Department of Physics

tu dortmund university

Photonic Band Theory of Moiré Crystals: A Two-Scale Approach

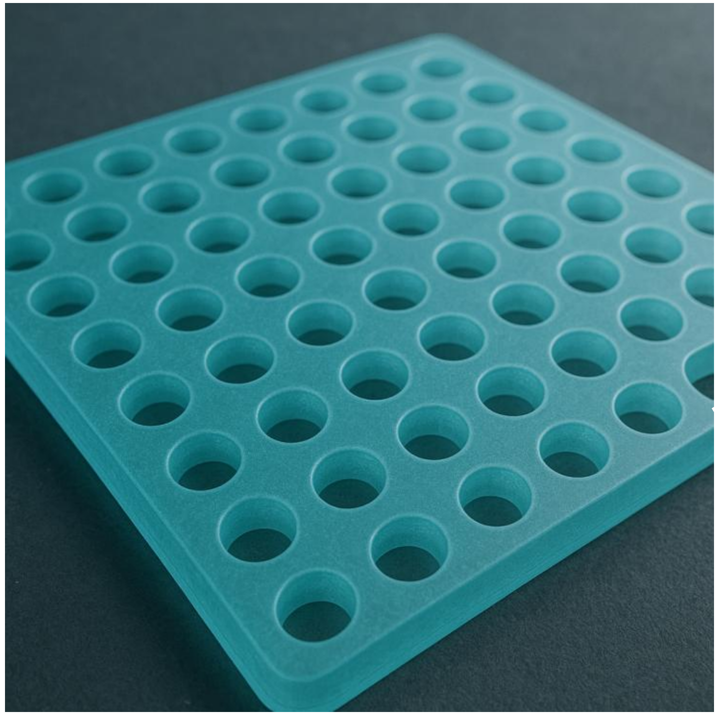
Master Thesis Presentation – CMT Seminar

Rene-Marcel Lehner

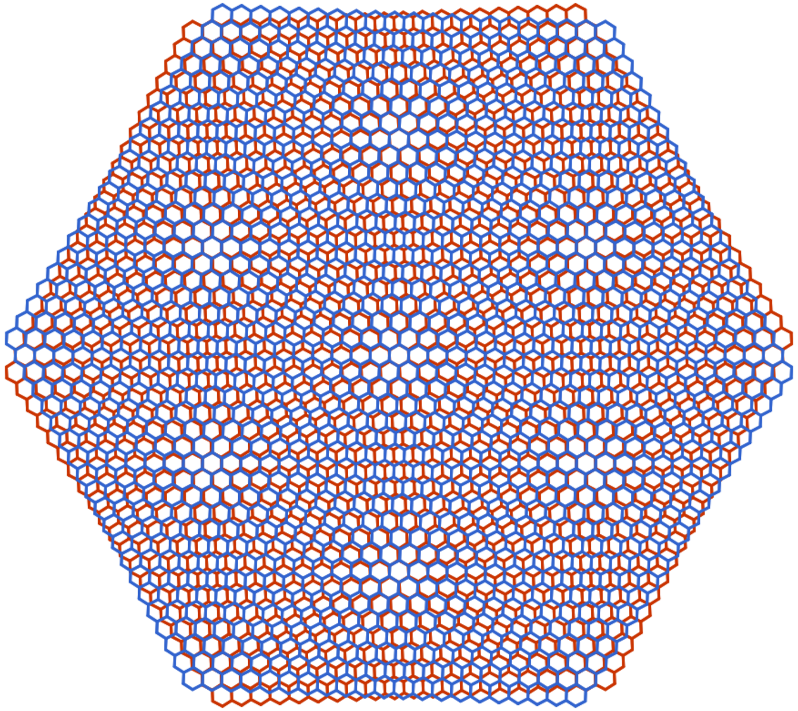
05/13/2026

Starting Point

Where	Nanostructures for Quantum Technologies Quantum Optics
What **System**	Photonic Crystals + Moiré Patterns
What **Goal**	Photonic Cavities; or other interesting properties



Illustrated with Dall·E



Cao et al., *Nature **556**, 80 (2018)*

Current Research on Photonic Moiré Crystals

2011, Bistritzer & McDonald (electronic; the starting point)

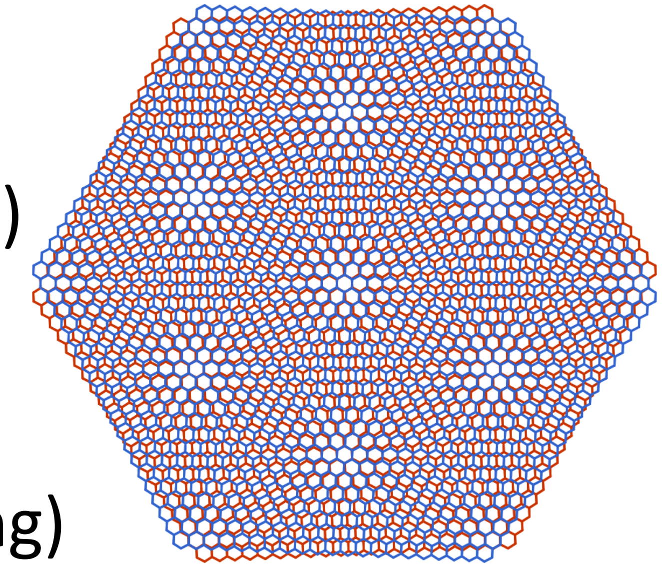
Continuum k·p model around graphene Dirac cones

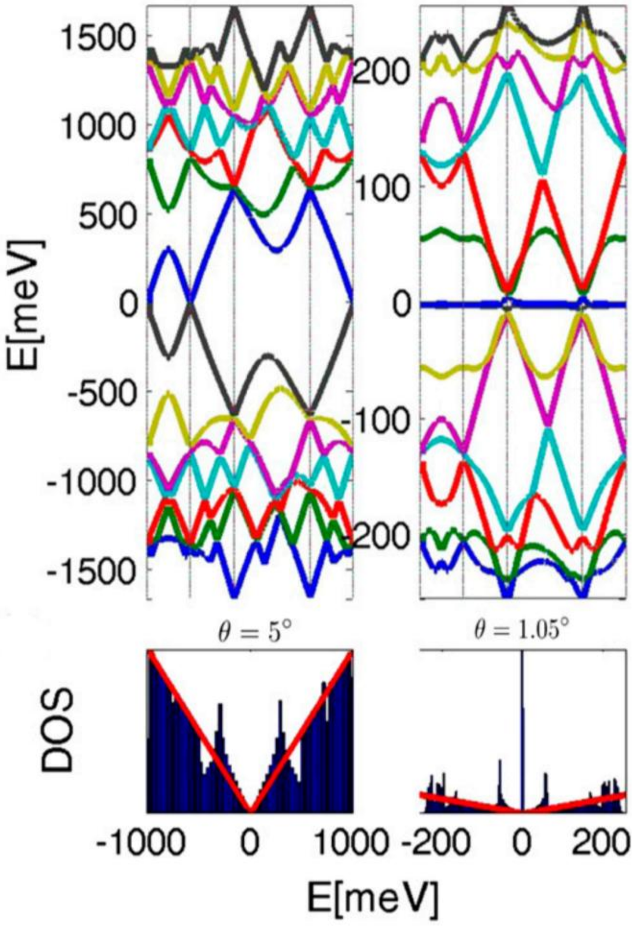
Found: Magic Angles

2021, Dong et al. (photonic continuum)

Photonic analogue of BM-Model

2021, Tang et al. (photonic tight-binding)

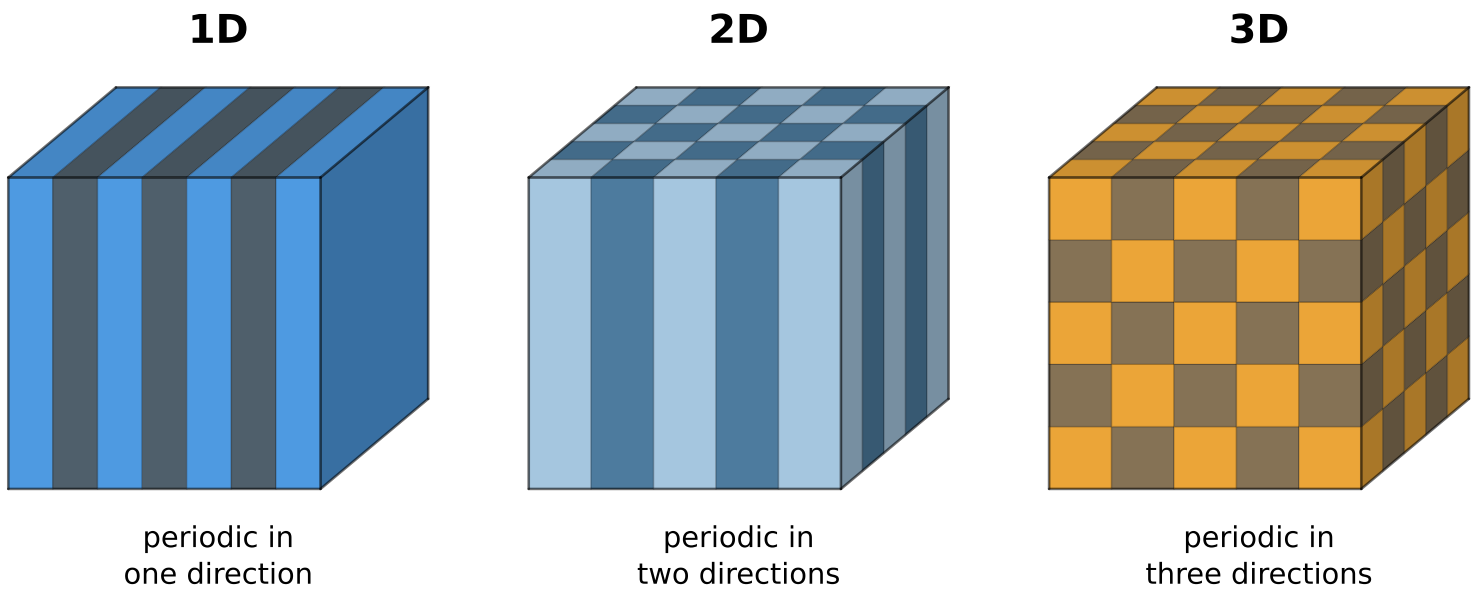




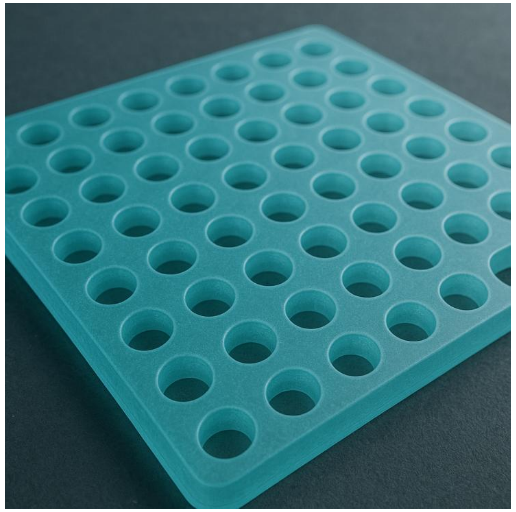
Bistritzer and MacDonald, *PNAS* ***108**, 30 (2011)*

Photonic Crystals

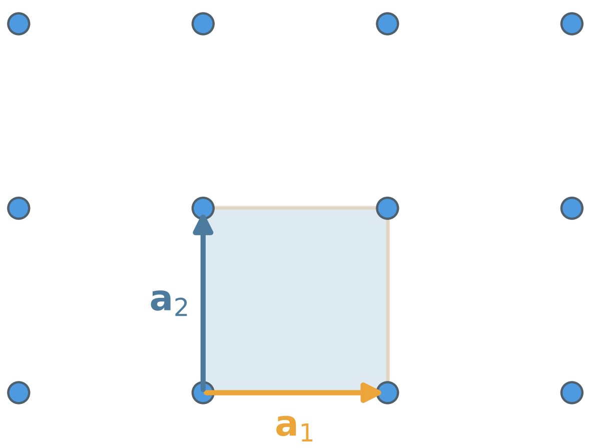
Dielectric Material + Periodicity = $\varepsilon(\boldsymbol{x})$



