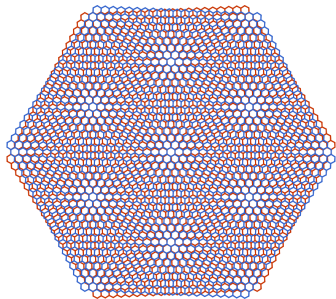


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Motivation: Twisted moiré materials

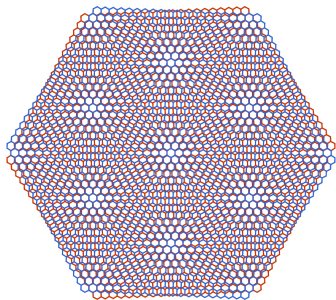


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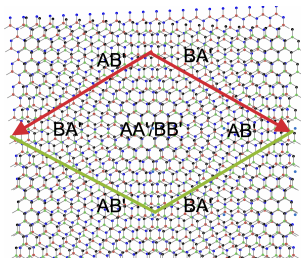


Moiré fundamental cell scales $\propto 1/\theta$.

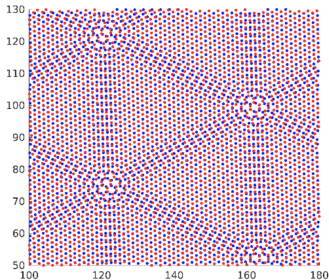
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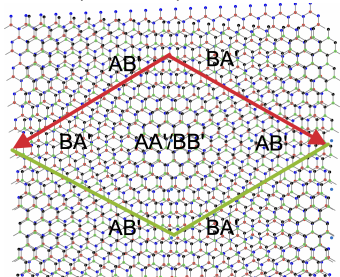
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Motivation: Twisted moiré materials are not inherently quasi-periodic, but periodic with large cells



Moiré fundamental cell scales $\propto 1/\theta$; Relaxation works by Carr, Kaxiras, Luskin, Massatt et al.



The Bistritzer-MacDonald Hamiltonian

The two main ground material types are semimetals (e.g. graphene) and semiconductors (e.g. WSe_2).

The Bistritzer-MacDonald Hamiltonian ('11,..) is given by

$$H_{\text{BM}} = \underbrace{H_0(D_x)}_{\text{Decoupled layers}} + \underbrace{V(\theta x)}_{\text{Coupling}}.$$

Substituting $\theta x \rightarrow x$ leads to a semiclassical operator with $\hbar = \theta$

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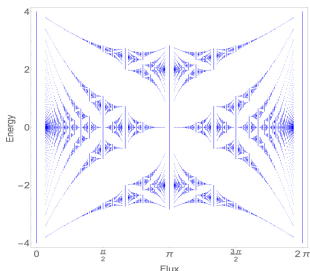
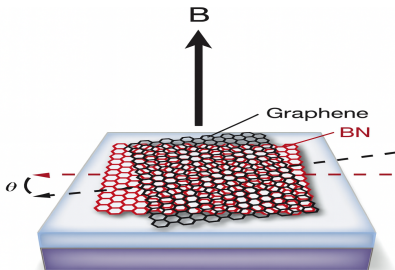
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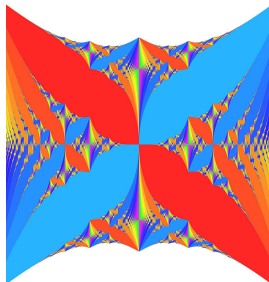
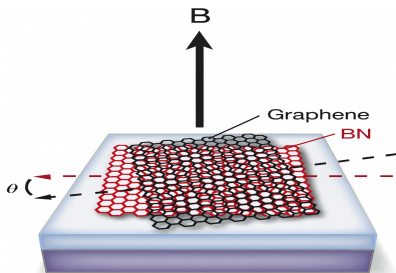
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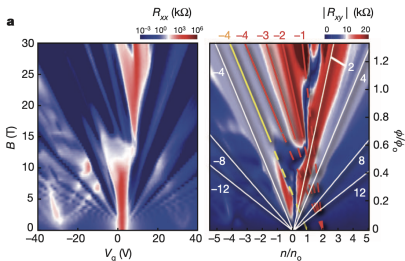
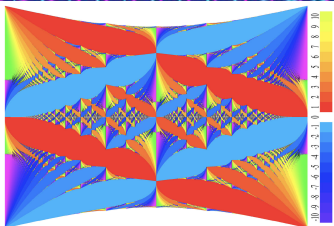
The Bistritzer-MacDonald Hamiltonian ('11,..) is an effective Hamiltonian

