Electronic properties of relaxed twisted bilayer graphene

Mitchell Luskin

Alex Watson, Tianyu Kong, Allan MacDonald, Daniel Massatt, Stephen Carr, cast of thousands

University of Minnesota

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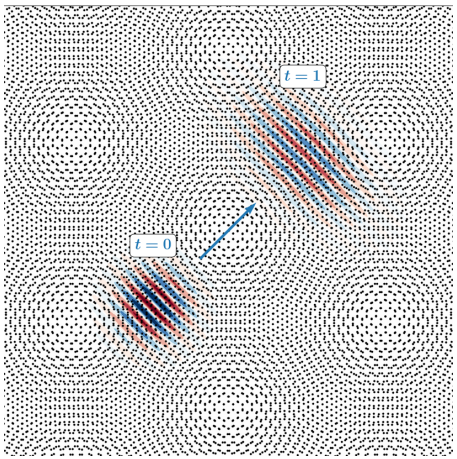


2D bilayer geometry

For layers $j \in \{1, 2\}$, we define the Bravais lattice

$$\mathcal{R}_j = \{A_j n : n \in \mathbb{Z}^2\}$$

where A_j is a 2×2 invertible matrix whose columns are primitive lattice vectors. We define the *unit cell* for layer j as

$$\Gamma_j = \{A_j x : x \in [0, 1)^2\}.$$

Reciprocal lattice: $\mathcal{R}_j^* := \{2\pi A^{-T} n : n \in \mathbb{Z}^2\}$.
Brillouin Zone: $\Gamma_j^* := BZ_j := \{2\pi A_j^{-T} x : x \in [0, 1)^2\}$.

Represent multilattices by $\mathcal{R}_1 \times \mathcal{A}_1$ and $\mathcal{R}_2 \times \mathcal{A}_2$
where $\mathcal{A}_i$ denotes the set of orbitals associated with each lattice point in layer i.

Tight-Binding Model

Tight-binding parameterizes the Hamiltonian into interactions between localized (Wannier) basis functions:

$$h_{\alpha\alpha'}(R - R') \sim \langle \phi_{(R,\alpha)} | \mathcal{H} | \phi_{(R',\alpha')} \rangle.$$

$R - R'$ can take any value in $\mathcal{R}_j$ for $R\alpha \in \mathcal{R}_j \times \mathcal{A}_j$, $R'\alpha' \in \mathcal{R}_j \times \mathcal{A}_j$, but $R - R'$ can take any value in $\mathbb{R}^2$ for $R\alpha \in \mathcal{R}_1 \times \mathcal{A}_1$, $R'\alpha' \in \mathcal{R}_2 \times \mathcal{A}_2$.

We can formally define an operator H such that

$$H_{R\alpha,R'\alpha'} = h_{\alpha\alpha'}(R - R'),$$

and an eigenproblem

$$H\psi = E\psi.$$

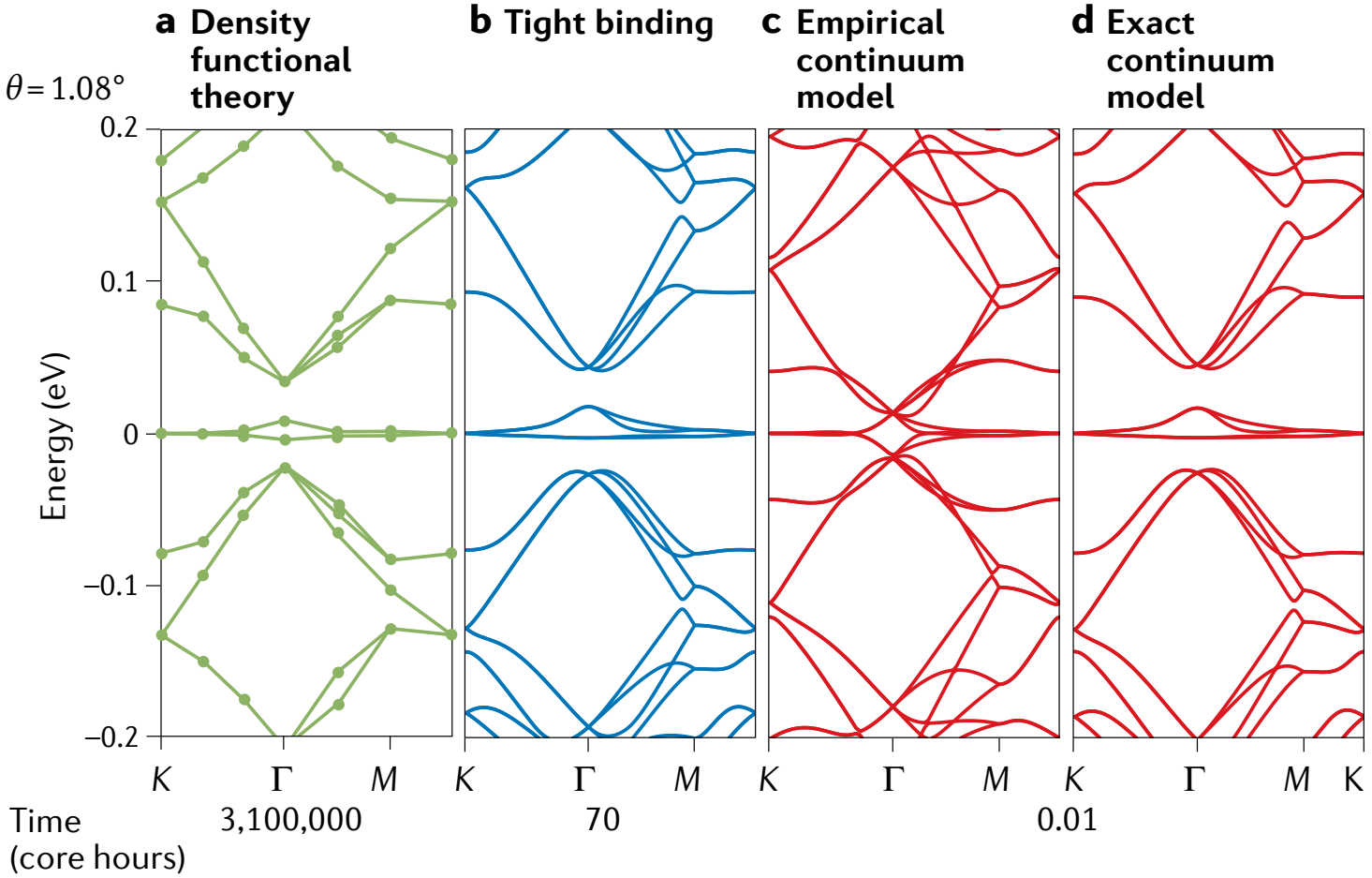
The operator H does not have translation symmetry and thus cannot diagonalized by a Bloch transform if $\mathcal{R}_1 \cup \mathcal{R}_2$ is not periodic.

- We assume an exponential localization of the Hamiltonian entries:

$$|h_{\alpha\alpha'}(x)| \leqslant Ce^{-\tilde{\gamma}|x|}.$$

Computing time of DFT versus Tight-Binding

Approximately $10,000$ atoms per moiré cell.



Electronic-structure methods for twisted moiré layers. Carr, S., Fang, S. & Kaxiras, E. Nat Rev Mater 5, 748–763 (2020).

Transform to Momentum Space

The multilayer wave function $\psi_{R,\alpha} = (\psi_{R_1\alpha_1}, \psi_{R_2\alpha_p})$ or $\psi := (\psi_1, \psi_2)$ is defined on $\Omega := \Omega_1 \cup \Omega_2 = \mathcal{R}_1 \times \mathcal{A}_1 \cup \mathcal{R}_2 \times \mathcal{A}_2$

Define the Bloch transform for each sheet

$$\check{\psi}_j(q) = |\Gamma_j^*|^{-1/2} \sum_{R_j \in \mathcal{R}_j} \psi_{R_j\alpha_j} e^{-iR_j\cdot q}, \qquad q \in \mathrm{BZ}_j,\ \alpha_j \in \mathcal{A}_j.$$

Transform the Hamiltonian to momentum space

$$\widetilde{H_{jj}\psi_j}(q) = c_j \widetilde{h_{jj}}(q)\check{\psi}_j(q), \qquad q \in \mathrm{BZ}_j,$$
$$\widetilde{H_{jk}\psi_k}(q) = \sum_{G_j \in \mathcal{R}_j^*} c_{jk} \widehat{h_{jk}}(q+G_j)\widetilde{\psi}_k(q+G_j), \qquad j \neq k,\ q \in \mathrm{BZ}_j,$$

where $c_j = |\Gamma_j^*|^{1/2}$, $c_{jk} = c_j \cdot c_k$, and

$$\widetilde{h_{jj}}(q) = |\Gamma_j^*|^{-1/2} \sum_{R_j \in \mathcal{R}_j} h_{\alpha_j\alpha_j}(R_j) e^{-iR_j\cdot q}, \qquad \alpha_j \in \mathcal{A}_j,\ q \in \mathrm{BZ}_j,$$

$$\widehat{h_{jk}}(q) = \frac{1}{2\pi} \int h_{\alpha\alpha'}(x) e^{-ix\cdot q} dx, \qquad j \neq k,\ \alpha_j \in \mathcal{A}_j,\ \alpha_k \in \mathcal{A}_k\ , q \in \mathbb{R}^2.$$

The proof follows from the Poisson summation formula:

$$|\Gamma_j^*|^{-1} \sum_{R_j \in \mathcal{R}_j} e^{iq\cdot R_j} = \sum_{G_j \in \mathcal{R}_j^*} \delta(q+G_j), \quad q \in \mathbb{R}.$$

Interlayer Scattering

Transform the Hamiltonian to momentum space

$$\widetilde{H_{jj}\psi_j}(q) = c_j \widetilde{h_{jj}}(q)\check{\psi}_j(q), \qquad q \in \mathrm{BZ}_j,$$
$$\widetilde{H_{jk}\psi_k}(q) = \sum_{G_j \in \mathcal{R}_j^*} c_{jk}\widehat{h_{jk}}(q+G_j)\widetilde{\psi}_k(q+G_j), \qquad j \neq k,\ q \in \mathrm{BZ}_j.$$

We thus see that

$$\check{\psi}_j(q) \text{ scatters to } \widetilde{\psi}_k(q+G_j) = \widetilde{\psi}_k(q+G_j-G_k), \quad G_j \in \mathcal{R}_j^*,\ G_k \in \mathcal{R}_k^*.$$

No periodicity if lattices are incommensurate!

Bilayer:

$$\widetilde{\psi}_1(q) \text{ scatters to } \widetilde{\psi}_2(q+G_1-G_2), \quad G_1 \in \mathcal{R}_1^*,\ G_2 \in \mathcal{R}_2^*.$$
$$\widetilde{\psi}_2(q+G_1-G_2) \text{ scatters to } \widetilde{\psi}_1(q+(G_1-G_2)+(G_2'-G_1'))$$
$$= \widetilde{\psi}_1(q+(G_1-G_1')-(G_2-G_2')), \quad G_2' \in \mathcal{R}_2^*,\ G_1' \in \mathcal{R}_1^*.$$

Interlayer Scattering

Transform the Hamiltonian to momentum space

$$\widetilde{H_{jj}\psi_j}(q) = c_j \widetilde{h_{jj}}(q)\check{\psi}_j(q), \qquad q \in \mathrm{BZ}_j,$$
$$\widetilde{H_{jk}\psi_k}(q) = \sum_{G_j \in \mathcal{R}_j^*} c_{jk}\widehat{h_{jk}}(q+G_j)\widetilde{\psi}_k(q+G_j), \qquad j \neq k,\ q \in \mathrm{BZ}_j.$$

We can substitute q by $q + G_k$ above to obtain

$$\widetilde{H_{jj}\psi_j}(q+G_k) = c_j \widetilde{h_{jj}}(q+G_k)\check{\psi}_j(q+G_k), \qquad j \neq k,$$
$$\widetilde{H_{jk}\psi_k}(q+G_k) = \sum_{G_j \in \mathcal{R}_j^*} c_{jk}\widehat{h_{jk}}(q+G_j+G_k)\widetilde{\psi}_k(q+G_j), \qquad j \neq k.$$

We can thus define the momentum Hamiltonian centered at q

$$[\widehat{H_{jj}}(q)]_{G_k,G_k'} = c_j \widetilde{h_{jj}}(q+G_k)\delta_{G_k,G_k'}, \qquad \text{if } j \neq k,\ G_k,\ G_k' \in \mathcal{R}_k^*,$$
$$[\widehat{H_{jk}}(q)]_{G_k,G_j} = c_{jk}\widehat{h_{jk}}(q+G_j+G_k), \qquad \text{if } j \neq k,\ G_j \in \mathcal{R}_j^*,\ G_k \in \mathcal{R}_k^*.$$