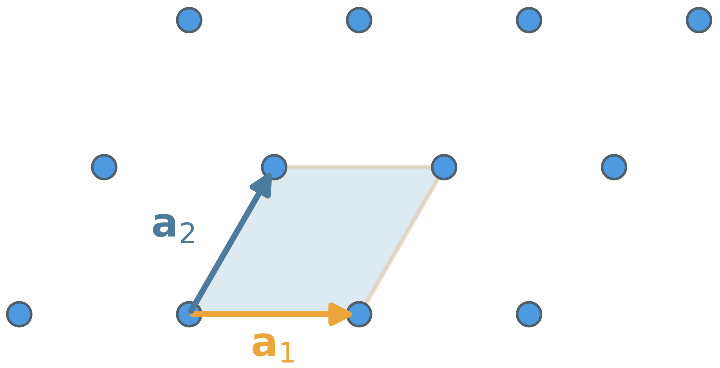
Photonic Crystals



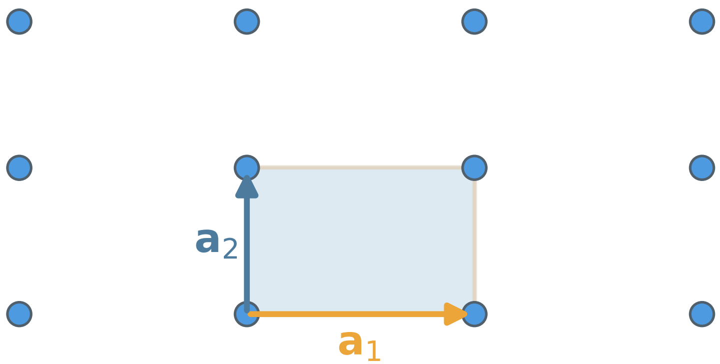
Square Lattice



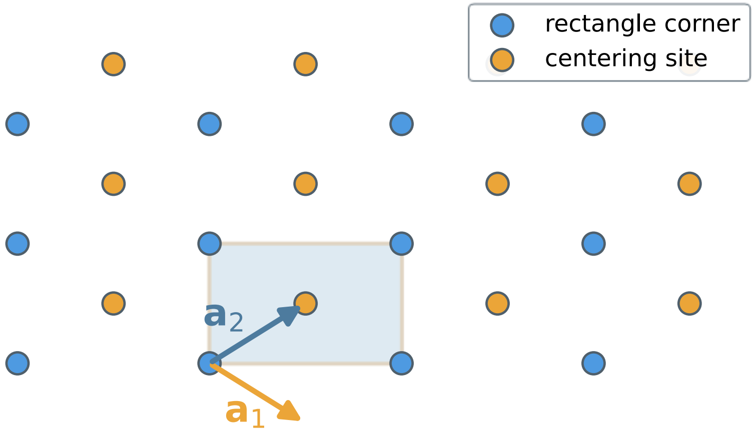
Hexagonal Lattice



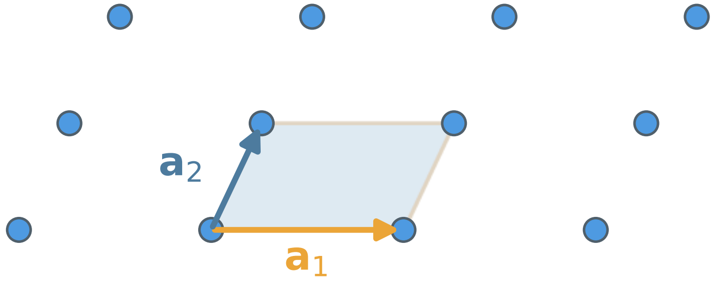
Rectangular Lattice



Centered-Rectangular Lattice



Oblique Lattice



Photonic Crystals

Maxwell's Equations + Time-Harmonic Fields

$$\boldsymbol{H}(\boldsymbol{x}, t) = \boldsymbol{H}(\boldsymbol{x})\mathrm{e}^{-\mathrm{i}\omega t}$$

Photonic Master Equation

$$\nabla \times \left(\frac{1}{\varepsilon(\boldsymbol{x})} \nabla \times \boldsymbol{H}(\boldsymbol{x}) \right) = \frac{\omega^2}{c^2} \boldsymbol{H}(\boldsymbol{x}),$$

This is an **Eigenvalue Equation**:

$$A\psi(\boldsymbol{x}) = \lambda B \psi(\boldsymbol{x}), \quad \lambda = \frac{\omega^2}{c^2}$$

Photonic Bands

Photonic Master Equation

$$\nabla \times \left(\frac{1}{\varepsilon(\boldsymbol{x})} \nabla \times \boldsymbol{H}(\boldsymbol{x}) \right) = \frac{\omega^2}{c^2} \boldsymbol{H}(\boldsymbol{x}),$$

Periodic Media: $\varepsilon(\boldsymbol{x} + \boldsymbol{T}) = \varepsilon(\boldsymbol{x})$

Bloch's Theorem: $\boldsymbol{H}_{n\boldsymbol{k}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \boldsymbol{u}_{n\boldsymbol{k}}(\boldsymbol{x})$

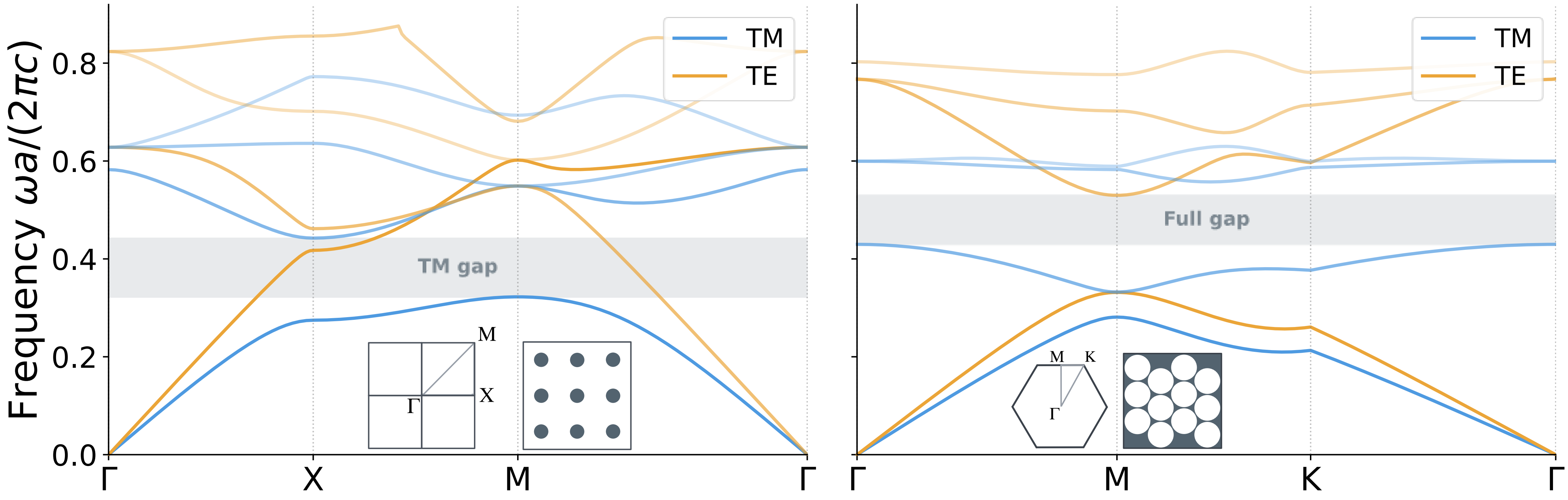
Photonic Band Equation

$$(\nabla + \mathrm{i}\boldsymbol{k}) \times \left[\frac{1}{\varepsilon(\boldsymbol{x})} (\nabla + \mathrm{i}\boldsymbol{k}) \times \boldsymbol{u}_{n\boldsymbol{k}}(\boldsymbol{x}) \right] = \frac{\omega_{n\boldsymbol{k}}^2}{c^2} \boldsymbol{u}_{n\boldsymbol{k}}(\boldsymbol{x}),$$

Photonic Bands

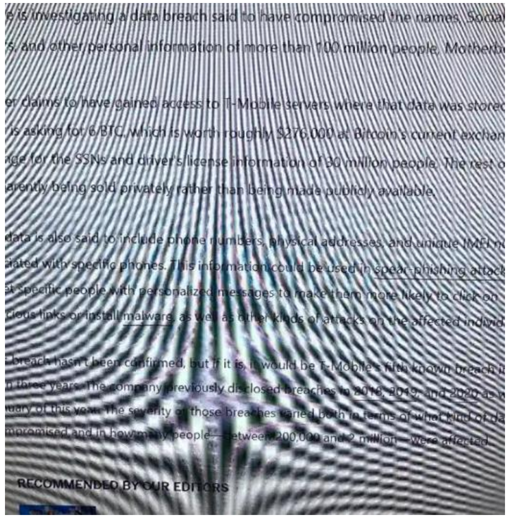
Photonic Band Equation

$$(\nabla + \mathrm{i}\boldsymbol{k}) \times \left[\frac{1}{\varepsilon(\boldsymbol{x})} (\nabla + \mathrm{i}\boldsymbol{k}) \times \boldsymbol{u}_{n\boldsymbol{k}}(\boldsymbol{x}) \right] = \frac{\omega_{n\boldsymbol{k}}^2}{c^2} \boldsymbol{u}_{n\boldsymbol{k}}(\boldsymbol{x}),$$