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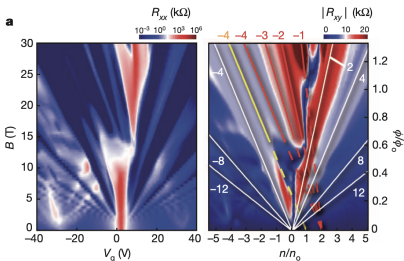
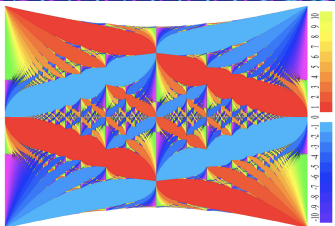


Agazzi et al (left); Dean et al '12. (right)

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The Hamiltonian

We consider a two-dimensional magnetic Schrödinger operator H_V with constant magnetic field $B = \partial_2 A_1 - \partial_1 A_2$, with $A(x) = Bx_1 e_2$ and a real-valued periodic potential $V \in C^\infty(\mathbb{R}^2/\Gamma_\mu)$ with

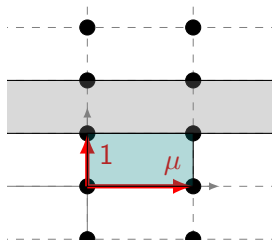
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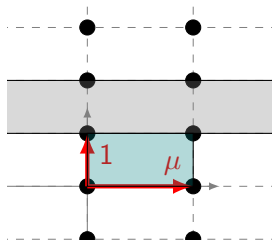
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Using $x \rightarrow x + e_2$ periodicity, the Bloch transform \mathcal{U}_c yields

$$\mathcal{U}_c H_V \mathcal{U}_c^{-1} = \int_{\mathbb{T}^*}^\oplus H_k dk; \quad H_k = h^2 D_{x_1}^2 + (h(D_{x_2} + k) - Bx_1)^2 + V(x).$$

How to see the (in)commensurability?

For $H_V = (-ih\nabla - A)^2 + V$, let

$$T_1 u(x) = e^{i\mu B x_2/h} u(x - \mu e_1) = e^{2\pi i \gamma x_2} u(x - \mu e_1) \text{ and } T_2 u(x) = u(x - e_2),$$

with $e_1 = (1, 0)$, $e_2 = (0, 1)$, and $\gamma := \mu B / (2\pi h)$. Then

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For $H_{V,k} = (-ih\nabla + hke_2 - A)^2 + V$, we introduce the regular translations $Tv(x) = v(x - \mu e_1)$ and observe that (H_k) is an ergodic family

$$TH_k = H_{k+2\pi\gamma} T.$$

We also observe that all $H_{k+2\pi\mathbb{Z}}$ are equivalent by

$$e^{-2\pi i n x_2} H_k e^{2\pi i n x_2} = H_{k+2\pi n},$$

where $x_2 \mapsto e^{2\pi i n x_2}$ is a unitary multiplication operator on $L^2(\mathbb{R}/\mathbb{Z})$.

Tight-binding reduction

To reduce the spectral analysis to a discrete operator, one starts by *filling the wells*. By this, we mean that one defines for $\alpha \in \mathbb{Z}^2$

$$H_V(\alpha) := H_V + \sum_{\beta \in \Gamma_\mu \setminus \{0\}} \theta(\bullet + \alpha_1 \mu \mathbf{e}_1 + \alpha_2 \mathbf{e}_2 + \beta).$$

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We take the eigenfunctions $(e_\alpha)_{\alpha \in \mathbb{Z}^2}$ associated with the lowest eigenvalue of $H_V(\alpha)$. We can project $v_\alpha := P e_\alpha := \mathbf{1}_I(H_V) e_\alpha$ and use Gram-Schmidt to find an orthonormal basis (φ_α) .

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$$H_V \text{ Proj} = \sum_{\alpha, \beta \in \mathbb{Z}^2} w_{\alpha, \beta} (\varphi_\alpha \otimes \varphi_\beta) \text{ with } w_{\alpha, \beta} := \langle H_V \varphi_\beta, \varphi_\alpha \rangle_{L^2(\mathbb{R}^2)}$$

with $w_{\alpha, \beta} = \mathcal{O}(e^{-|\alpha - \beta|/h})$.