Momentum Space Hamilton

We can thus define the momentum Hamiltonian centered at q

$$[\widehat{H_{jj}}(q)]_{G_k,G_k'} = c_j \widetilde{h_{jj}}(q+G_k)\delta_{G_k,G_k'}, \qquad \text{if } j \neq k,\ G_k,\ G_k' \in \mathcal{R}_k^*,$$

$$[\widehat{H_{jk}}(q)]_{G_k,G_j} = c_{jk}\widehat{h_{jk}}(q+G_j+G_k), \qquad \text{if } j \neq k,\ G_j \in \mathcal{R}_j^*,\ G_k \in \mathcal{R}_k^*.$$

We then have the following theorem based on the ergodicity property:

Theorem

,

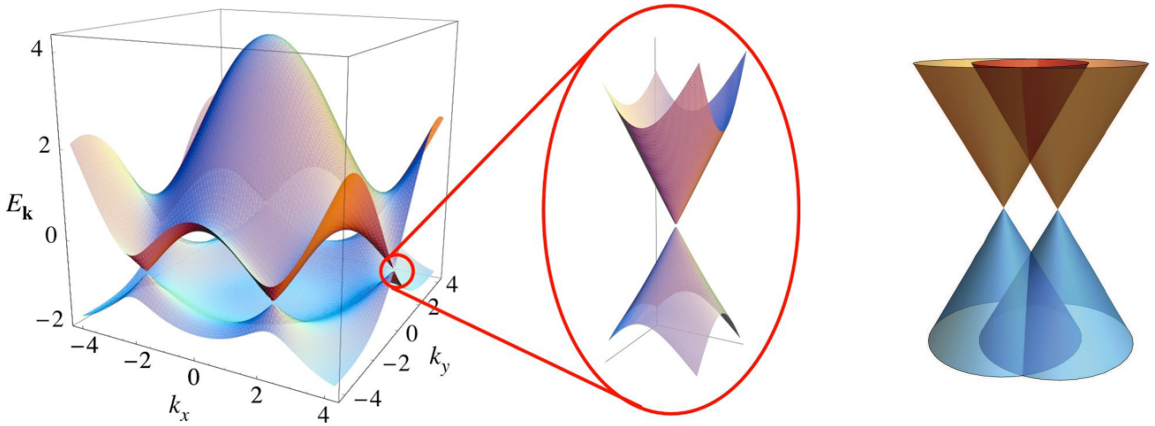
$$Tr\ g(H) = Tr\ g(\hat{H}(0)) = \nu^* \sum_{j=1}^{2} \sum_{\alpha \in \mathcal{A}_j} \int_{\Gamma_j^*} [g \circ \hat{H}(q)]_{0\alpha,0\alpha},$$

where

$$\nu^* = \left[|\Gamma_2^*| \cdot |\mathcal{A}_1| + |\Gamma_1^*| \cdot |\mathcal{A}_2| \right]^{-1}.$$

Incommensurate heterostructures in momentum space. Daniel Massatt, Stephen Carr, Mitchell Luskin, and Christoph Ortner. Multiscale Model. Simul., 16:429–451, 2018.

Incommensurate Band Structure — Local Momentum DoS



[*The electronic properties of graphene*, Neto, Geim, et al, *Rev. Mod. Phys*]
[*Correlated insulator behaviour at half-filling in magic-angle graphene superlattices*,Cao, Jarillo-Herroro, et al, *Nature*]

Figure: L: Monolayer graphene bands at the Fermi level. The Dirac cone. R: Band structure for non-interacting twisted bilayer graphene.

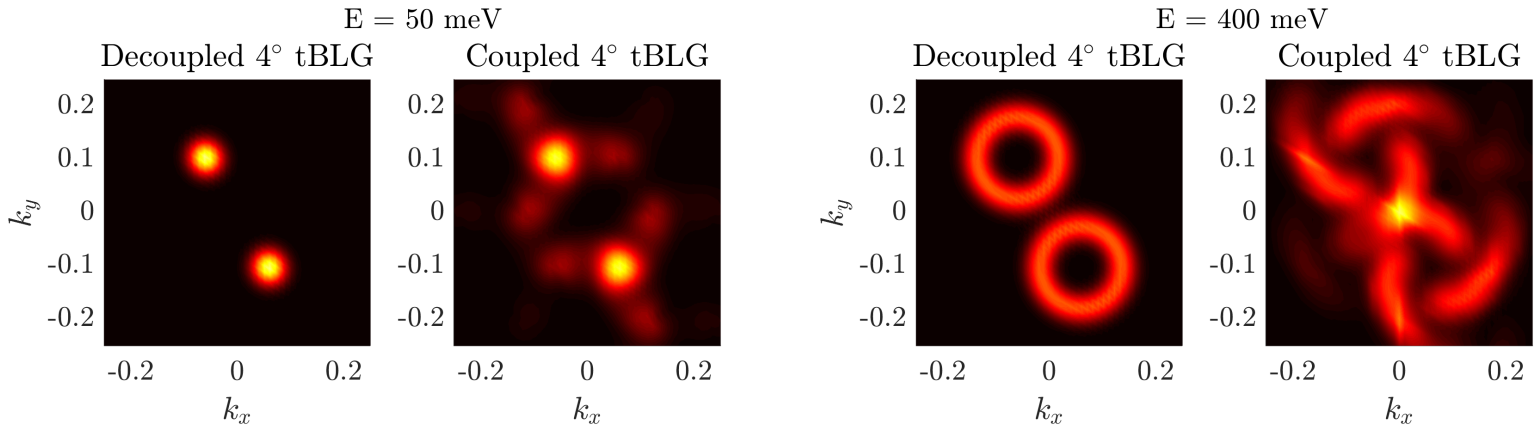
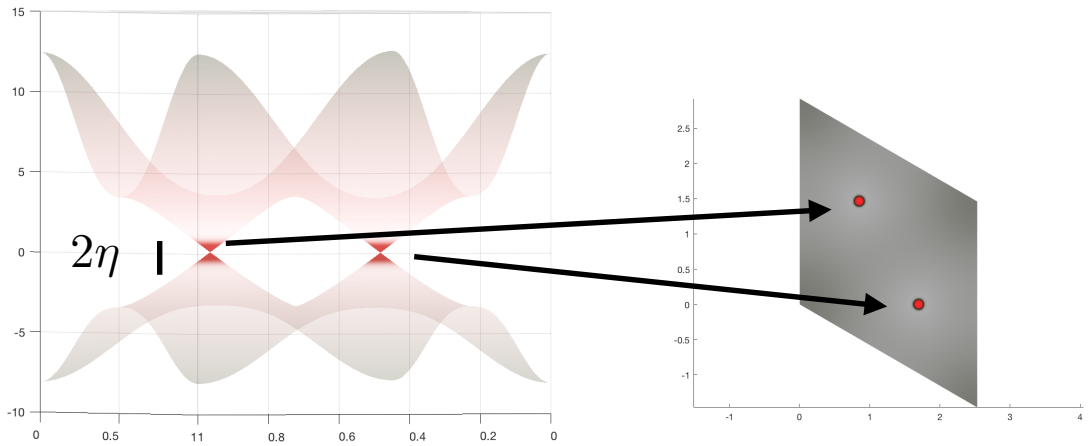
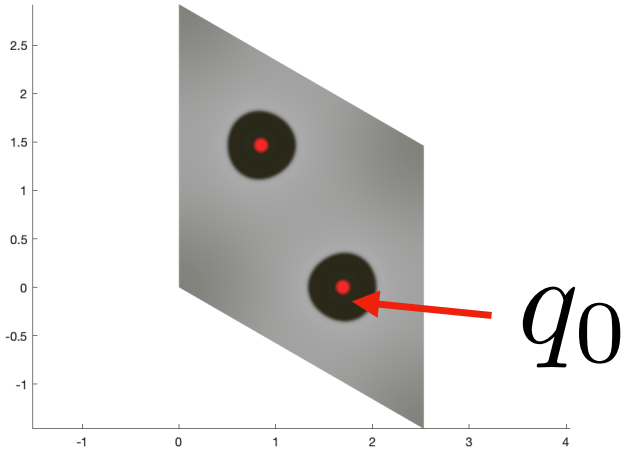


Figure: Twisted bilayer graphene momentum local DoS

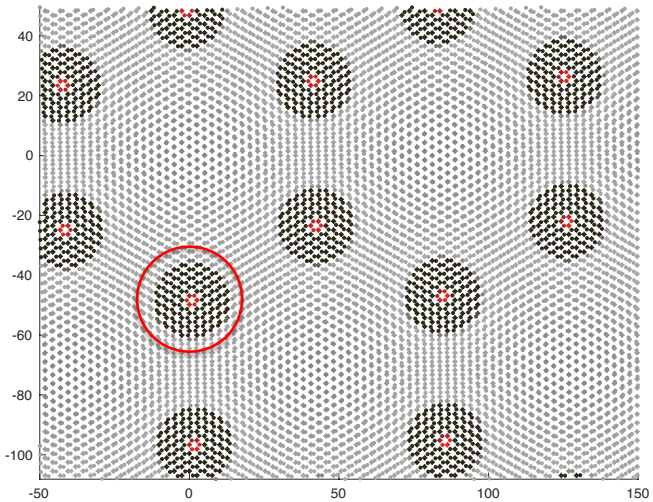
Choice of Truncation



Momenta corresponding to energy of interest (η is coupling strength between sheets).



We add buffer region of radius r in momentum space



We map to truncated reciprocal lattice region.

Momentum Space Hamiltonian Domain Reduction

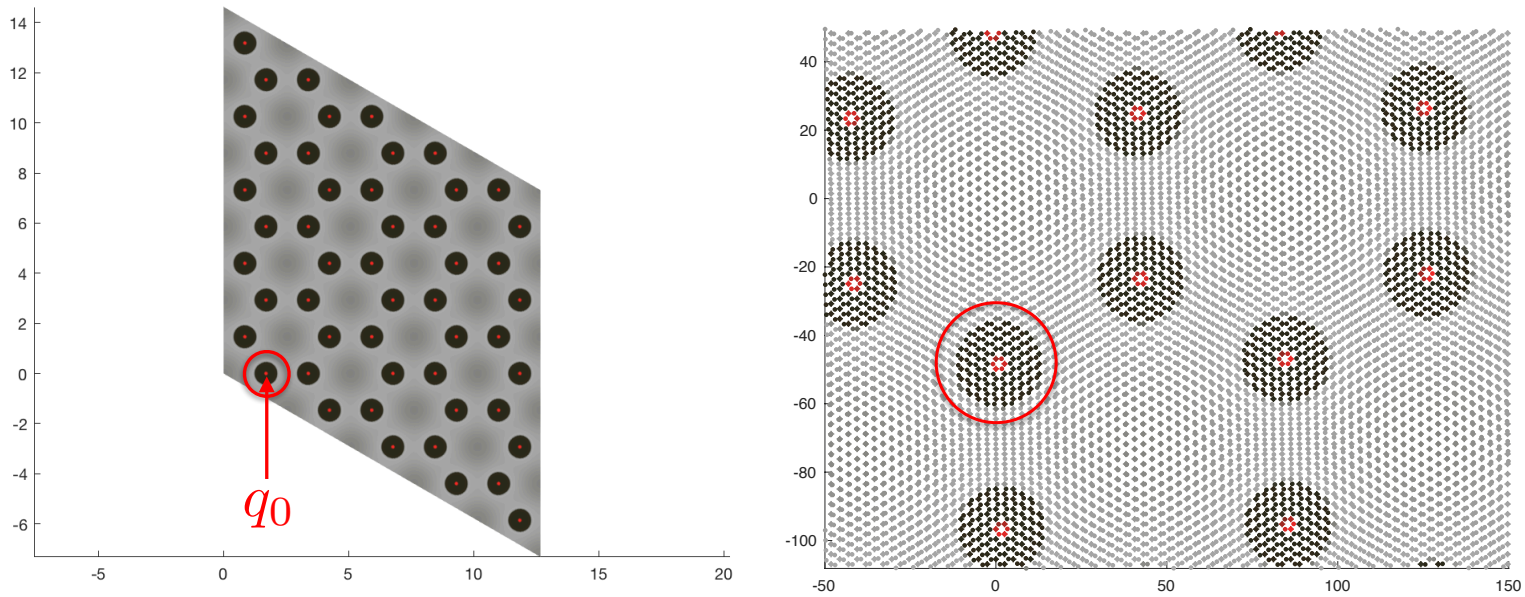


Figure: Low energy momenta in momentum space (left) and reciprocal space (right).