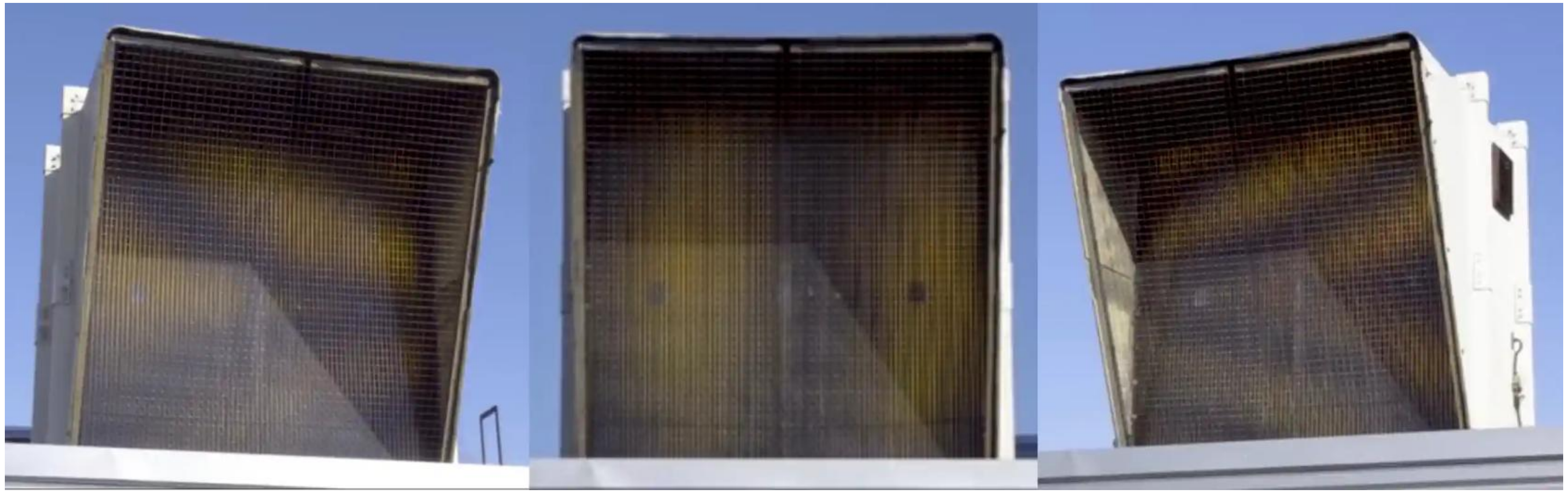


Moiré Effect

Day-to-Day examples: Images of periodic patterns

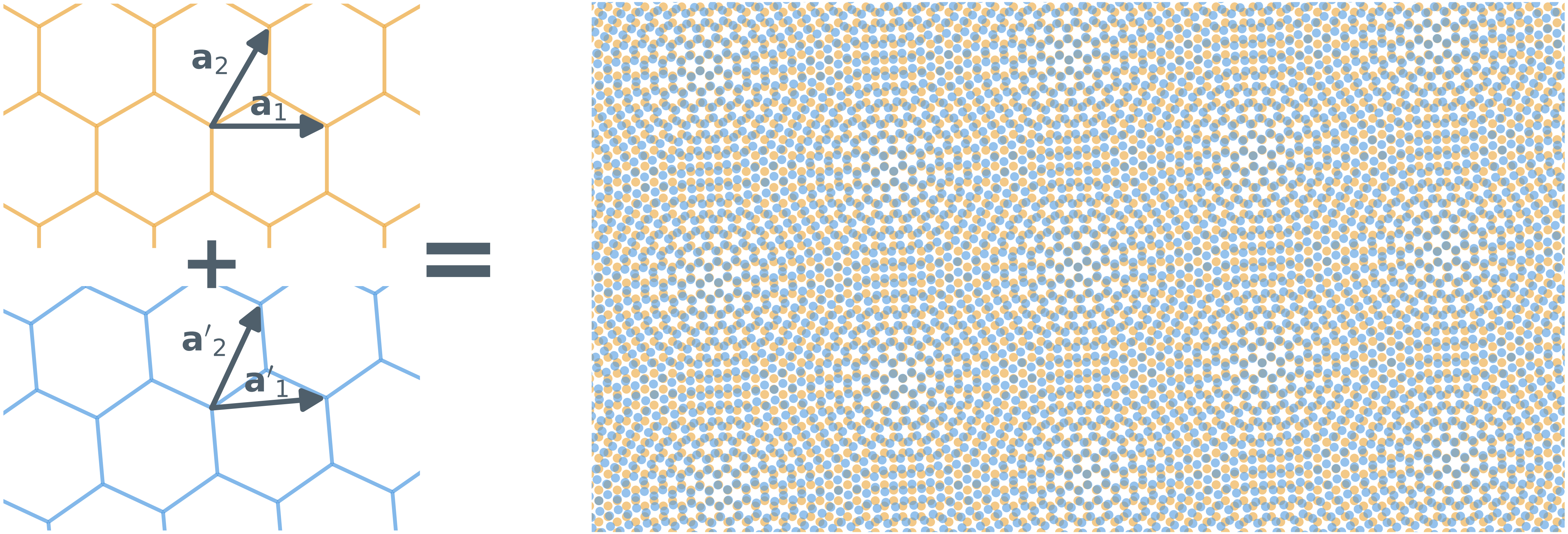


Inogon Lights (1980s)



Images from the web: *Reddit [1], Photography Blog [2], Wikipedia [3]*

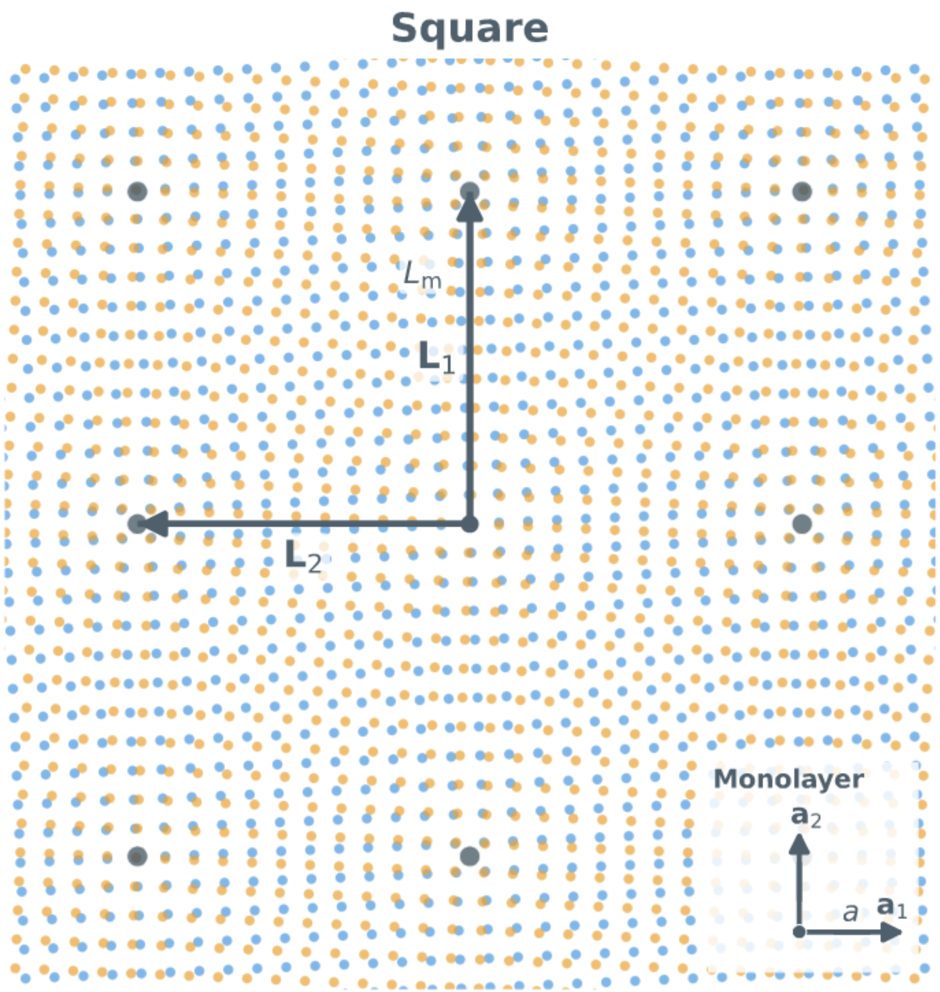
(Two) *Twisted* Bravais Lattices = Moiré Lattice

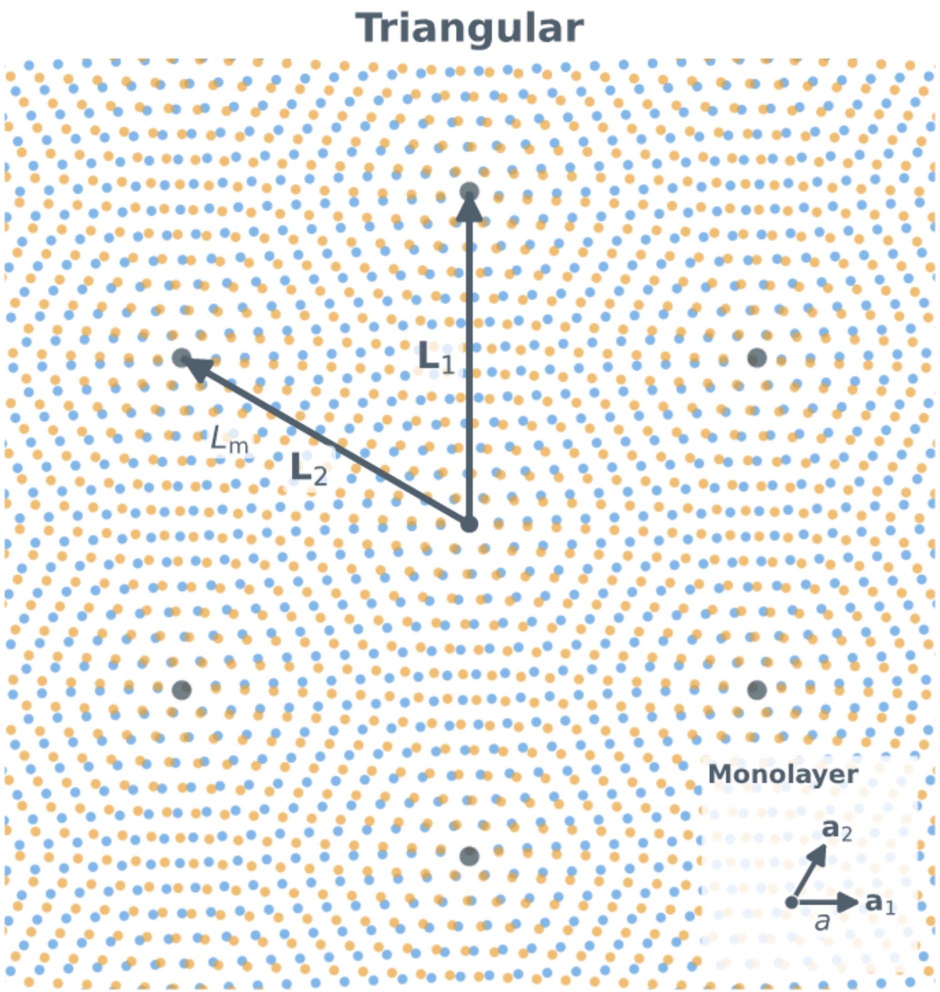


$\Theta = 5°$ Twist

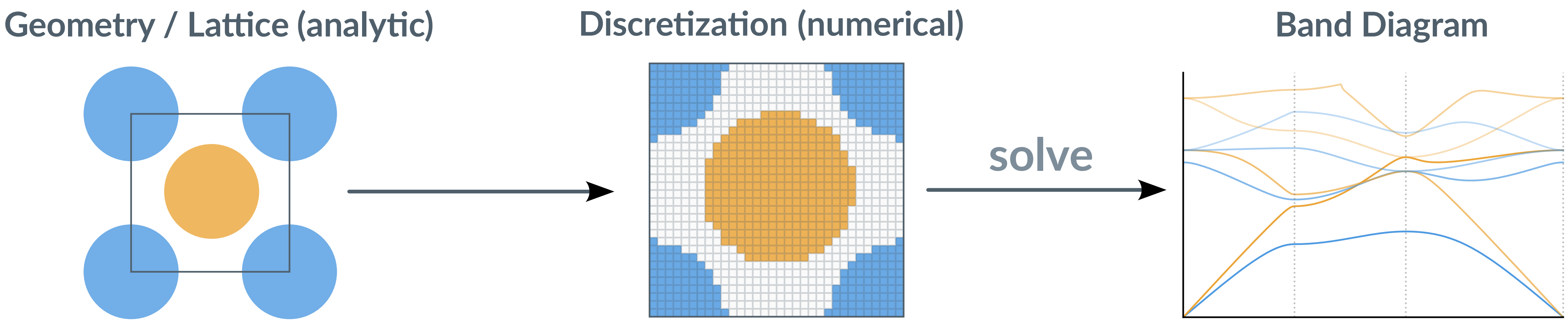
(Two) *Twisted* Bravais Lattices = Moiré Lattice
"Twisted Bilayer"