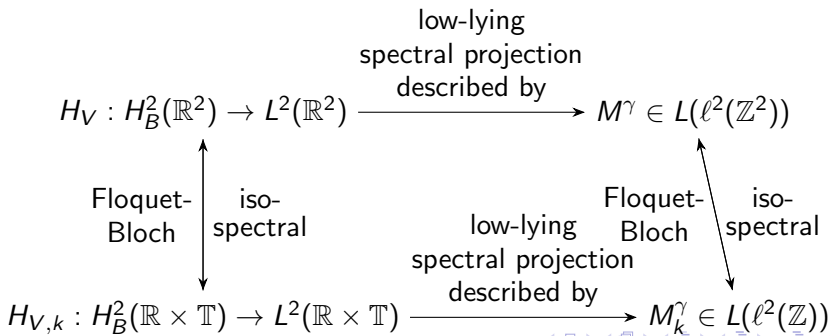
The gDML is the discrete operator $M^\gamma : \ell^2(\mathbb{Z}^2) \rightarrow \ell^2(\mathbb{Z}^2)$

$$M^\gamma u(\alpha) := \sum_{\beta \in \mathbb{Z}^2} w_{\alpha, \beta} u(\beta).$$

A similar Bloch reduction that allowed us to go from H_V to $H_{k, V}$ allows us to reduce M^γ to a one-dimensional operator with

$$f_\beta := w_{0, \beta}$$

$$M_k^\gamma u(n_1) = \sum_{\beta_1 \in \mathbb{Z}} v_{\beta_1}(k - 2\pi n_1 \gamma) u(n_1 + \beta_1) \text{ with } v_{\beta_1}(x) = \sum_{\beta_2 \in \mathbb{Z}} f_{\beta_2} e^{i\beta_2 x}.$$



Nearest-neighbour approximation

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The nearest neighbour approximations of the operators M^γ and M_k^γ are the discrete magnetic Laplacian $\text{DML} \in L(\ell^2(\mathbb{Z}))$

$$(\text{DML } \psi)_\alpha = \psi_{\alpha+e_1} + \psi_{\alpha-e_1} + \lambda (e^{2\pi i \gamma \alpha_1} \psi_{\alpha+e_2} + e^{-2\pi i \gamma \alpha_1} \psi_{\alpha-e_2})$$

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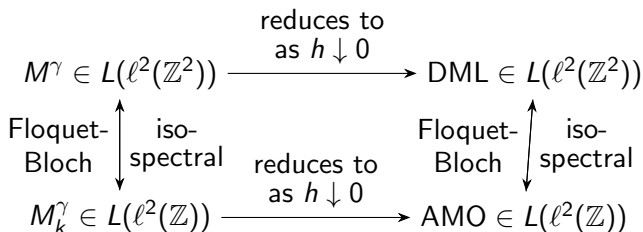
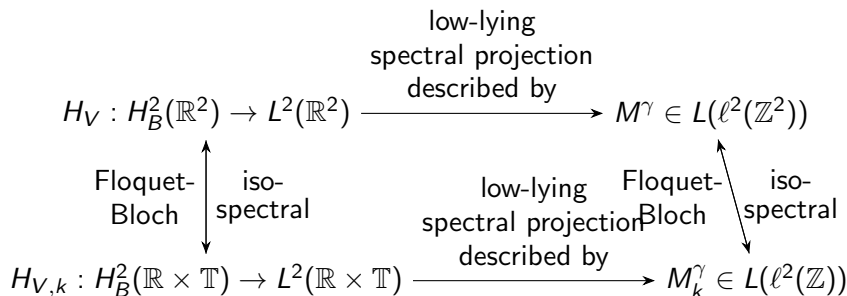
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and the AMO family $\text{AMO} \in L(\ell^2(\mathbb{Z}))$ with

$$(\text{AMO } \psi)_{k,n} = \psi_{n+1} + \psi_{n-1} + 2\lambda \cos(2\pi \gamma n + k) \psi_n$$

for $k \in \mathbb{R}/(2\pi\mathbb{Z})$.

Tight-binding reduction



Spectral convergence properties of continuum models

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In addition,

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- ▶ **B-Ge-Jitomirskaya'26:** *The same holds by changing μ in the continuum for low energies, $h > 0$ small, and $H_{k,v}$.*

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We studied the limit from continuous magnetic operators in the plane to discrete graphs and showed that spectral properties are preserved.

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- ▶ Part 1: How is mechanical strain correctly included in quantum graphs? - How do spectral properties change upon "straining"?
- ▶ Part 2: What happens for high energies in the continuum model

$$H_V = \hbar^2 D_{x_1}^2 + (\hbar D_{x_2} - Bx_1)^2 + V?$$

Summary & Open questions

We studied the limit from continuous magnetic operators in the plane to discrete graphs and showed that spectral properties are preserved.

- ▶ Part 1: Are there interesting quantum graph model for twisted materials? - See for instance for planar graphene (Kuchment-Post '07).
- ▶ Part 1: How is mechanical strain correctly included in quantum graphs? - How do spectral properties change upon "straining"?
- ▶ Part 2: What happens for high energies in the continuum model

$$H_V = h^2 D_{x_1}^2 + (hD_{x_2} - Bx_1)^2 + V?$$

- ▶ Part 2: Can we approximate the metric graph using continuum models and exhibit spectral stability?