Can approximate $\widehat{H}(q)$ by $\widehat{H}|_{\Omega^*_{r,\tau}}(q)$ in

$$\operatorname{Tr} g(H) = \operatorname{Tr} g(\widehat{H}) \approx \nu^* \sum_{j=1}^{2} \sum_{\alpha \in \mathcal{A}_j} \int_{\Gamma_j^*} [g \circ \widehat{H}|_{\Omega^*_{r,\tau}}(q)]_{0\alpha,0\alpha},$$

for momentum basis truncation r and interlayer tunneling truncation τ.

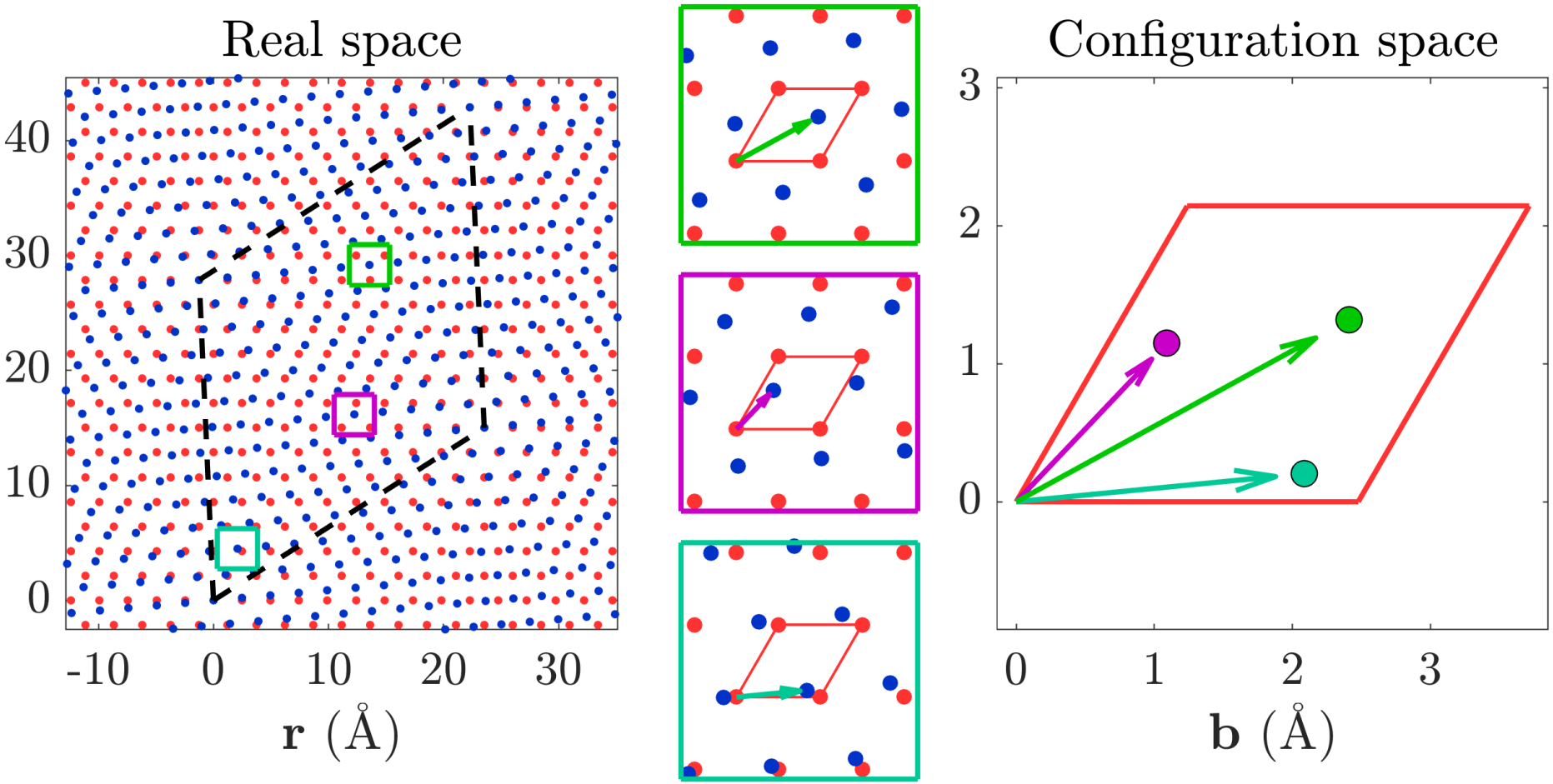
Disregistry

The disregistry of an atom R_1 of layer 1 with respect to layer 2 is given by

$$b_{1\to 2}(R_1) = \mathrm{mod}_{\Gamma_2}(R_1), \qquad R_1 \in \mathcal{R}_1.$$

Since $A_2 A_1^{-1} R_1 \in \mathcal{R}_2$, we can smoothly interpolate to $\mathbb{R}^2$ by

$$b_{1\to 2}(x) = \mathrm{mod}_{\Gamma_2}\left[(I - A_2 A_1^{-1})x\right].$$



Moiré Unit Cell and Superlattice

$b_{1\to 2}(x)$ and $b_{2\to 1}(x)$ are isomorphisms

$$b_{1\to 2}: \begin{cases} \Gamma_{\mathcal{M}} \to \Gamma_2, \\ \quad x \mapsto (I - A_2A_1^{-1})x = (I - A_2A_1^{-1})x + A_2(e_1 + e_2) = A_2(A_2^{-1} - A_1^{-1})x, \end{cases}$$

$$b_{2\to 1}: \begin{cases} \Gamma_{\mathcal{M}} \to \Gamma_1, \\ \quad x \mapsto (I - A_1A_2^{-1})x = A_1(A_1^{-1} - A_2^{-1})x, \end{cases}$$

where $\Gamma_{\mathcal{M}}$ is the periodic moiré cell:

$$\Gamma_{\mathcal{M}} := \mathbb{R}^2/\mathcal{R}_{\mathcal{M}} = A_{\mathcal{M}}[0,1)^2 = (A_1^{-1} - A_2^{-1})^{-1}[0,1)^2,$$

and $\mathcal{R}_{\mathcal{M}}$ is the moiré superlattice given by

$$\mathcal{R}_{\mathcal{M}} := A_{\mathcal{M}}\mathbb{Z}^2 = (A_1^{-1} - A_2^{-1})^{-1}\mathbb{Z}^2.$$

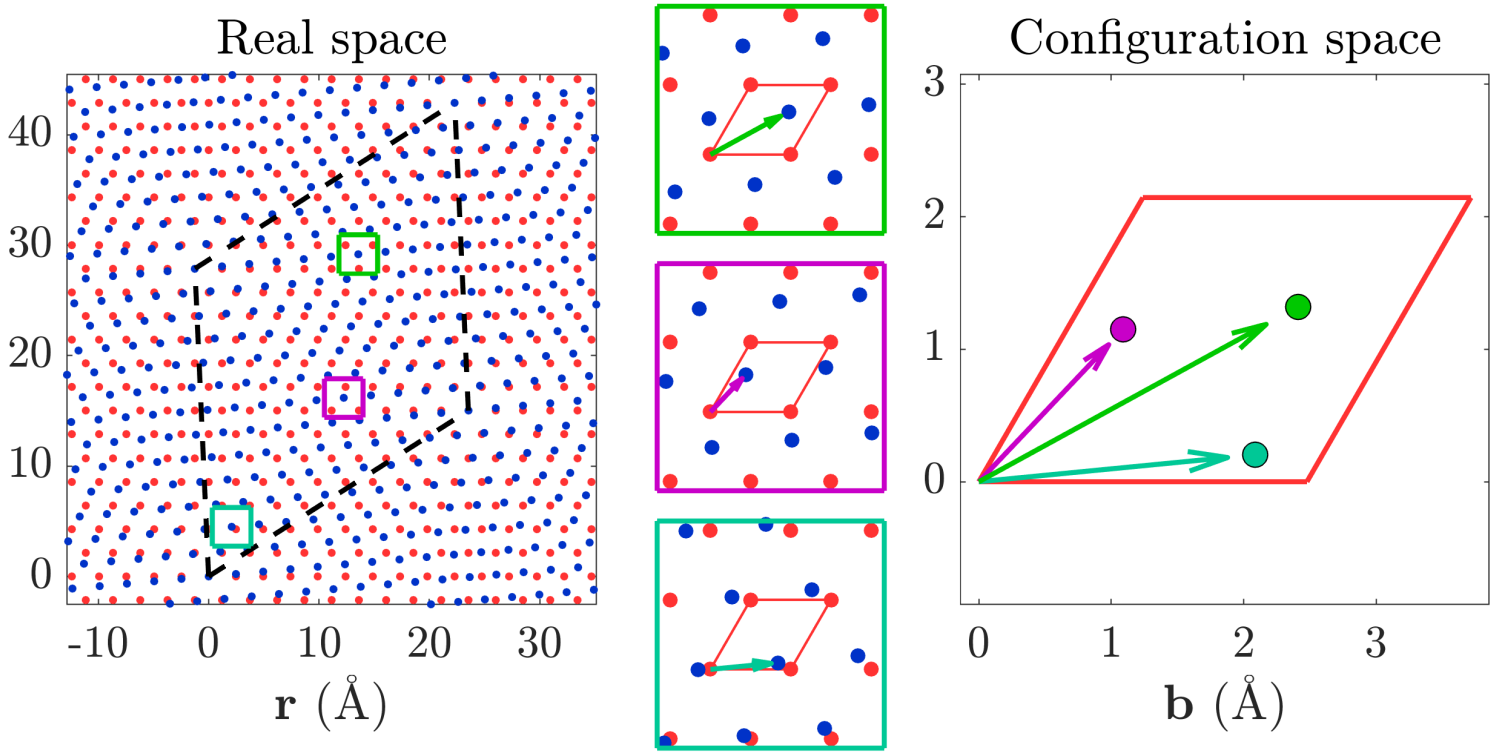
Reciprocal moiré lattice is then given by

$$\mathcal{R}^*_{\mathcal{M}} := 2\pi A_{\mathcal{M}}^{-T}\mathbb{Z}^2 = 2\pi(A_1^{-T} - A_2^{-T})\mathbb{Z}^2.$$

Ergodicity of Disregistries for Incommensurate 2D Layers

For $h \in C_{\text{per}}(\Gamma_2)$, we thus have that $h(R_1) = h(b_{1\to 2}(R_1))$ and