$\Theta = 5°$ Twist





Intuition: Apply the monolattice workflow



Not possible: Computationally *AND* Conceptually

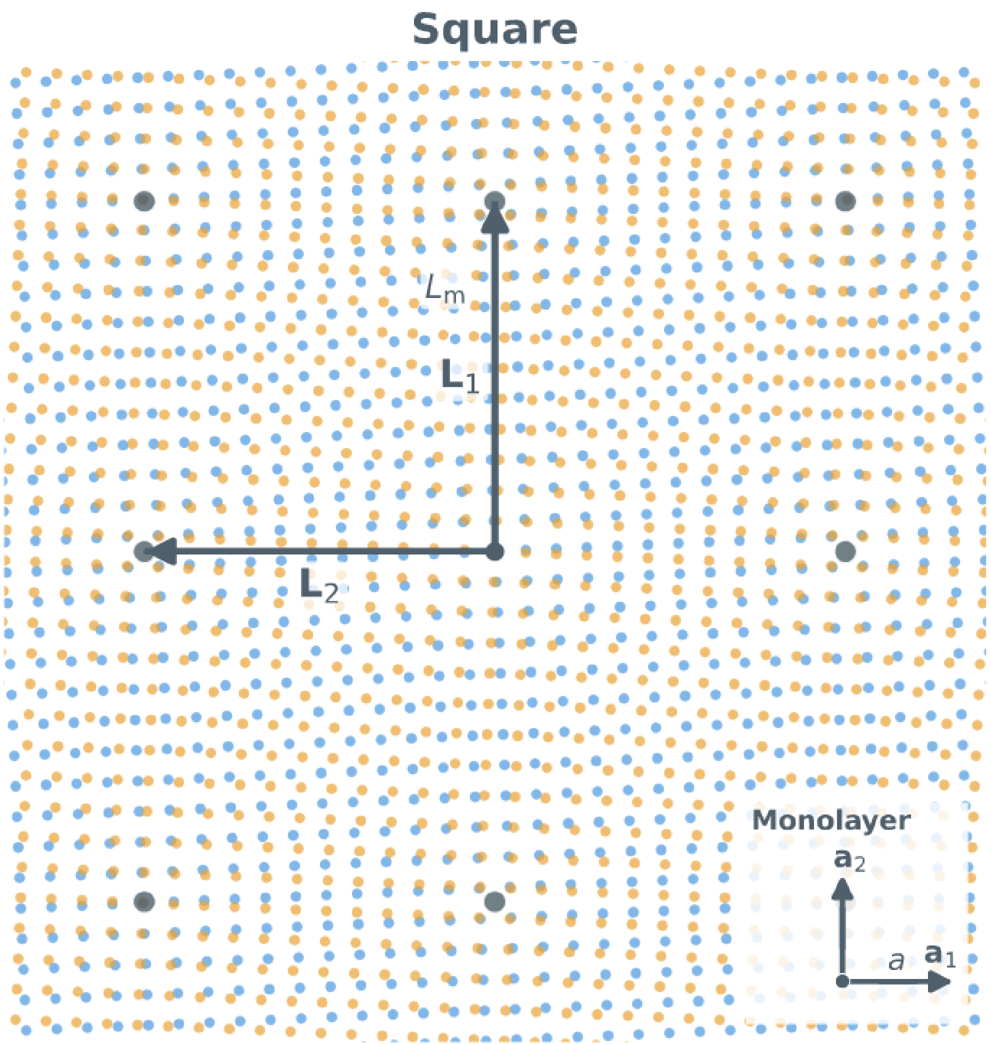
Conceptual Mismatch

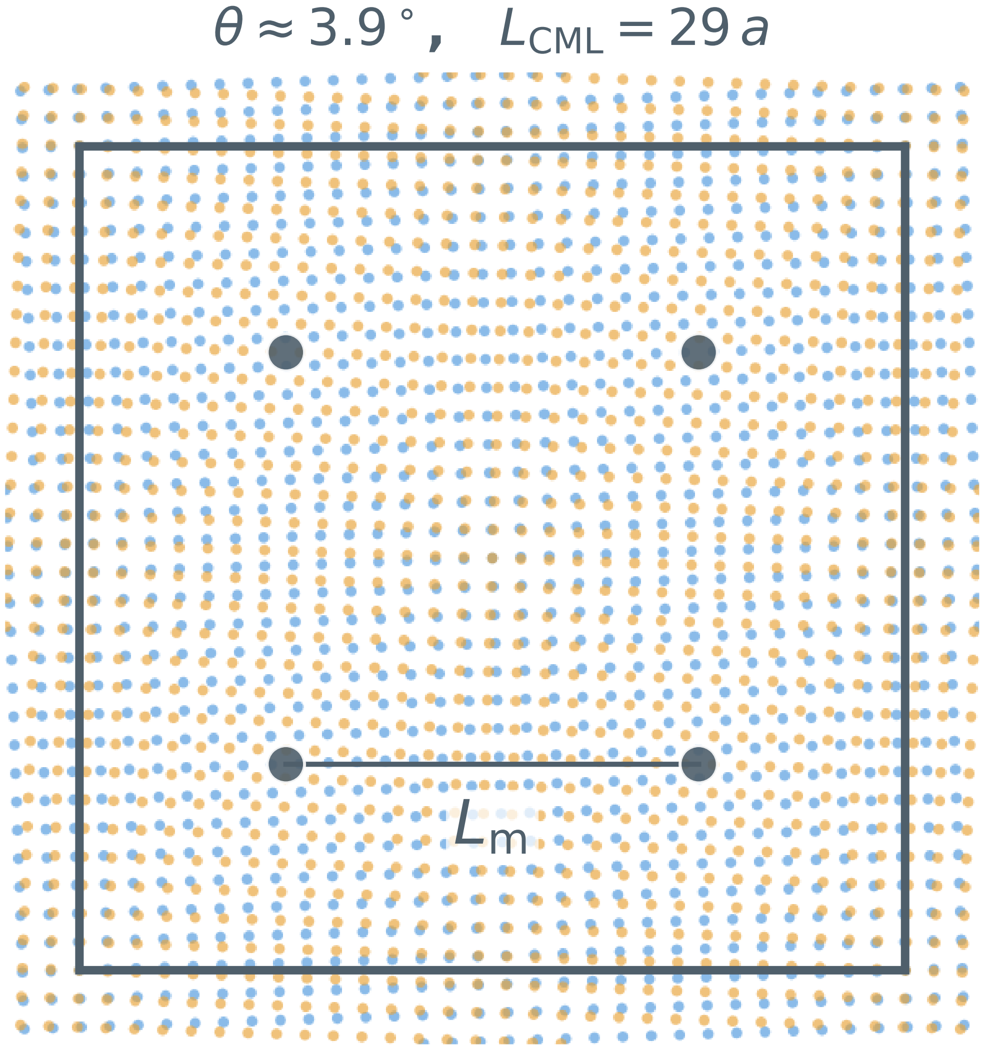
Needed:

Commensurability

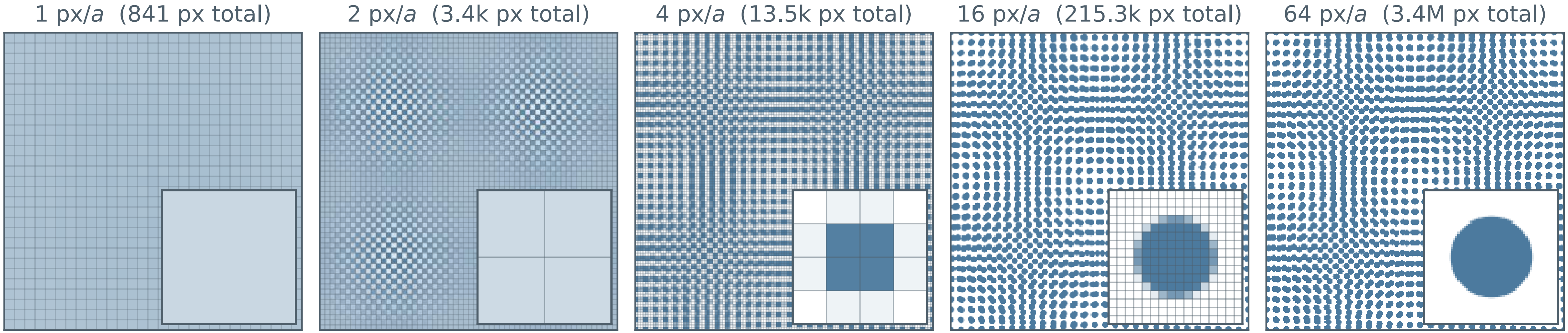
Moiré Lattices are generally

Quasi-Periodic





Computational Bottleneck

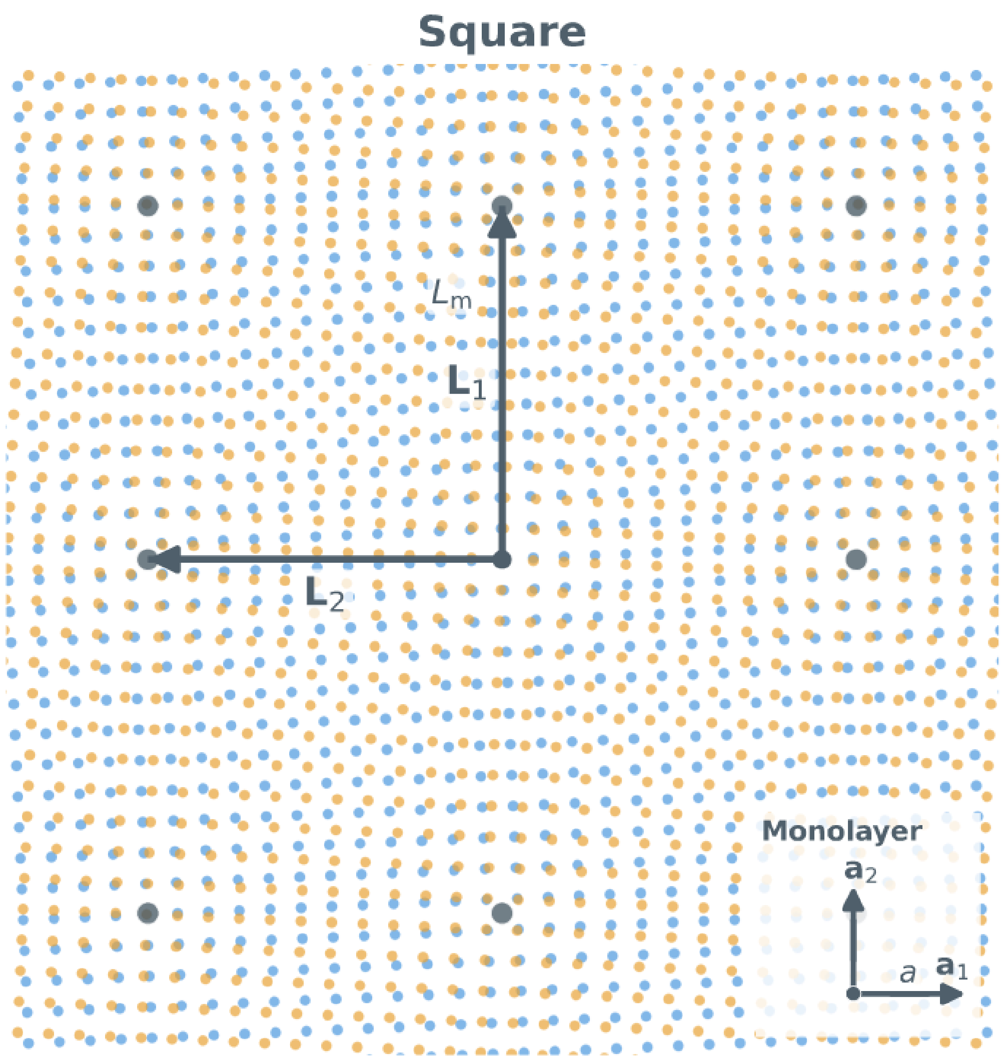


$\Theta = 2°$ twisted square bilayer

Moiré Grid Size

$$N_{\text{grid}} = \left(\frac{N_{\text{px}}}{a}\right)^2 \times \left(\frac{L_m}{a}\right)^2 \approx \frac{N_{\text{px}}^2}{\theta^2}$$