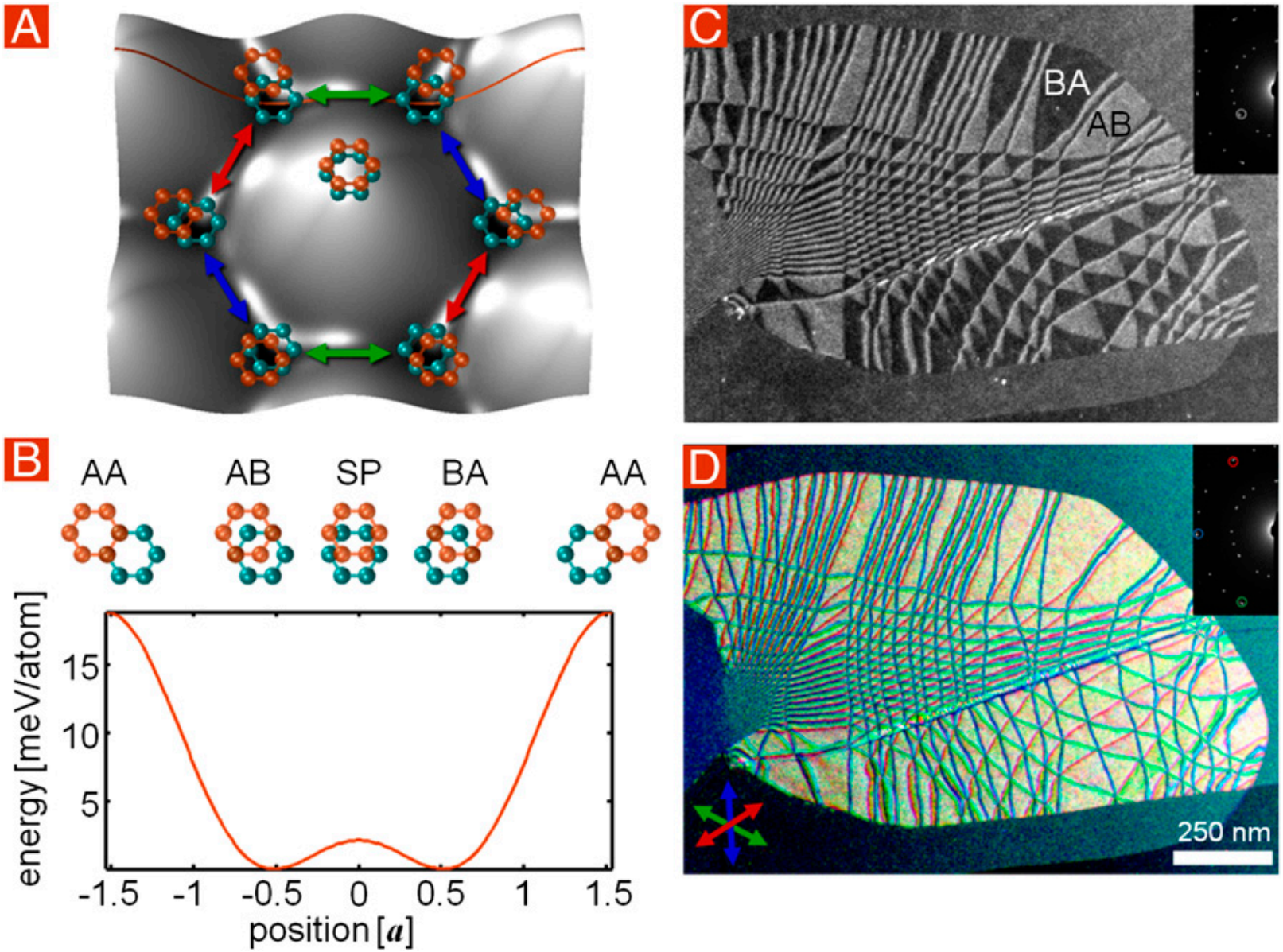
$$\frac{1}{\#\mathcal{R}_1 \cap B_r} \sum_{R_1 \in \mathcal{R}_1 \cap B_r} h(R_1) = \frac{1}{\#\mathcal{R}_1 \cap B_r} \sum_{R_1 \in \mathcal{R}_1 \cap B_r} h(b_{1\to 2}(R_1)) \to \frac{1}{|\Gamma_2|} \int_{\Gamma_2} h(b)db.$$



Generalized Kubo formulas for the transport properties of incommensurate 2D atomic heterostructures. E. Cancés, P. Cazeaux, and M. Luskin. Journal of Mathematical Physics, 58:063502, 2017.

Electronic density of states for incommensurate layers. Daniel Massatt, Mitchell Luskin, and Christoph Ortner. SIAM J. Multiscale Modeling & Simulation, 15:476–499, 2017.

Energy landscape in twisted bilayer graphene



Strain solitons and topological defects in bilayer graphene. PNAS, 2013, Alden, . . . , McEuen

Continuum Model for Relaxation of Incommensurate 2D Bilayers

The relation between displacement in configuration space coordinates and real space coordinates is assumed to be given by

$$U_1(x) = u_1(b_{1\to 2}(x)) \quad \text{and} \quad U_2(x) = u_2(b_{2\to 1}(x)),$$

where u_1 is periodic on Γ_2 and u_2 is periodic on Γ_1. Since $b_{1\to 2}(x)$ and $b_{2\to 1}(x)$ are isomorphisms

$$b_{1\to 2} : \begin{cases} \Gamma_{\mathcal{M}} \to \Gamma_2, \\ \quad x \mapsto (I - A_2 A_1^{-1})x, \end{cases} \qquad b_{2\to 1} : \begin{cases} \Gamma_{\mathcal{M}} \to \Gamma_1, \\ \quad x \mapsto (I - A_1 A_2^{-1})x, \end{cases}$$

we have that $U_1(x)$ and $U_2(x)$ are periodic on $\Gamma_{\mathcal{M}}$ and

$$E_{\text{tot}}(U_1, U_2) = \int_{\Gamma_{\mathcal{M}}} dx \Big[\mathcal{E}^1_{\text{intra}}(\nabla U_1(x)) + \mathcal{E}^2_{\text{intra}}(\nabla U_2(x)) + \frac{1}{2}\mathcal{E}^1_{\text{inter}}(b_{1\to 2}(x) + U_1(x) - U_2(x)) + \frac{1}{2}\mathcal{E}^2_{\text{inter}}(b_{2\to 1}(x) + U_2(x) - U_1(x)) \Big].$$

where $\mathcal{E}^1_{\text{inter}} : \Gamma_2 \to \mathbb{R}$ is the relaxed Generalized Stacking Fault Energy.

Energy minimization of 2D incommensurate heterostructures. P. Cazeaux , M. Luskin, and D. Massatt. Arch. Rat. Mech. Anal., 235:1289–1325, 2019.

Generalized Stacking Fault Energy

The interlayer energy density of layer 2 with respect to layer 1 can be accurately modeled by the Generalized Stacking Fault Energy, F_{GSFE},

$$\mathcal{E}^2_{\text{inter}}(b_{2\to1}(x) + U_2(x) - U_1(x)) = F_{\text{GSFE}}(b_{2\to1}(x) + U_2(x) - U_1(x)),$$

where $b_{2\to1}(x)$ is the disregistry. F_{GSFE} can be fit by DFT.

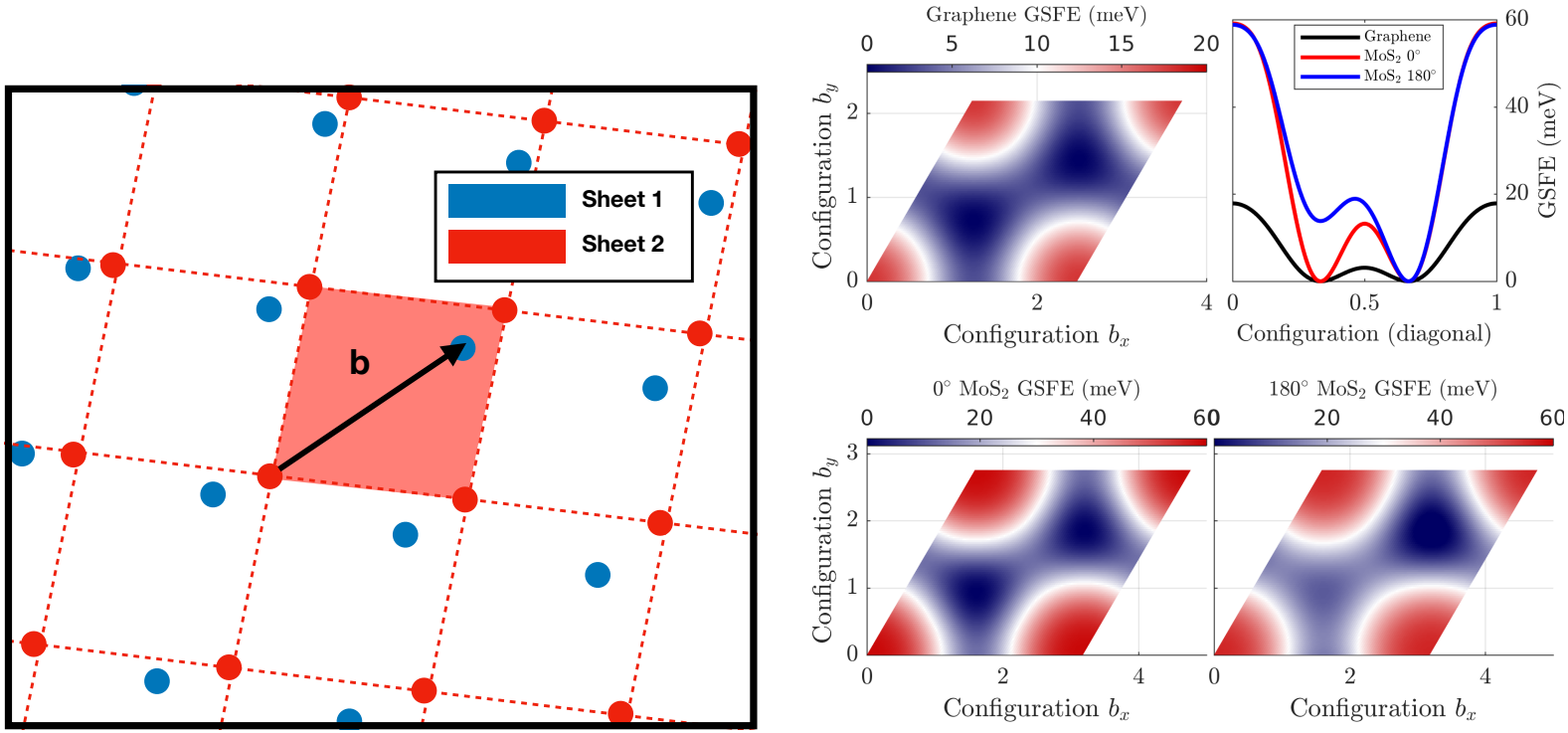


Figure: How the Generalized Stacking Fault Energy, which represents the interlayer coupling energy, depends on the disregistry b for three different materials.

Bilayer Graphene or MoS_2 Configuration Space Model

For bilayer graphene or MoS_2, $\mathcal{E}_{\text{intra}} = \mathcal{E}^1_{\text{intra}} = \mathcal{E}^2_{\text{intra}}$ since the intralayer energy is isotropic and

$$\mathcal{E}^1_{\text{inter}}(b_{1\to 2}(x)) = \mathcal{E}^2_{\text{inter}}(b_{2\to 1}(x))$$

by symmetry.

We can then obtain from the uniqueness of solutions to the energy minimization problem that $U_1 = -U_2$ and U_1 is the minimum displacement for the energy

$$E_{\text{tot}}(U) := \frac{1}{|\Gamma_M|}\int_{\Gamma_M} dx\big[\mathcal{E}_{\text{intra}}(\nabla U(x)) + \mathcal{E}^1_{\text{inter}}(b_{1\to 2}(x) + 2U(x))\big].$$

Rescale to $\Gamma_0 := 2\sin(\theta/2)\Gamma_{\mathcal{M}}$ to get Ginzburg-Landau type equation:

$$E_{\text{tot}}(U) := \int_{\Gamma_0} dx\big[\mathcal{E}_{\text{intra}}(\nabla U(x)) + \frac{1}{(2\sin\theta/2)^2}\mathcal{E}^1_{\text{inter}}(b_{1\to 2}(x) + 2U(x))\big].$$

Hence,

$$\int_{\Gamma_2} |\nabla u_1(b)|^2\, db \leqslant C\theta^{-2}, \quad \int_{\Gamma_{\mathcal{M}}} |\nabla U_1(x)|^2 dx \leqslant C\theta^{-2}.$$

Regularity of Displacement

$$\int_{\Gamma_2} |\nabla u_1(b)|^2 \, db \leqslant C\theta^{-2}, \qquad \int_{\Gamma_{\mathcal{M}}} |\nabla U_1(x)|^2 dx \leqslant C\theta^{-2}.$$

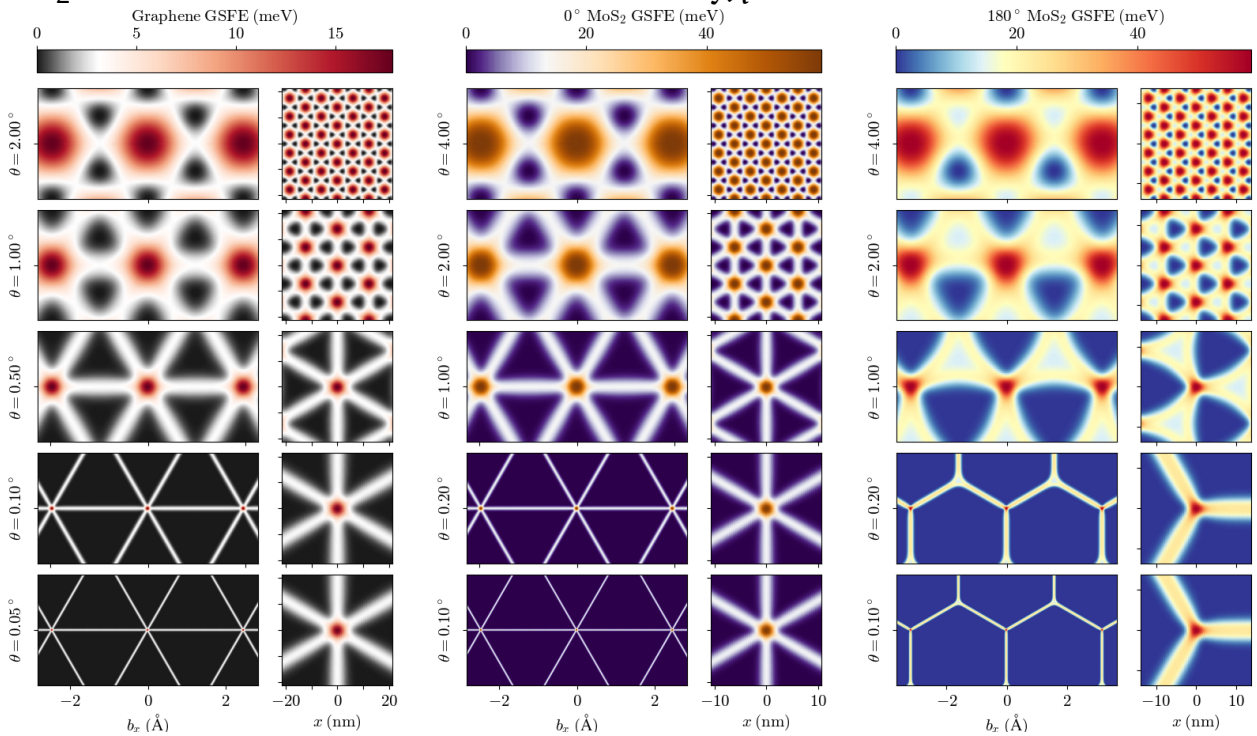


Figure: Relaxation results for twisted bilayers with five incommensurate twist angles each. The left panel of each column shows $F_{\mathrm{GSFE}}(\mathbf{b} + 2\mathbf{u}(\mathbf{b}))$ over Γ (the relaxation pattern in configuration space) and the right panel shows $F_{\mathrm{GSFE}}(\mathbf{r})$ (over real space).

Relaxation and Domain Formation in Incommensurate 2D Heterostructures. S. Carr, D. Massatt, S. B. Torrisi, P. Cazeaux, M. Luskin and E. Kaxiras). Physical Review B, page 224102 (7 pp), 2018.

Relaxation and domain wall structure of bilayer moiré systems. Paul Cazeaux, Drake Clark, Rebecca Engelke, Philip Kim, and Mitchell Luskin. Journal of Elasticity, 2023.

Hamiltonian for Relaxed Bilayer Structures

We assume that the relaxed position for an atom on site $R_1 \in \mathcal{R}_1$ is given by

$$R_1 \mapsto R_1 + u_1(R_1), \qquad u_1 \in C_{\text{per}}(\Gamma_2).$$

If $R_1 \in \mathcal{R}_1$ and $R_2 \in \mathcal{R}_2$, we have by periodicity of u_1 and u_2:

$$\begin{aligned} H^u_{R_1,R_2} &= h_{12}(R_1 + u_1(R_1) - R_2 - u_{P_2}(R_2)) \\ &= h_{12}(R_1 - R_2 + u_1(R_1 - R_2) - u_2(R_2 - R_1)) \\ &= h^u_{12}(R_1 - R_2), \end{aligned}$$

where the relaxed interlayer coupling function is

$$h^u_{12}(x) = h_{12}(x + u_1(x) - u_2(-x)).$$

For intralayer coupling, $R, R' \in \mathcal{R}_j$,

$$H^u_{R,R'} = h_{jj}(R + u_j(R) - R' - u_j(R')),$$

which is not periodic!

Momentum Space Relaxed Hamiltonian

The shifted Hamiltonian has the same structure for interlayer coupling:

$$[\hat{H}^u(q)]_{G_1,G_2} = c_{12}\hat{h}^u_{12}(q + G_1 + G_2) \qquad \text{if } G_1 \in \mathcal{R}_1^*,\ G_2 \in \mathcal{R}_2^*.$$

For intralayer coupling, $R_1,\ R_1^{'} \in \mathcal{R}_1$,

$$H^u_{R_1,R_1^{'}} = h_{11}(R_1 + u_1(R_1) - R_1^{'} - u_1(R_1^{'}))$$

is not periodic! How to apply Bloch transform?

We propose to approximate the Hamiltonian H^u with so that we can compute the intralayer scattering due to relaxation.

Approximation of Intralayer Coupling

For $R_1,\ R_1^{'} \in \mathcal{R}_1$

$$
\begin{aligned}
H^u_{R_1,R_1^{'}} &= h_{11}(R_1 + u_1(R_1) - R_1^{'} - u_1(R_1^{'})) \\
&= h_{11}(R_1 - R_1^{'} + u_1(R_1) - u_1\left(R_1 + (R_1^{'} - R_1)\right) && \textit{Ie} \\
&\approx h_{11}(R_1 - R_1^{'}) + \nabla h_{11}(R_1 - R_1^{'}) \cdot \left(u_1\left((R_1 - R_1^{'}) + R_1^{'}\right) - u_1(R_1^{'})\right).
\end{aligned}
$$

We thus define the approximate Hamiltonian $\tilde{H}^u$ as

$$
\begin{aligned}
[\tilde{H}^u]_{R_1,R_2} &= h^u_{12}(R_1 - R_2), && R_1 \in \mathcal{R}_1,\ R_2 \in \mathcal{R}_2, \\
[\tilde{H}^u]_{R_1,R_1^{'}} &= h_{11}(R_1 - R_1^{'}) \\
&\quad + \nabla h_{11}(R_1 - R_1^{'}) \cdot \left(u_1\left((R_1 - R_1^{'}) + R_1^{'}\right) - u_1(R_1^{'})\right), && \text{if } R_1,\ R_1^{'} \in \mathcal{R}_1.
\end{aligned}
$$

Scattering from Relaxation

Recall that u_1 is periodic on Γ_2. The Fourier coefficients of $u_1(b_2)$ are

$$\hat{u}_1^{G_2} = |\Gamma_2|^{-1} \int_{\Gamma_2} u_1(b_2) e^{-iG_2 \cdot b_2} \, db_2, \qquad G_2 \in \mathcal{R}_2^*,$$

and the Fourier coefficients of $u_1(b_2 + (R_1 - R_1^{'}))$ are thus $e^{iG_2 \cdot (R_1 - R_1^{'})} \hat{u}_1^{G_2}$. It follows that

$$u_1(R_1) - u_1(R_1^{'}) = \sum_{G_2 \in \mathcal{R}_2^*} \left(e^{iG_2 \cdot (R_1 - R_1^{'})} - 1 \right) \hat{u}_1^{G_2} e^{iG_2 \cdot R_1^{'}}$$

and thus

$$\begin{aligned} [\tilde{H}^u]_{R_1, R_1^{'}} &= h_{11}(R_1 - R_1^{'}) \\ &\quad + \nabla h_{11}(R_1 - R_1^{'}) \cdot \sum_{G_2 \in \mathcal{R}_2^*} \left(e^{iG_2 \cdot (R_1 - R_1^{'})} - 1 \right) \hat{u}_1^{G_2} e^{iG_2 \cdot R_1^{'}}. \end{aligned}$$

Approximate Momentum Space Relaxed Intralayer Hamiltonian

Since

$$[\tilde{H}^u]_{R_1,R_1'} = h_{11}(R_1 - R_1') + \nabla h_{11}(R_1 - R_1') \cdot \sum_{G_2 \in \mathcal{R}_2^*} \left(e^{iG_2 \cdot (R_1 - R_1')} - 1 \right) \hat{u}_1^{G_2} e^{iG_2 \cdot R_1'},$$

we have that the Bloch transform of $\sum_{R_1'} [\tilde{H}^u]_{R_1,R_1'} \psi_1(R_1')$ is

$$\widetilde{h_{11}}(q)\widetilde{\psi_1}(q) + \sum_{G_2 \neq 0} \left[\widetilde{\nabla h_{11}}(q - G_2) - \widetilde{\nabla h_{11}}(q) \right] \hat{u}_1^{G_2} \widetilde{\psi_1}(q - G_2).$$

Electronic band structure: unrelaxed vs. relaxed

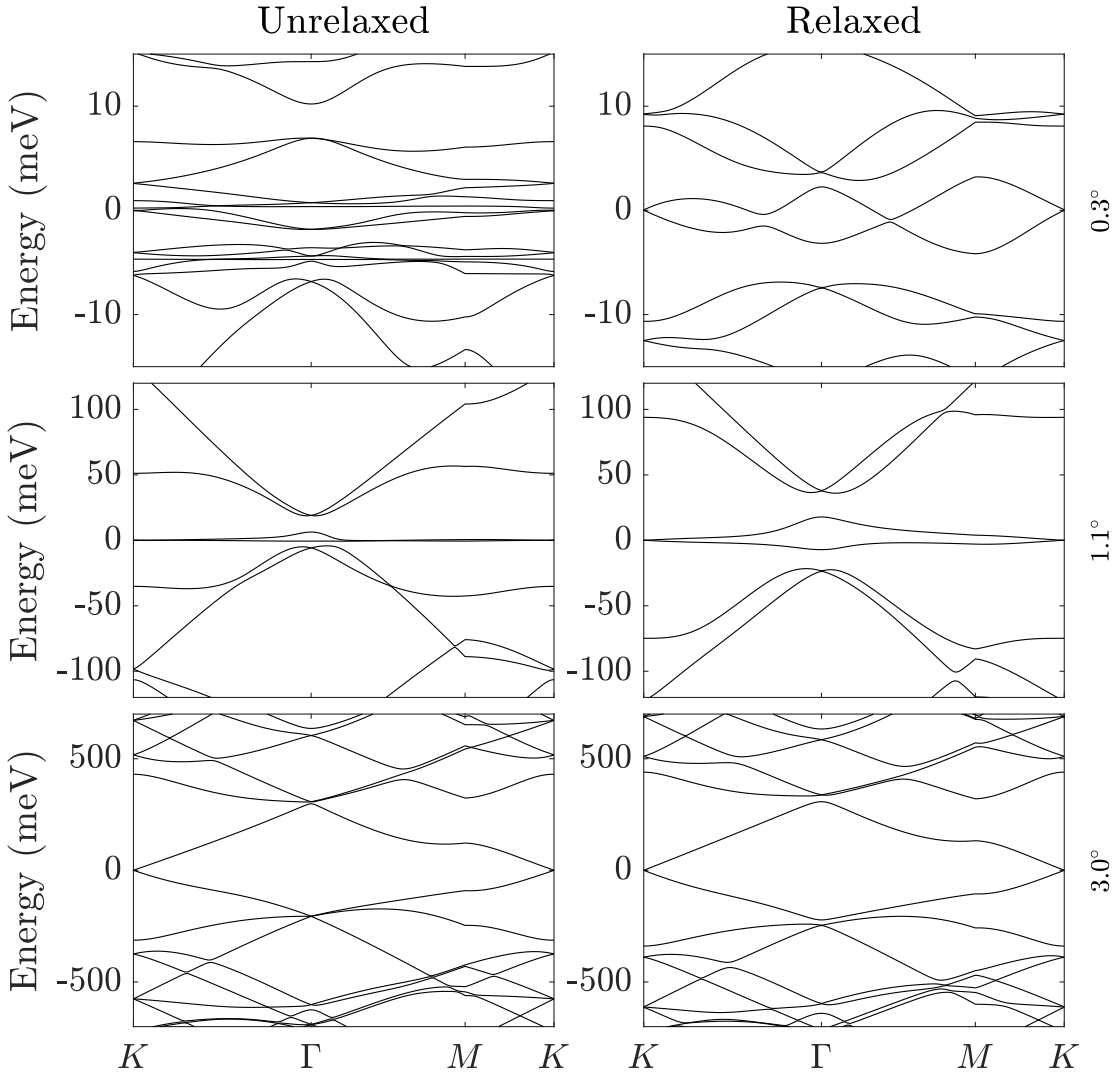


Figure: Electronic band structure along high-symmetry lines of the moiré Brillouin zone at a single monolayer K valley for 0.3° (top), 1.1° (middle), and 3.0° (bottom).