Ansatz for a New Description: Recognizing Two Scales



Scaling Parameter

$$\eta := \frac{a}{L} \ll 1$$

Dimensionless Coordinates

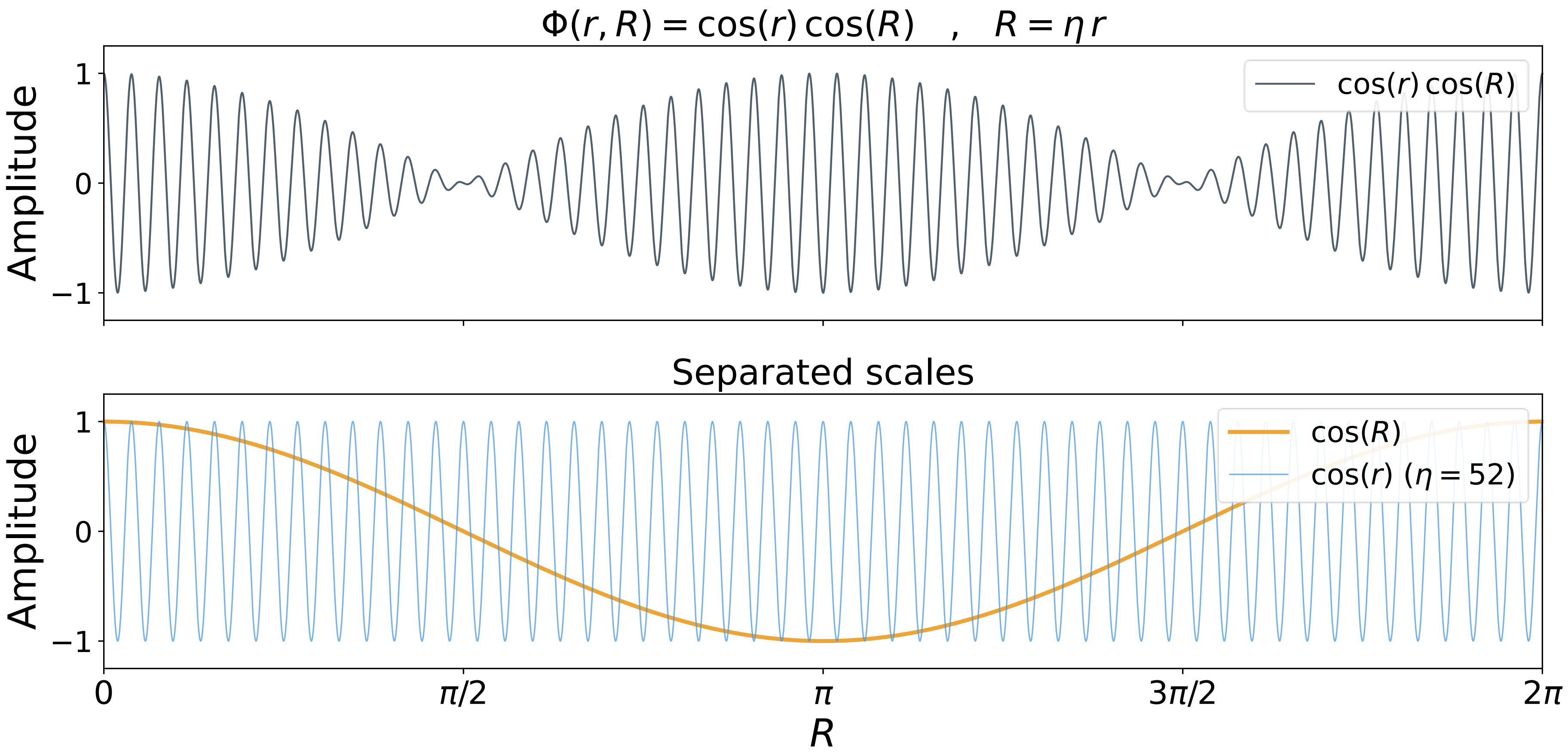
$$\boldsymbol{r} := \frac{\boldsymbol{x}}{a}, \quad \boldsymbol{R} := \frac{\boldsymbol{x}}{L}$$

$$\boldsymbol{R} = \eta \boldsymbol{r}$$

$$\varepsilon(\boldsymbol{x}) \to \varepsilon(\boldsymbol{r}, \boldsymbol{R})$$

$$\nabla_{\boldsymbol{x}} \to \frac{1}{a}(\nabla_{\boldsymbol{r}} + \eta \nabla_{\boldsymbol{R}})$$

Recognizing Two Scales



Envelope Approximation

Photonic Master Equation

$$\nabla \times \left(\frac{1}{\varepsilon(\boldsymbol{x})} \nabla \times \boldsymbol{H}(\boldsymbol{x}) \right) = \frac{\omega^2}{c^2} \boldsymbol{H}(\boldsymbol{x}),$$

Multi-Band Envelope Ansatz

$$H_{\boldsymbol{k}_0 \boldsymbol{q}}(\boldsymbol{r}, \boldsymbol{R}) \approx \mathrm{e}^{\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{r}} \sum_{n=1}^{N} F_{n\boldsymbol{q}}(\boldsymbol{R}) u_{n\boldsymbol{k}_0}(\boldsymbol{r}; \boldsymbol{R}).$$

Result: Effective Hamiltonian

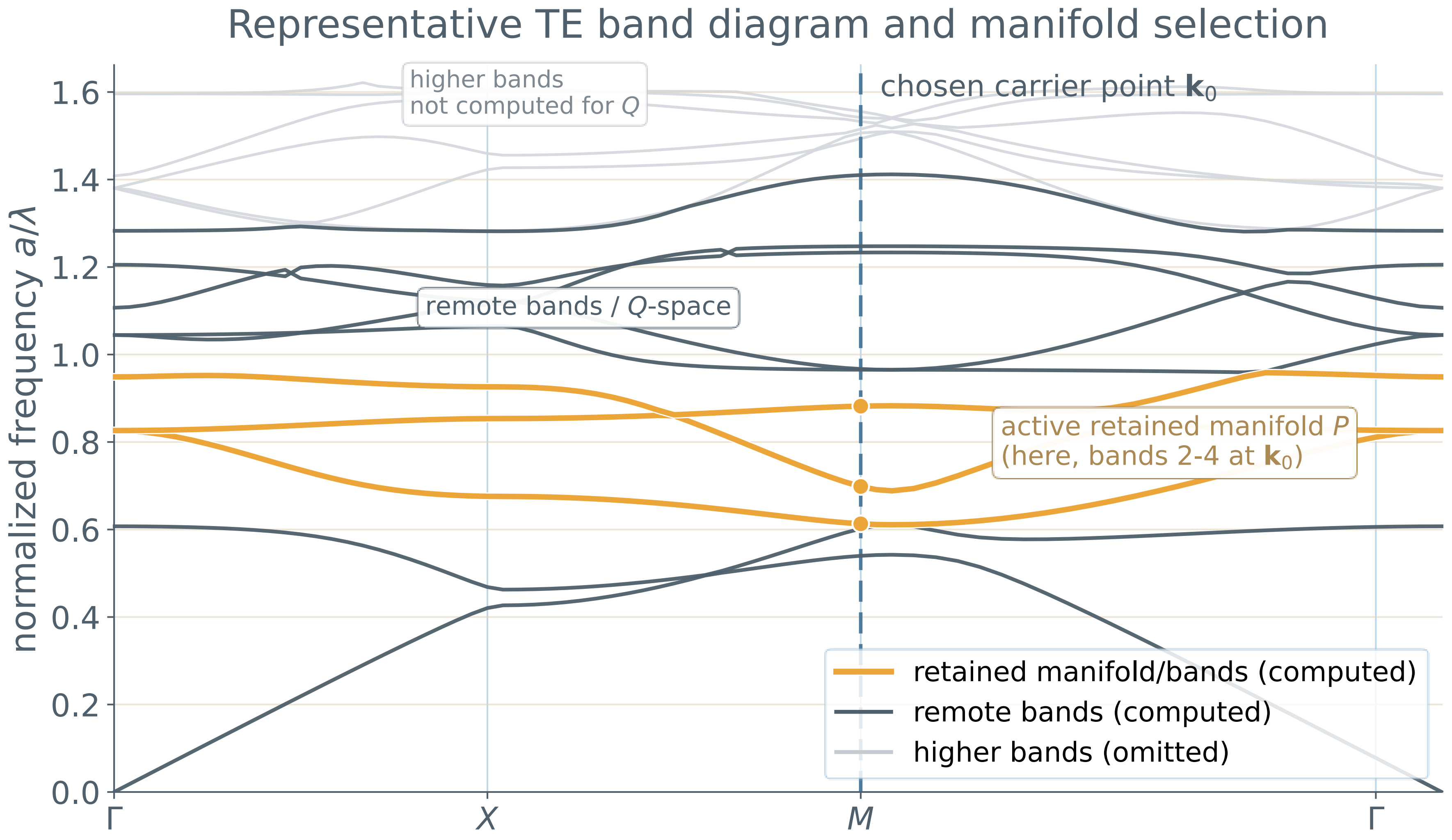
Effective Hamiltonian

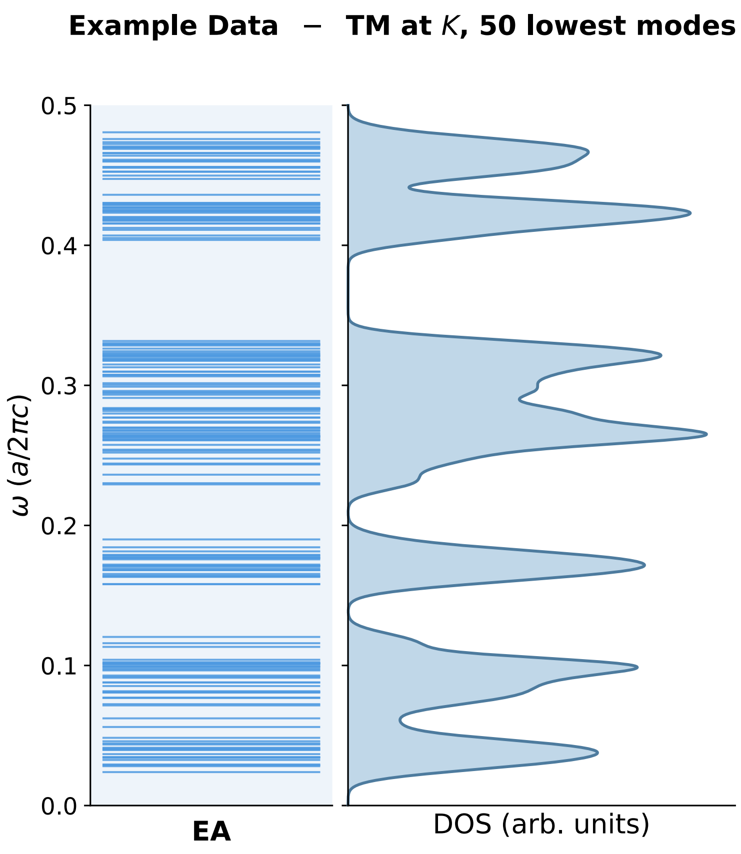
$$\mathcal{H}_{\text{eff}} \approx \Lambda + \eta \mathcal{H}_1 + \eta^2 \mathcal{H}_2$$

$$\mathcal{H}_{\text{eff}} \boldsymbol{f}_{\boldsymbol{q}} = \lambda \boldsymbol{f}_{\boldsymbol{q}}$$

How to **Use** the Envelope Approximation

$$\mathcal{H}_{\text{eff}} \boldsymbol{f_q} = \lambda \boldsymbol{f_q}$$





Problem: Data is ***unavailable***

Missing term	Why MPB cannot provide it
$v_{mn}^{(i)}$ velocity matrix elements	MPB is matrix-free and never builds the operator explicitly; inner products are inaccessible.
M_{ij}^{-1} inverse mass tensor	Requires off-diagonal couplings between retained and remote bands; blocked by matrix-free architecture.
$\Xi_i^{\dagger}\varepsilon^{-1}\Xi_i$ Born-Huang potential	The ε^{-1}-weighted overlap needs the explicit dielectric operator; MPB does not expose it.
Registry sweep throughput	MPB's geometry setup penalizes dense registry computations.