Electronic Observables for Relaxed Bilayer 2D Heterostructures in Momentum Space, Daniel Massatt, Stephen Carr, Mitchell Luskin, arXiv:2109.15296v3, 2021

Interlayer hopping functions for unrelaxed and relaxed 2D bilayers

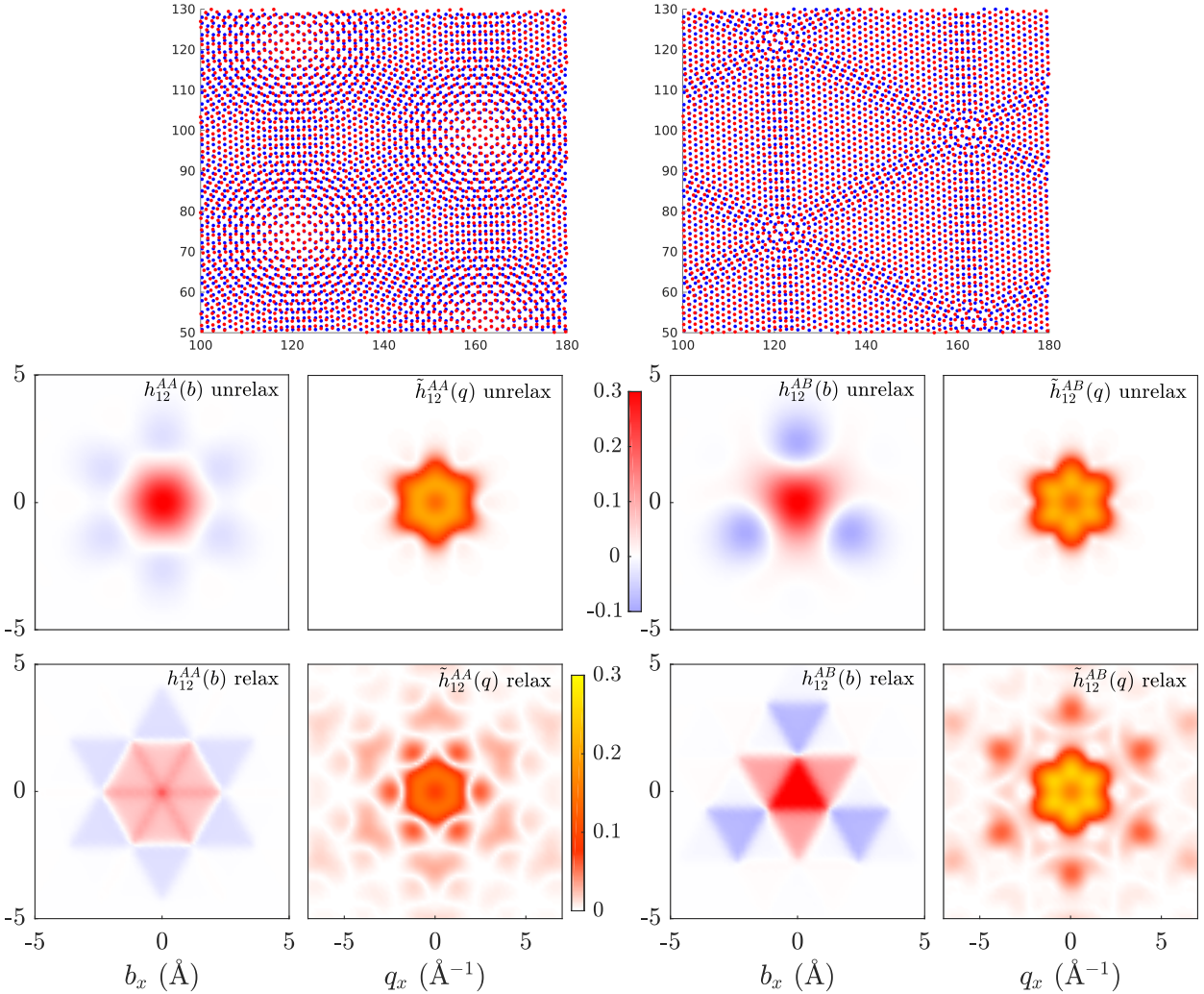
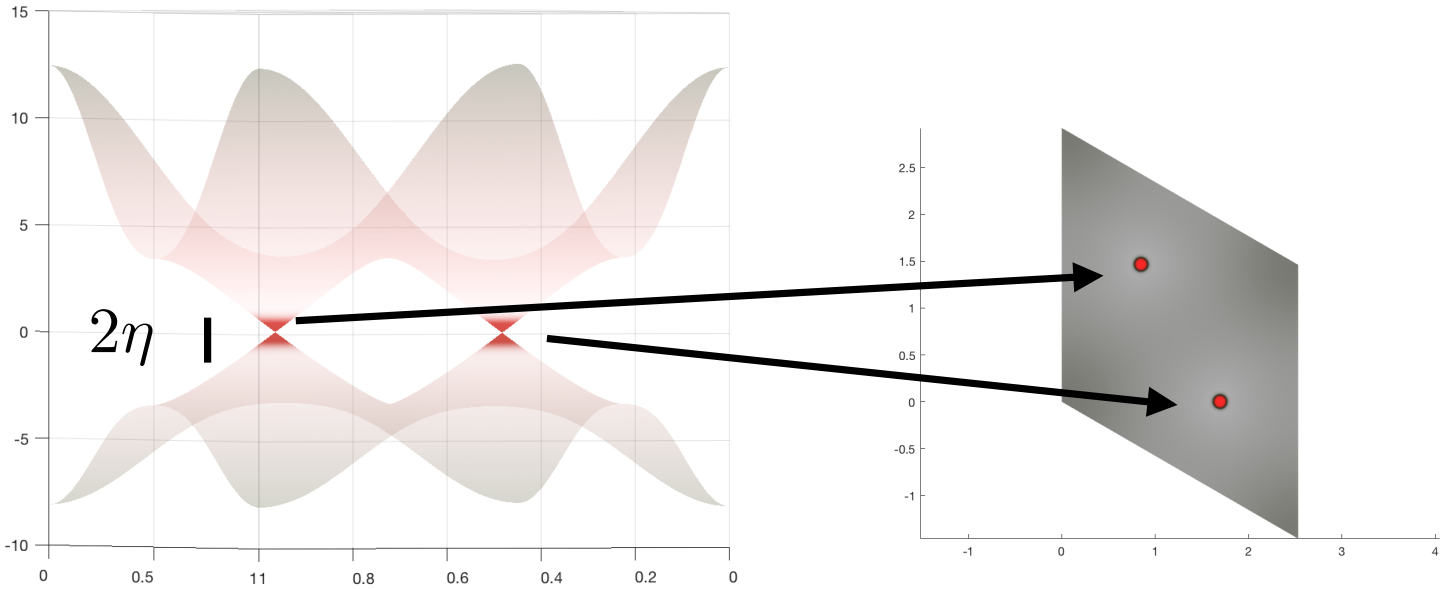


Figure: Interlayer coupling for small twist angle $\theta = 0.3^\circ$ in real and momentum space. Real space methods suffer a loss of regularity with respect to configuration, while momentum space suffers with slower reciprocal space localization.

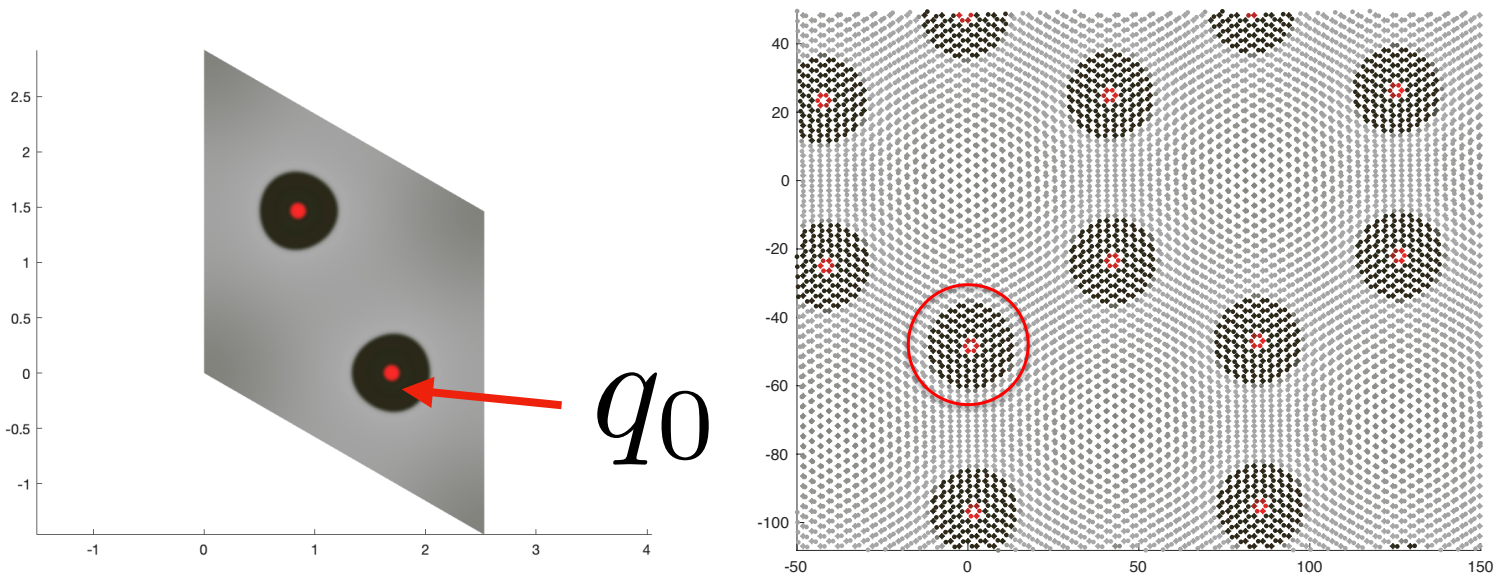
Electronic Observables for Relaxed Bilayer 2D Heterostructures in Momentum Space, Daniel Massatt, Stephen Carr, Mitchell Luskin, MMS, to appear.

Energy Window & Momenta



- We fix a small energy window of interest, η strength of relaxation & interlayer coupling.
- Weak Van der Waals forces allow all scattering hoppings to be considered 'perturbative.'

Low Energy Reciprocal Latttice Approximation



Mapping from momentum space (left) to reciprocal lattice space (right)

Reciprocal lattice TB model forms isolated small matrix pockets, allowing band structure.

Convergence of Electronic Structure

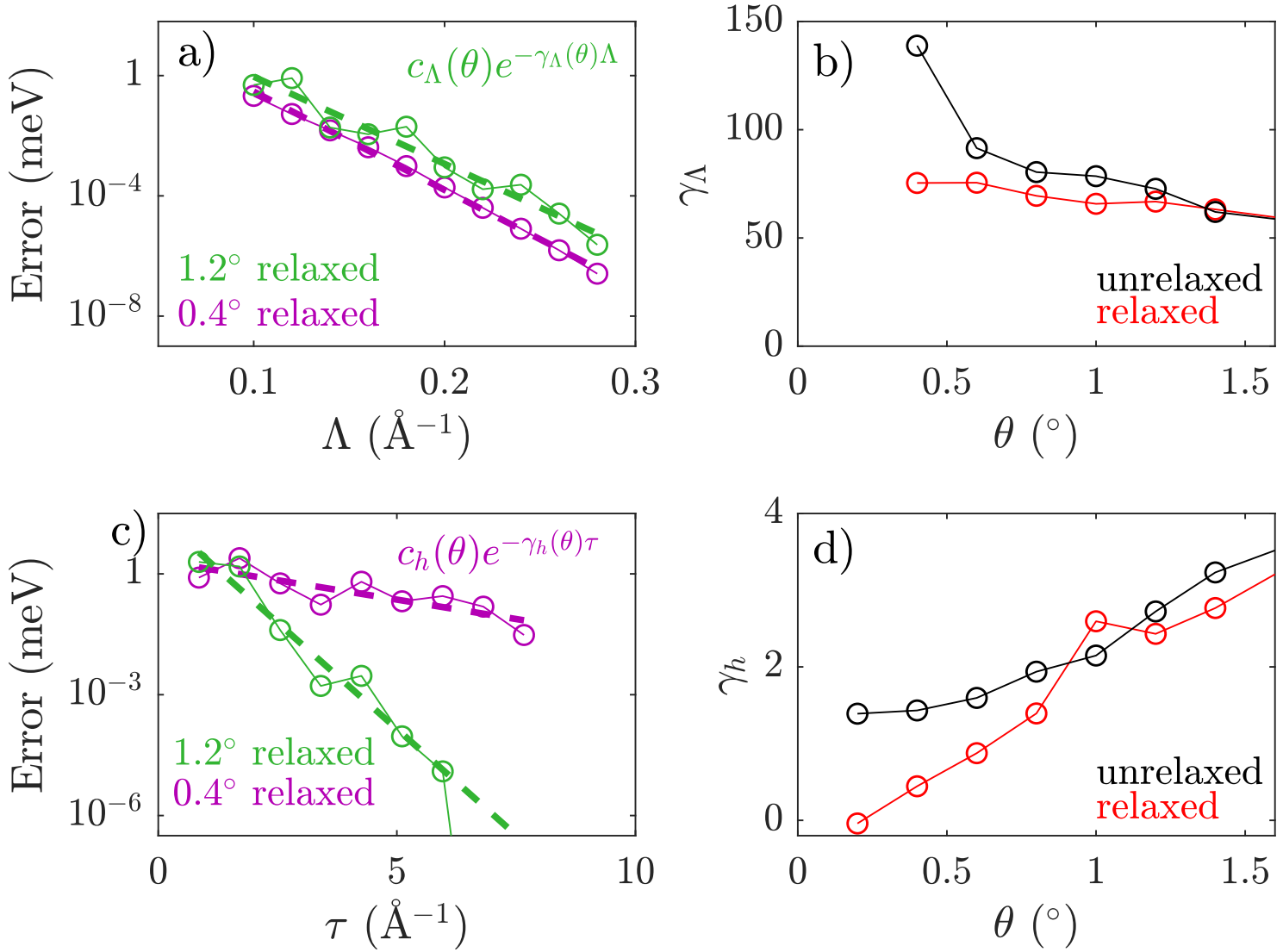


Figure: The relative error for the Γ-point electron eigenvalue closest to the Fermi energy as a function of the momentum basis truncation radius Λ and interlayer truncation radius τ.