Solution: Blaze2D

A New Custom Maxwell Solver

```
pip install blaze2d
```

Method: Plane-Wave Expansion

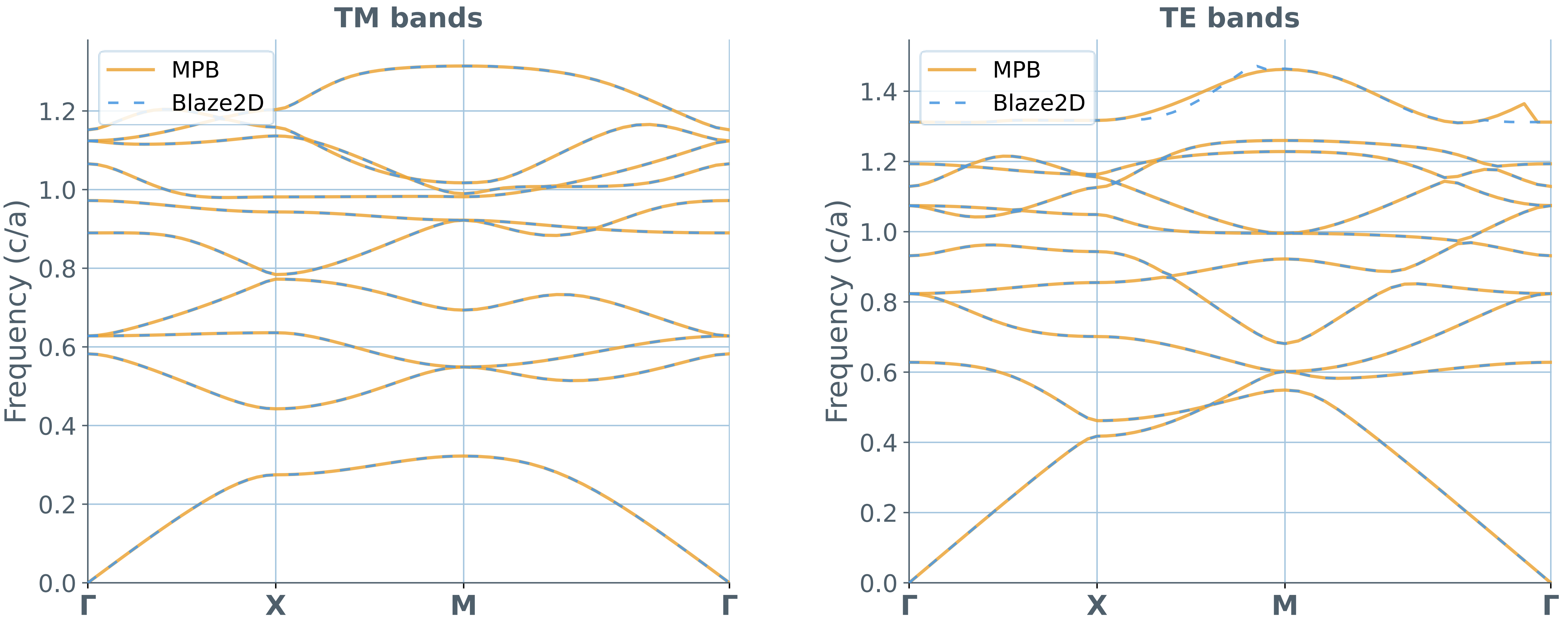
+

Algorithm: LOBPCG

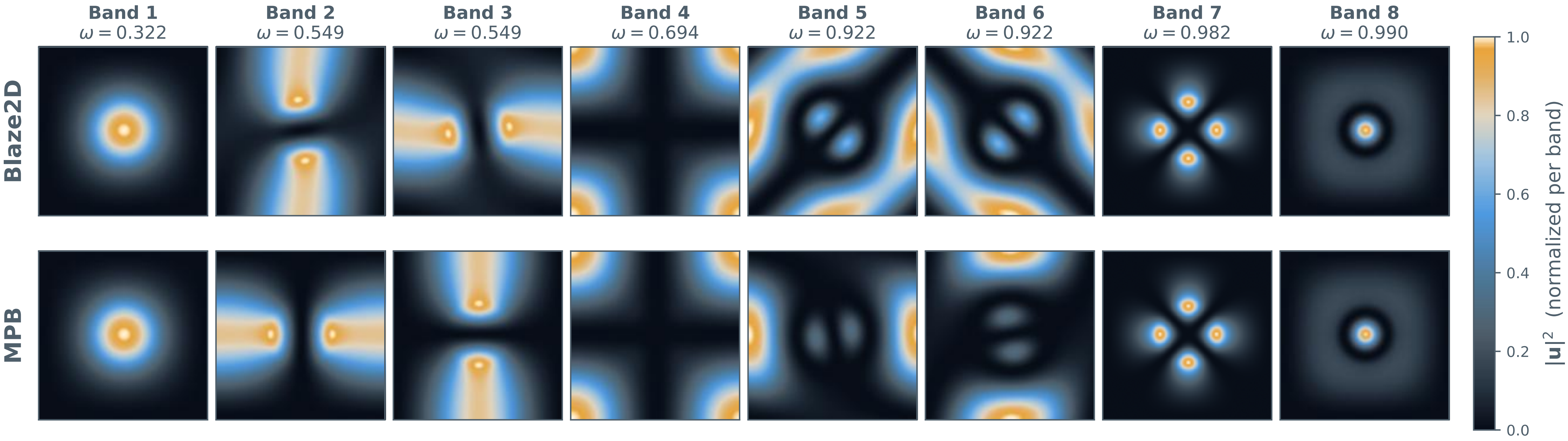
+

Language: Rust

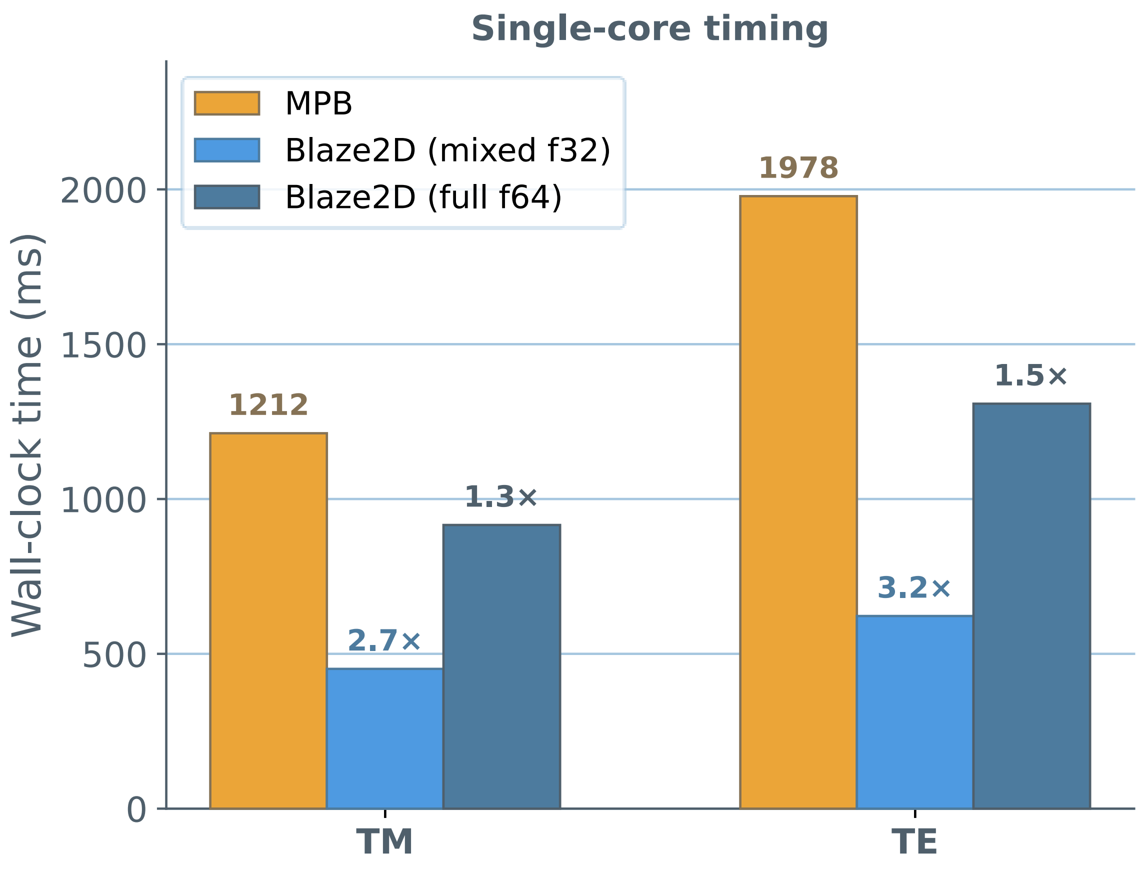
Validating Blaze with MPB

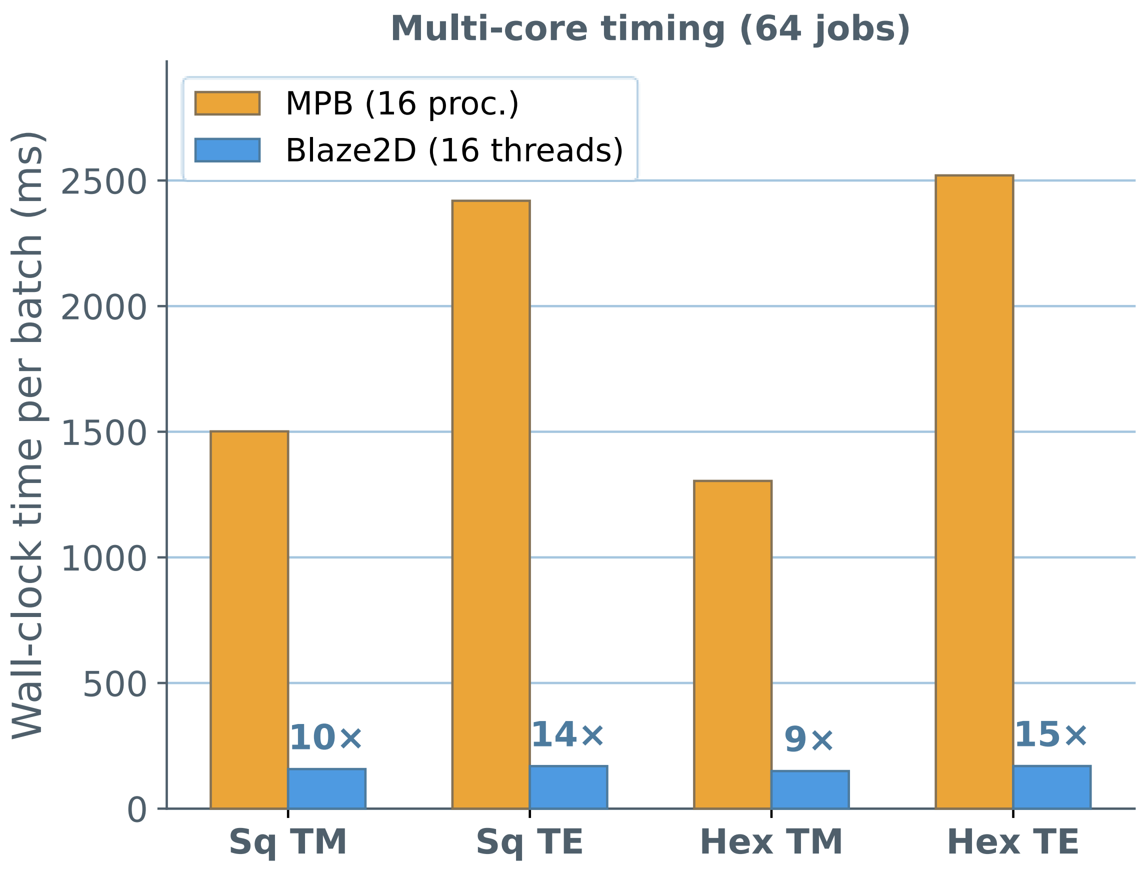


Validating Blaze with MPB



Benchmarking Blaze against MPB

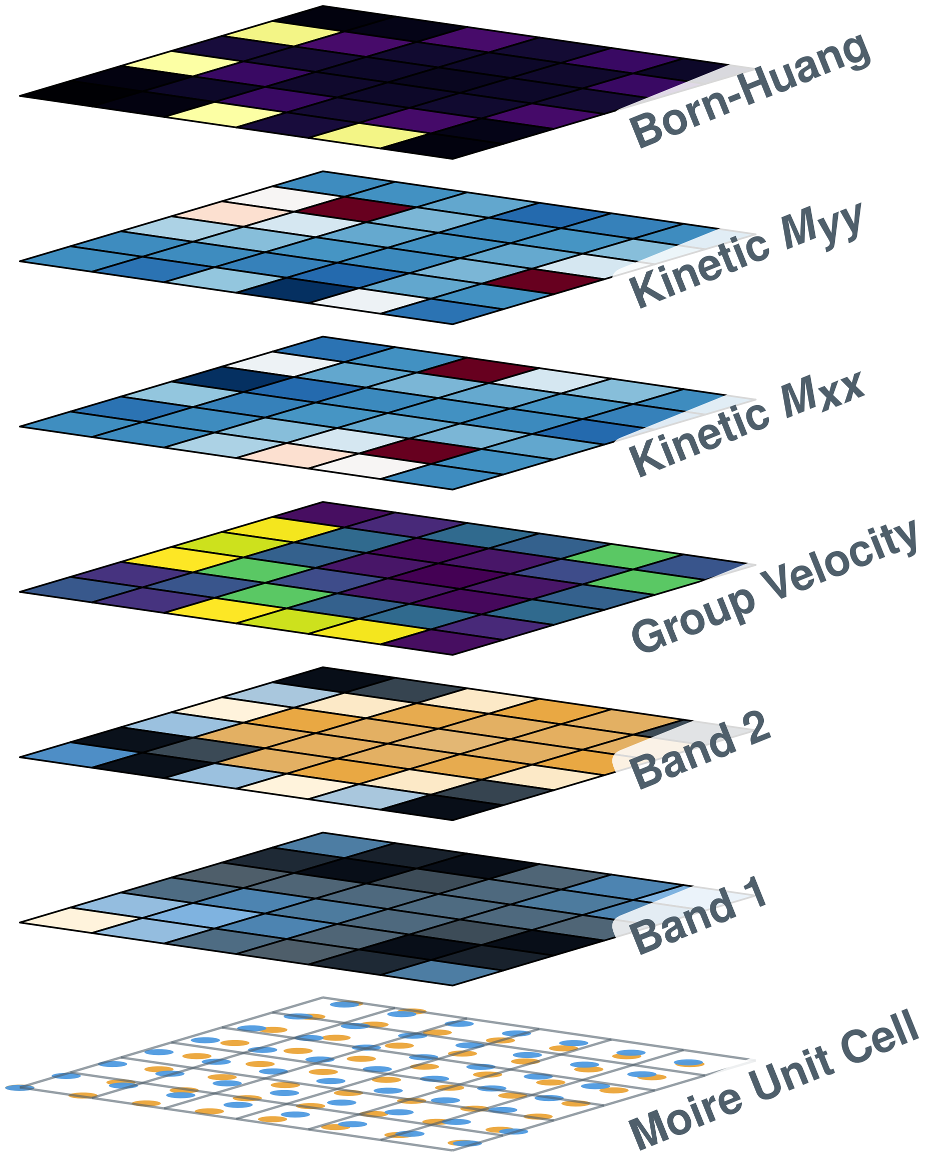




We can compute the **data**.

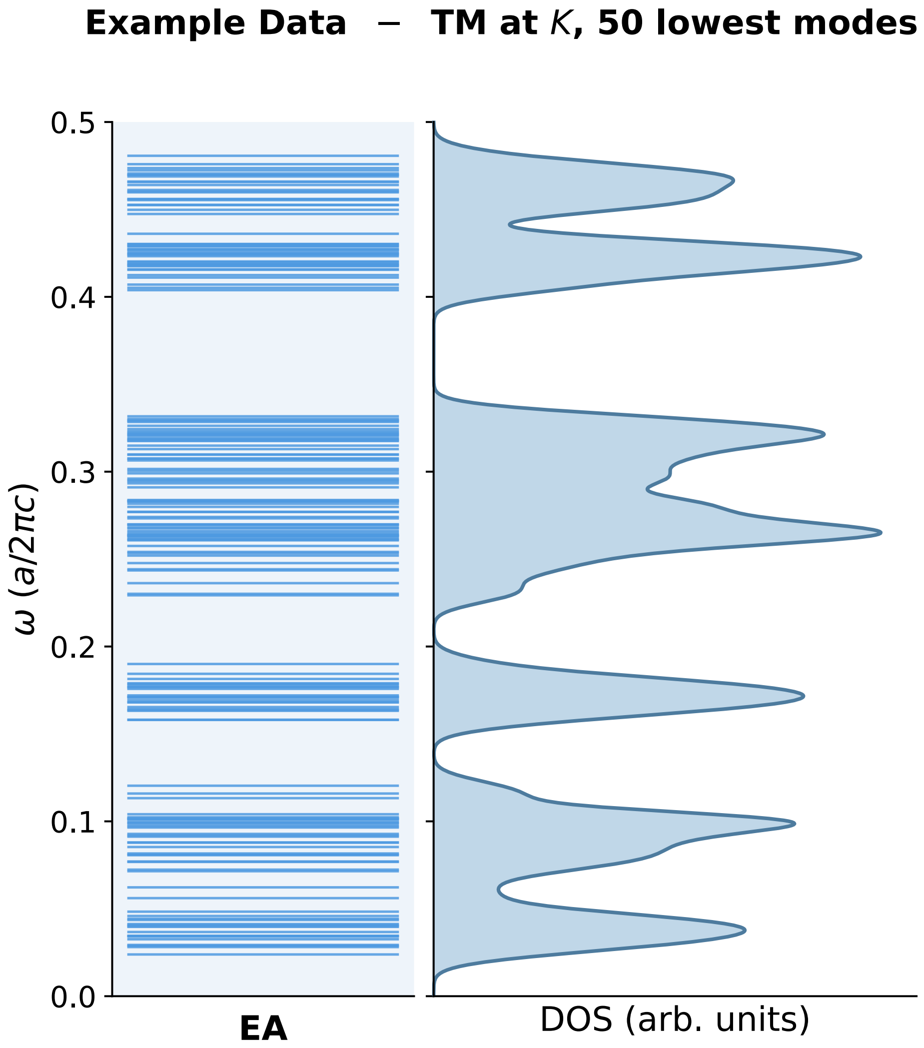
What now?

Building the EA Hamiltonian



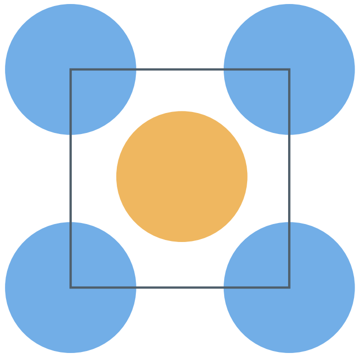
$$\mathcal{H}_{\text{eff}} \boldsymbol{f}_{\boldsymbol{q}} = \lambda \boldsymbol{f}_{\boldsymbol{q}}$$

$\mathcal{H}_{\text{eff}}$ `scipy.eigsh` →

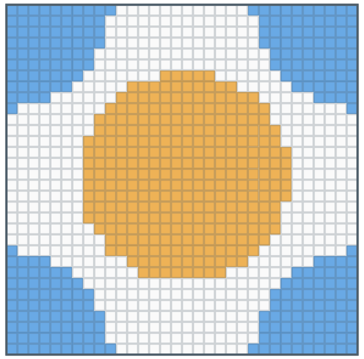


Building the EA Hamiltonian with *Blaze2D*

Geometry / Lattice (analytic)

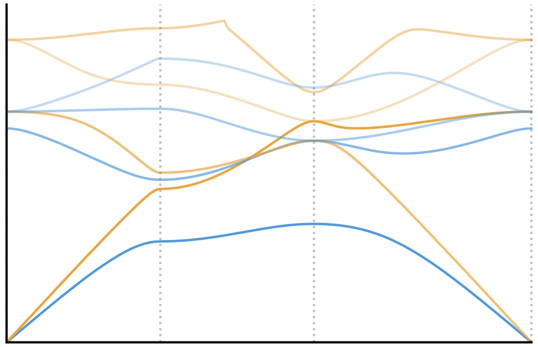


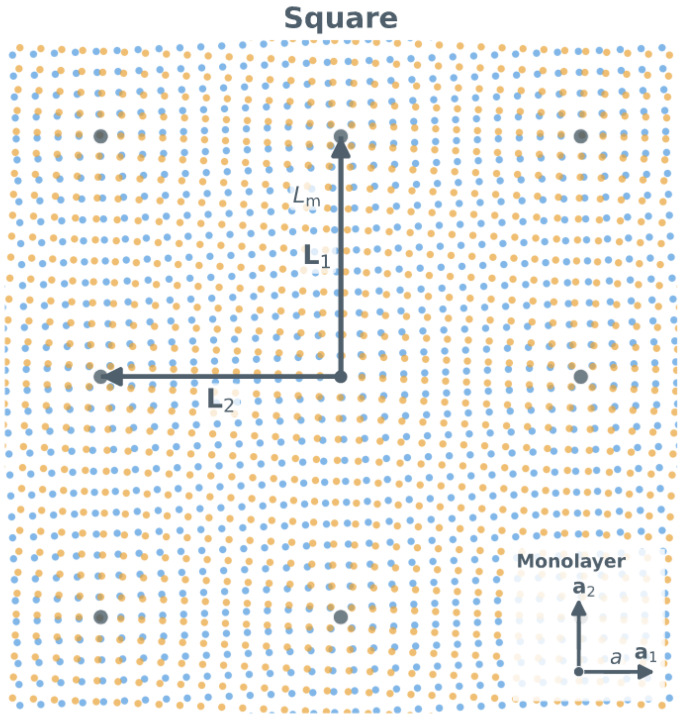
Discretization (numerical)