Convergence of Electronic Structure

Error estimate for the band structure (local density of states) as a function of the momentum basis truncation radius Λ and interlayer truncation radius τ :

$$\left|\epsilon_\Gamma(\Lambda,\tau)-\epsilon_\Gamma\right| \lesssim e^{-\gamma_h \tau}+e^{-\gamma_\Lambda \Lambda},$$

where the exponential rates of convergence for the unrelaxed structure is

$$\gamma_h \lesssim 1, \qquad \gamma_\Lambda \lesssim \theta^{-1},$$

and the exponential rates of convergence for the relaxed structure since

$$\gamma_h \lesssim \theta, \qquad \gamma_\Lambda \lesssim 1,$$

since

$$\int_{\Gamma_2} |\nabla u_1(b)|^2\, db \leqslant C\theta^{-2}, \quad \int_{\Gamma_{\mathcal{M}}} |\nabla U_1(x)|^2 dx \leqslant C\theta^{-2}.$$

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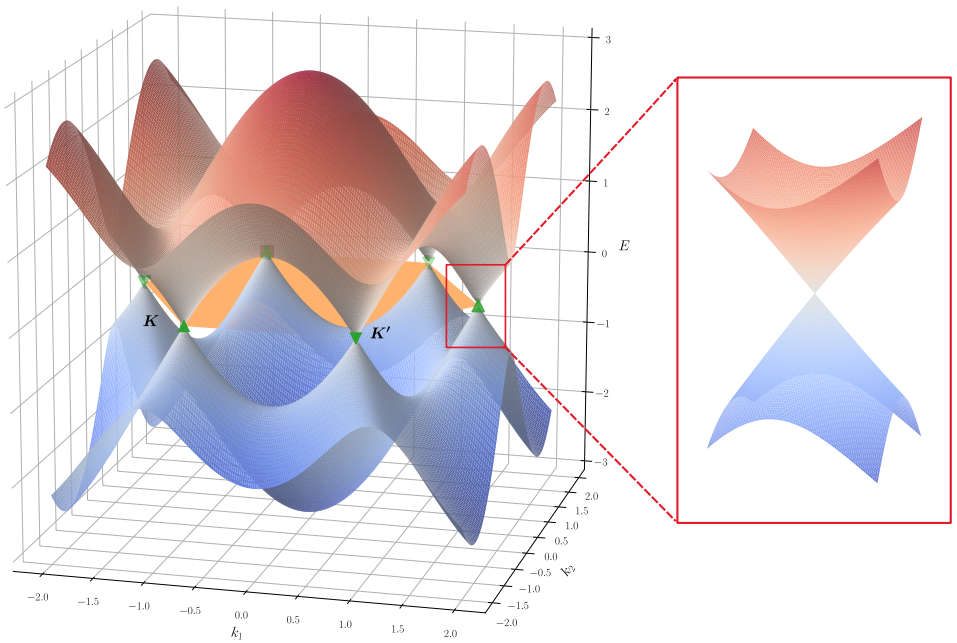
Dirac points for Graphene

Physically relevant part of dispersion relation is ≈ 0 frequency, at Brillouin zone corners Dirac points $\boldsymbol{K}, \boldsymbol{K}'$ (green triangles).



Can we derive an effective description of dynamics at these points?

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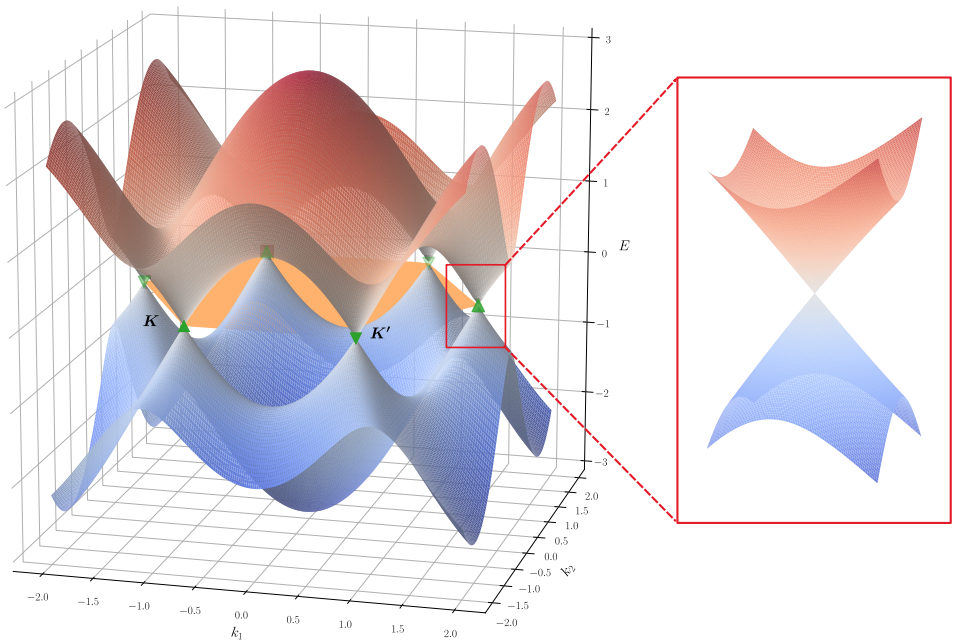

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Consider the tight-binding model of graphene $i\partial_t\psi = H\psi$, with initial data a wave-packet localized at $\boldsymbol{K}$, with spectral width $\epsilon \ll 1$

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The solution evolves as a wave-packet up to $t \sim \epsilon^{-2+\delta}$ (any $\delta > 0$)

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envelopes modulated by the massless Dirac equation ($D := -i\partial$)

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Tight-binding model for twisted bilayer graphene

Define the bilayer Hilbert space $\mathcal{H} := \ell^2(\Lambda_1; \mathbb{C}^2) \oplus \ell^2(\Lambda_2; \mathbb{C}^2)$,

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \psi_i = (\psi_{\boldsymbol{R}_i})_{\boldsymbol{R}_i \in \Lambda_i}, \quad \psi_{\boldsymbol{R}_i} = \begin{pmatrix} \psi^A_{\boldsymbol{R}_i} \\ \psi^B_{\boldsymbol{R}_i} \end{pmatrix}, \quad i \in \{1, 2\}.$$

We consider the model $i\partial_t \psi = H\psi$, with

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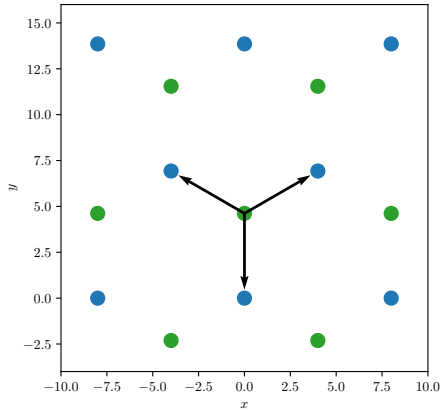
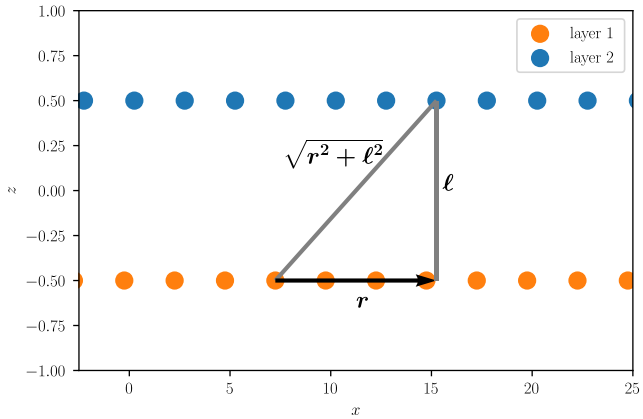
For the intralayer terms, we take the monolayer Hamiltonian with nearest-neighbor hopping.





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$$(H_{12}\psi_2)^{\sigma}_{\boldsymbol{R}_1} := \sum_{\boldsymbol{R}_2 \in \Lambda_2} \sum_{\sigma' \in \{A,B\}} h\left(\sqrt{\left|\boldsymbol{R}_1 + \boldsymbol{\tau}_1^{\sigma} - \boldsymbol{R}_2 - \boldsymbol{\tau}_2^{\sigma'}\right|^2 + \ell^2}\right) \psi^{\sigma'}_{\boldsymbol{R}_2},$$

where $h : \mathbb{R}_{\geqslant 0} \to \mathbb{R}$ decays, and $\ell > 0$ is the interlayer distance.

We emphasize that H is aperiodic for generic (irrational) θ!

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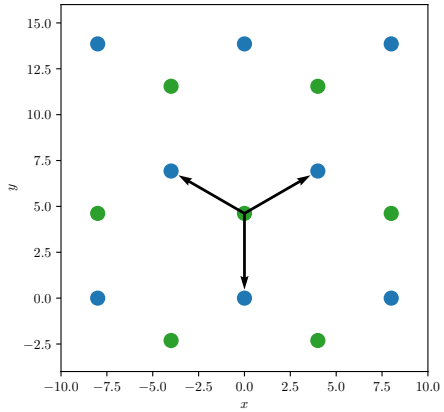

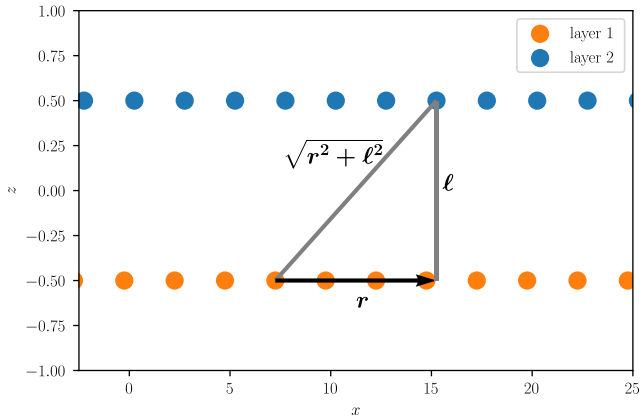

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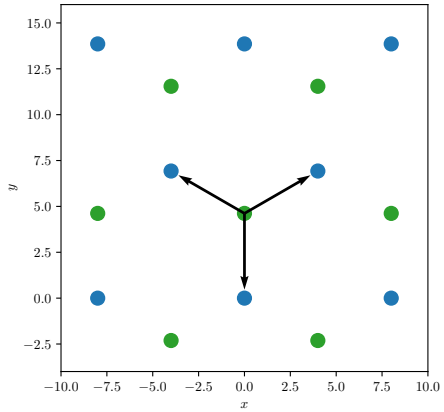

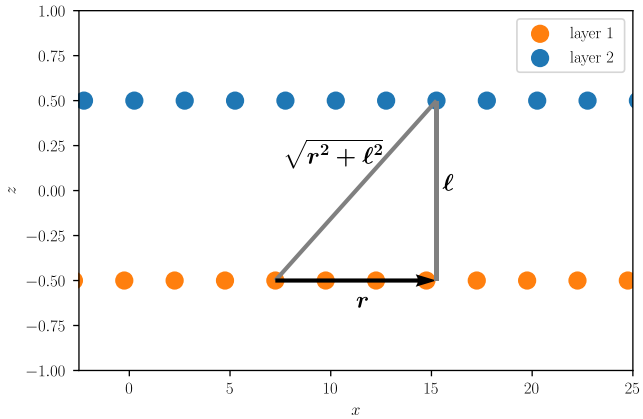

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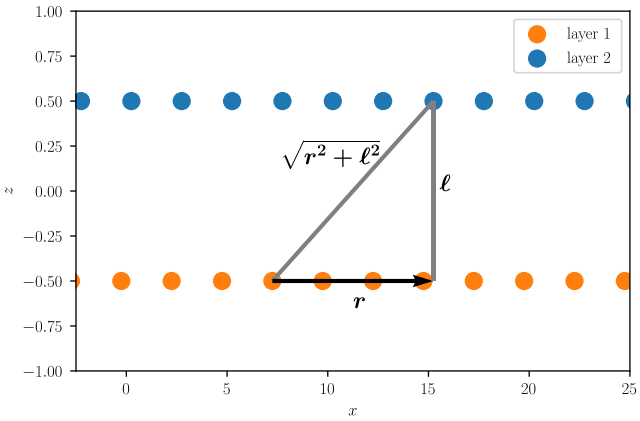
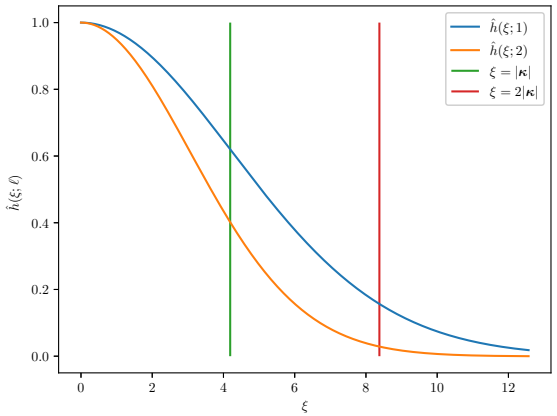
Key assumption

Consider the two-dimensional Fourier transform of the interlayer hopping function, depending on interlayer distance $\ell > 0$

$$\hat{h}(\boldsymbol{\xi}; \ell) := \int_{\mathbb{R}^2} e^{-i\boldsymbol{\xi}\cdot\boldsymbol{r}} h\left(\sqrt{|\boldsymbol{r}|^2 + \ell^2}\right) \, \mathrm{d}\boldsymbol{r}.$$





Assumption (roughly stated)

$\hat{h}(\xi;\ell)$ is Lipschitz in ξ, and $|\hat{h}(\xi;\ell)| \sim e^{-\ell|\xi|}$

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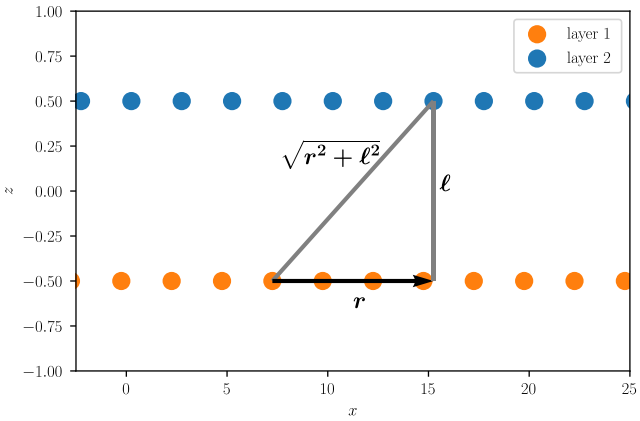

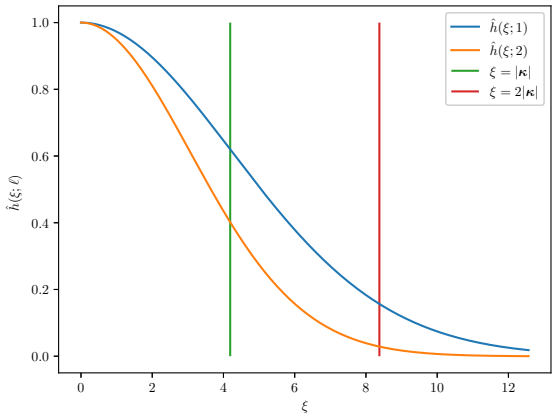

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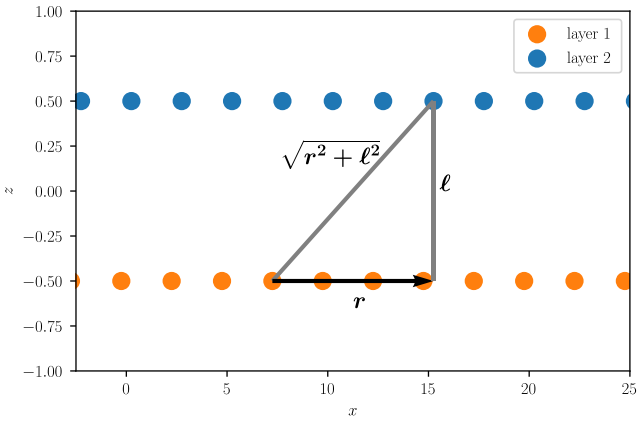

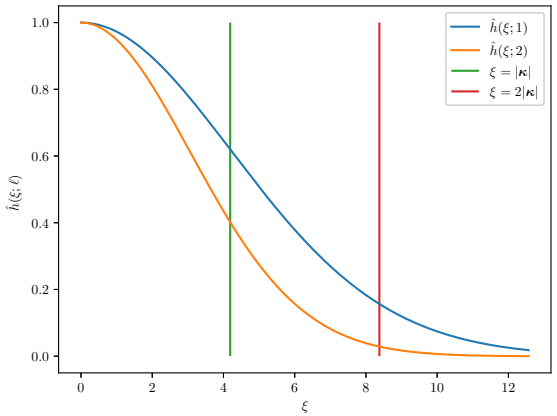

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Consider the tight-binding model of twisted bilayer graphene $i\partial_t\psi = H\psi$, with wave-packet initial data $\psi(0) = \psi_0$ localized at $\boldsymbol{K}_i$ in layer i, with spectral width $\epsilon \ll 1$.

Suppose h satisfies the assumption, and ℓ and θ satisfy

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Then, $\psi(t)$ evolves as wave-packet up to $t \sim \epsilon^{-2+\delta}$ (any $\delta > 0$), with envelopes $f = (f_1^A, f_1^B, f_2^A, f_2^B)^\top$ modulated by

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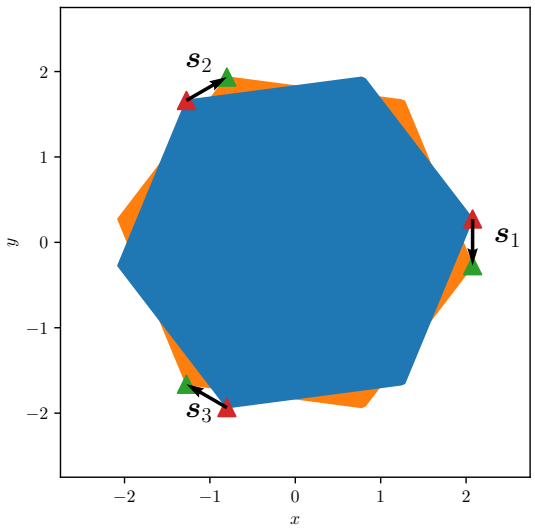
Moiré potential

Difficult part: simplifying interlayer terms using properties of momentum space interlayer hopping $\hat{h}$ to moiré potential

$$T(\boldsymbol{r}) := \hat{h}(|\boldsymbol{K}|;\ell)\left(T_1 e^{i\boldsymbol{s}_1\cdot\boldsymbol{r}} + T_2 e^{i\boldsymbol{s}_2\cdot\boldsymbol{r}} + T_3 e^{i\boldsymbol{s}_3\cdot\boldsymbol{r}}\right),$$

$\boldsymbol{s}_1, \boldsymbol{s}_2, \boldsymbol{s}_3$ displacements between twisted Dirac points, $\propto\theta$!



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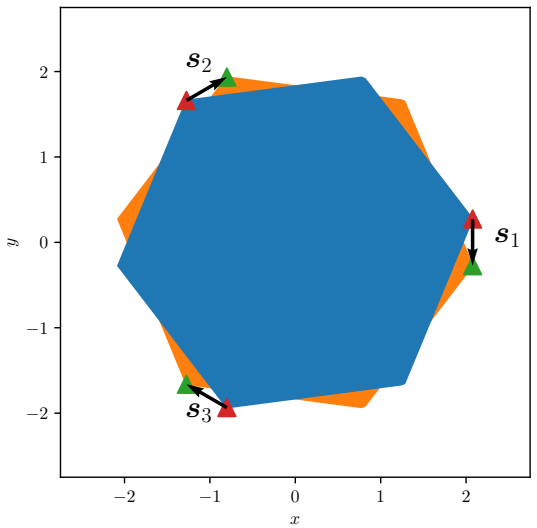
$$T(\boldsymbol{r}) := \hat{h}(|\boldsymbol{K}|;\ell)\left(T_1 e^{i\boldsymbol{s}_1\cdot\boldsymbol{r}} + T_2 e^{i\boldsymbol{s}_2\cdot\boldsymbol{r}} + T_3 e^{i\boldsymbol{s}_3\cdot\boldsymbol{r}}\right),$$

$\boldsymbol{s}_1, \boldsymbol{s}_2, \boldsymbol{s}_3$ displacements between twisted Dirac points, $\propto\theta$!



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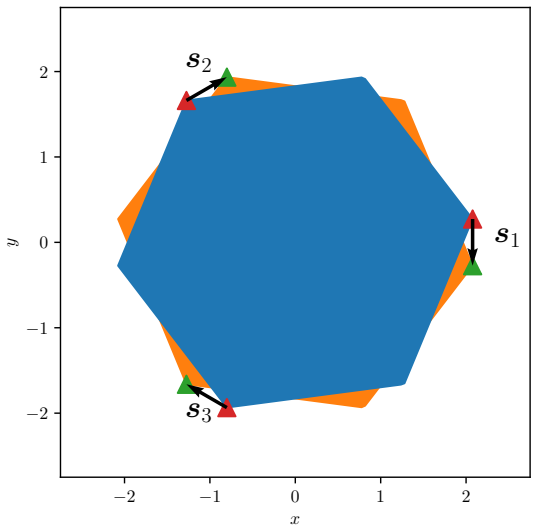

Relevance to for twisted bilayer graphene

Given the estimated physical value of $\hat{h}(|\boldsymbol{\kappa}|;\ell)$*, and* θ *near to the first magic angle, does there exist a range of* ϵ *values, with* $\epsilon \ll 1$*, such that both conditions of our theorem hold*

$$|\hat{h}(|\boldsymbol{K}|;\ell)| \sim \epsilon, \quad \theta \lesssim \epsilon.$$

The interlayer hopping energy and monolayer graphene π-band energy scale is

$$\frac{\hat{\mathfrak{h}}(|\boldsymbol{K}|;L)}{|\Gamma|} \approx 110 \text{ meV}, \quad \frac{\hbar v_D}{a} \approx 2.6 \text{ eV},$$

so

$$\hat{h}(|\boldsymbol{\kappa}|;\ell) = \frac{\hat{\mathfrak{h}}(|\boldsymbol{K}|;L)}{|\Gamma|\left(\frac{\hbar v_D}{a}\right)} \approx \frac{110 \text{ meV}}{2.6 \text{ eV}} \approx 0.042.$$

On the other hand, the first magic angle is at

$$\theta \approx 1^\circ \approx 0.017 \text{ radians}.$$

Relevance to strongly-correlated (many-body) electronic phases in TBG

Coulomb e-e interactions in hBN (which typically encapsulates TBG in experiments) at the magic angle moiré scale has energy scale

$$\frac{e^2}{4\pi\epsilon_{\text{hBN}}\left(\frac{a}{\theta}\right)} \approx 23 \text{ meV},$$

where ϵ_{hBN} is the permittivity of hBN $\approx 5\epsilon_0$. The interlayer hopping energy 110 meV suggests that e-e interaction terms couple only states that are described accurately by the BM model.

Coulomb e-e interactions do significantly affect the dynamics in TBG's flat moiré bands since their width can be as small as ≈ 10 meV.

Similar considerations apply to lattice-mediated interactions between electrons, which are characterized by a smaller energy scale ~ 1 meV .

Bistritzer-MacDonald dynamics in twisted bilayer graphene, Alexander B. Watson, Tianyu Kong, Allan H. MacDonald, and Mitchell Luskin. J. Math. Phys, 64:031502 (38pp), 2023.