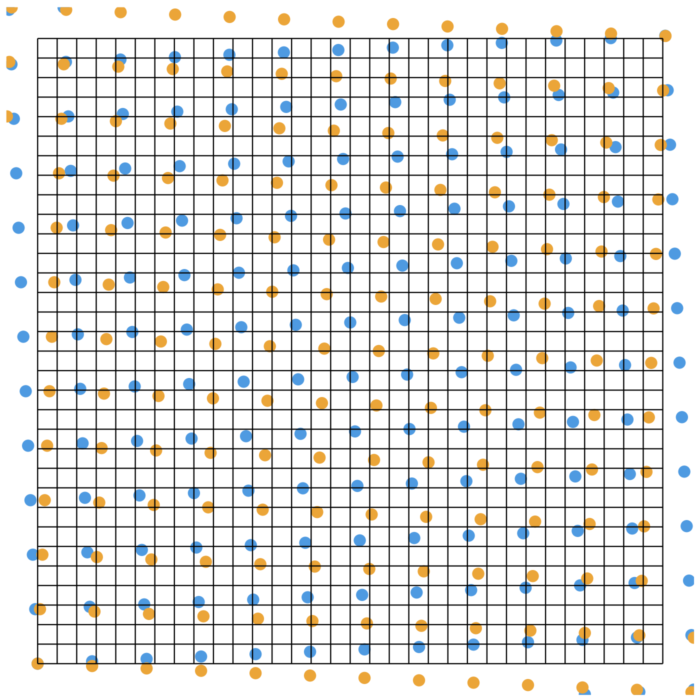


solve

Band Diagram



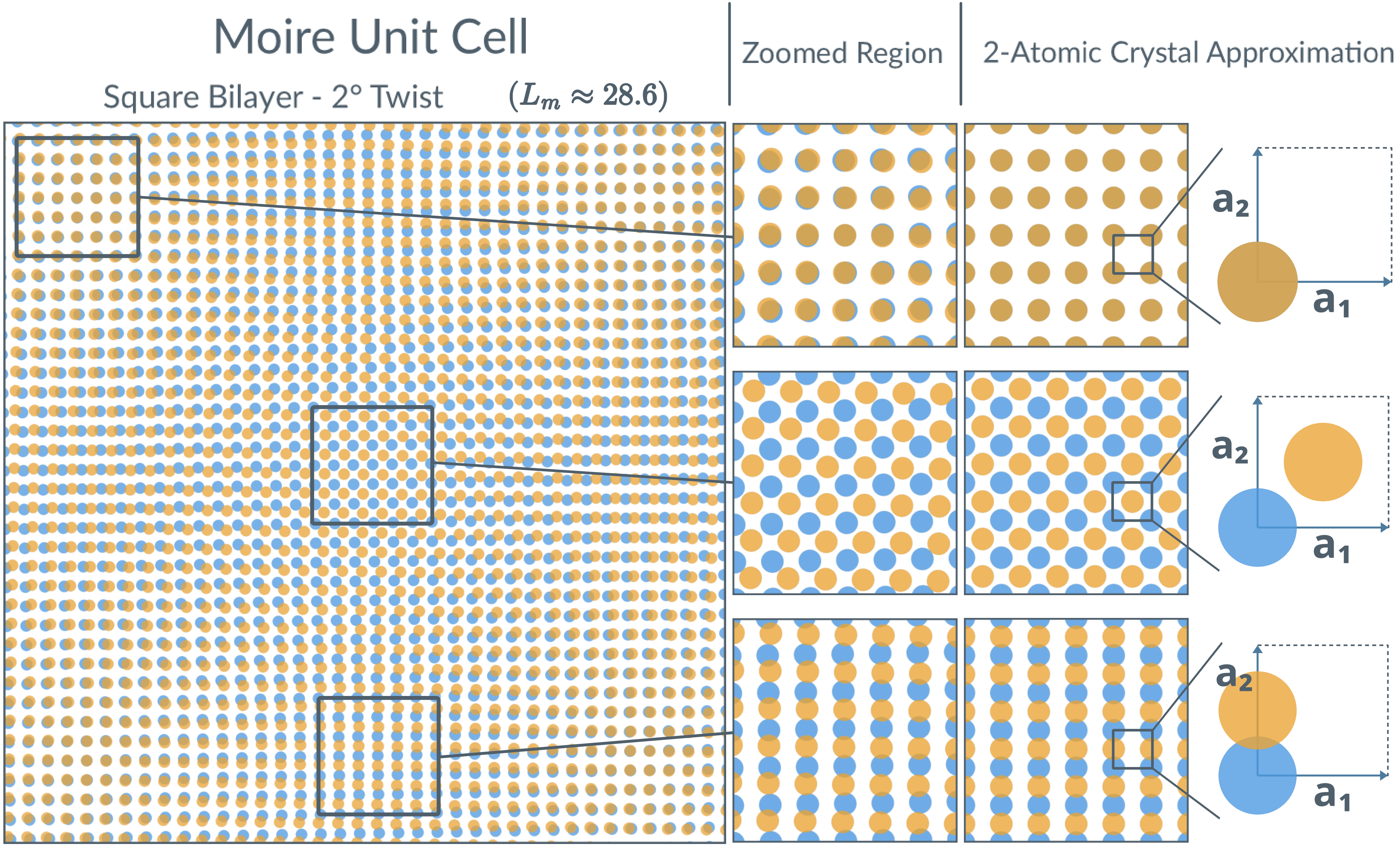




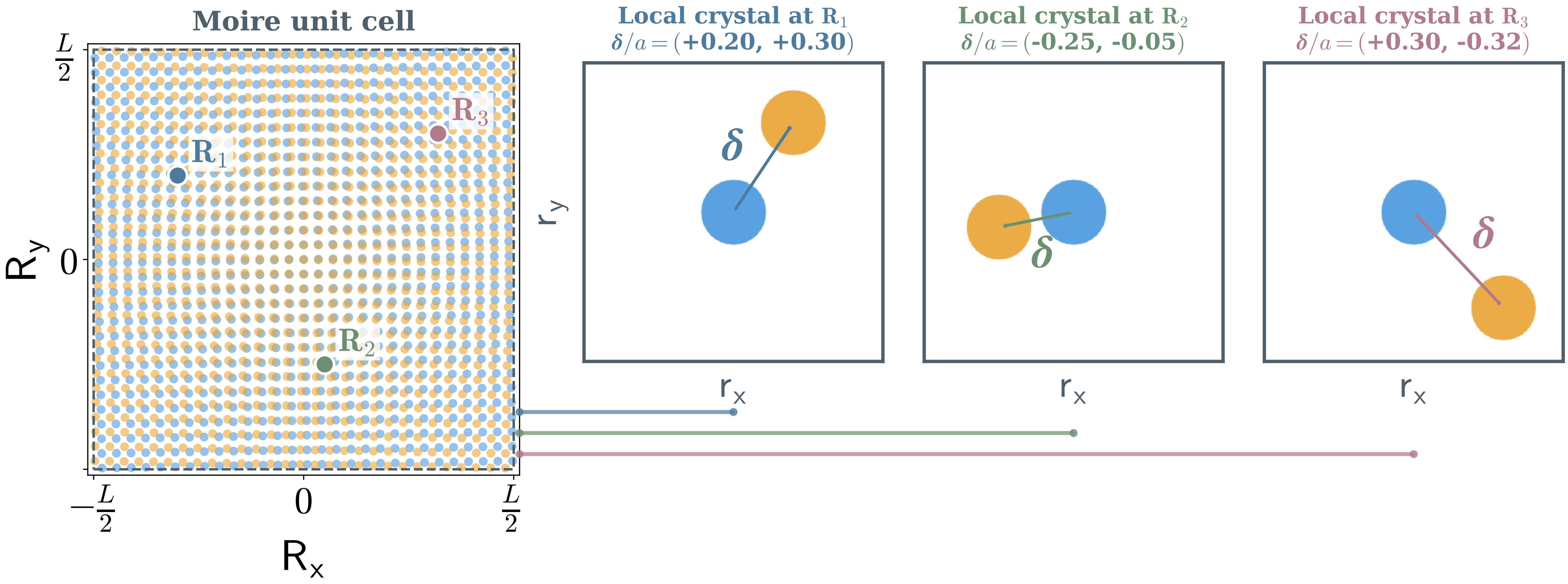
+ Operator Data

$\mathcal{H}_{\mathrm{eff}}$

2-Atomic Crystal Approximation



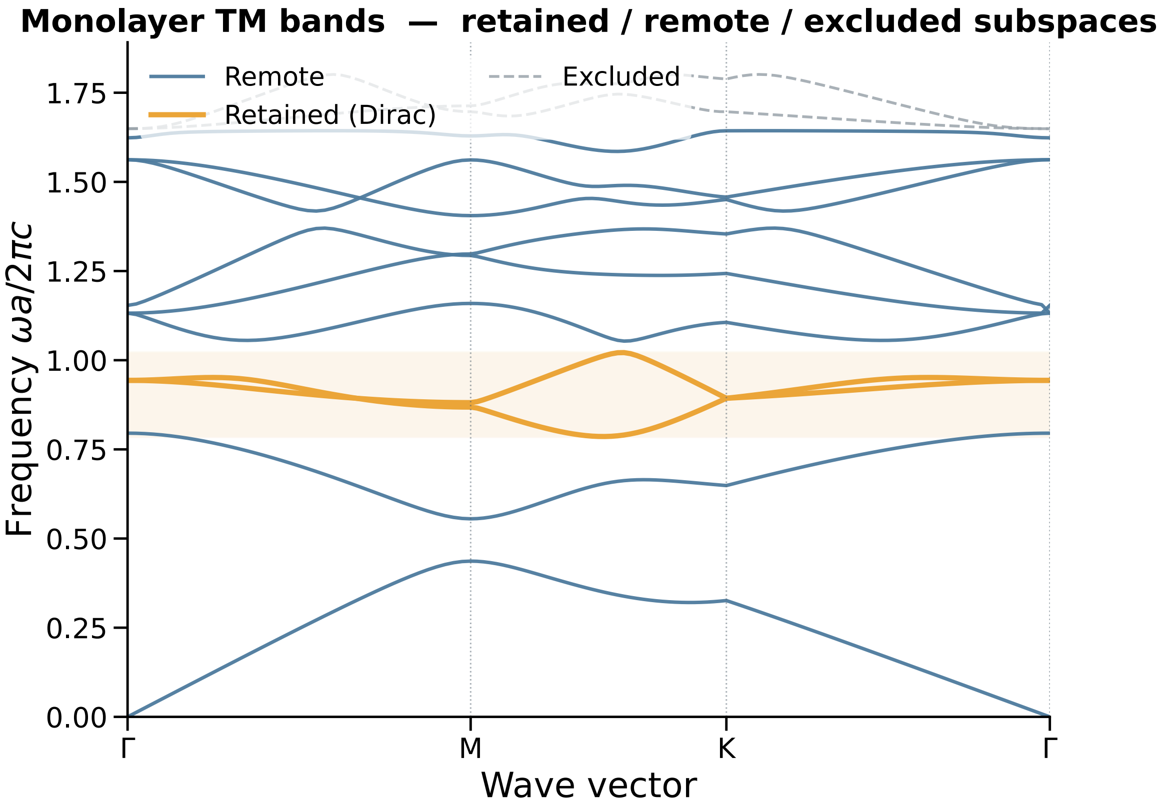
2-Atomic Crystal Approximation

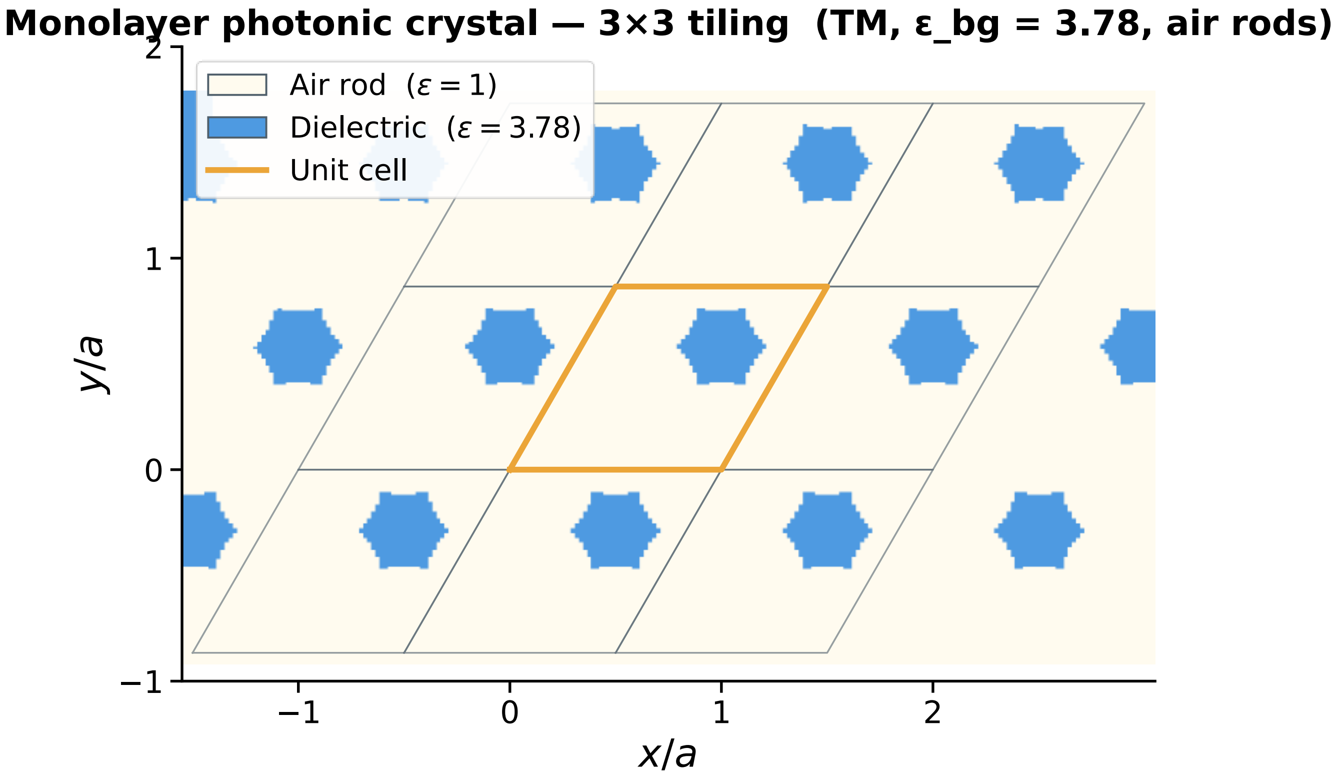


One Concrete Example

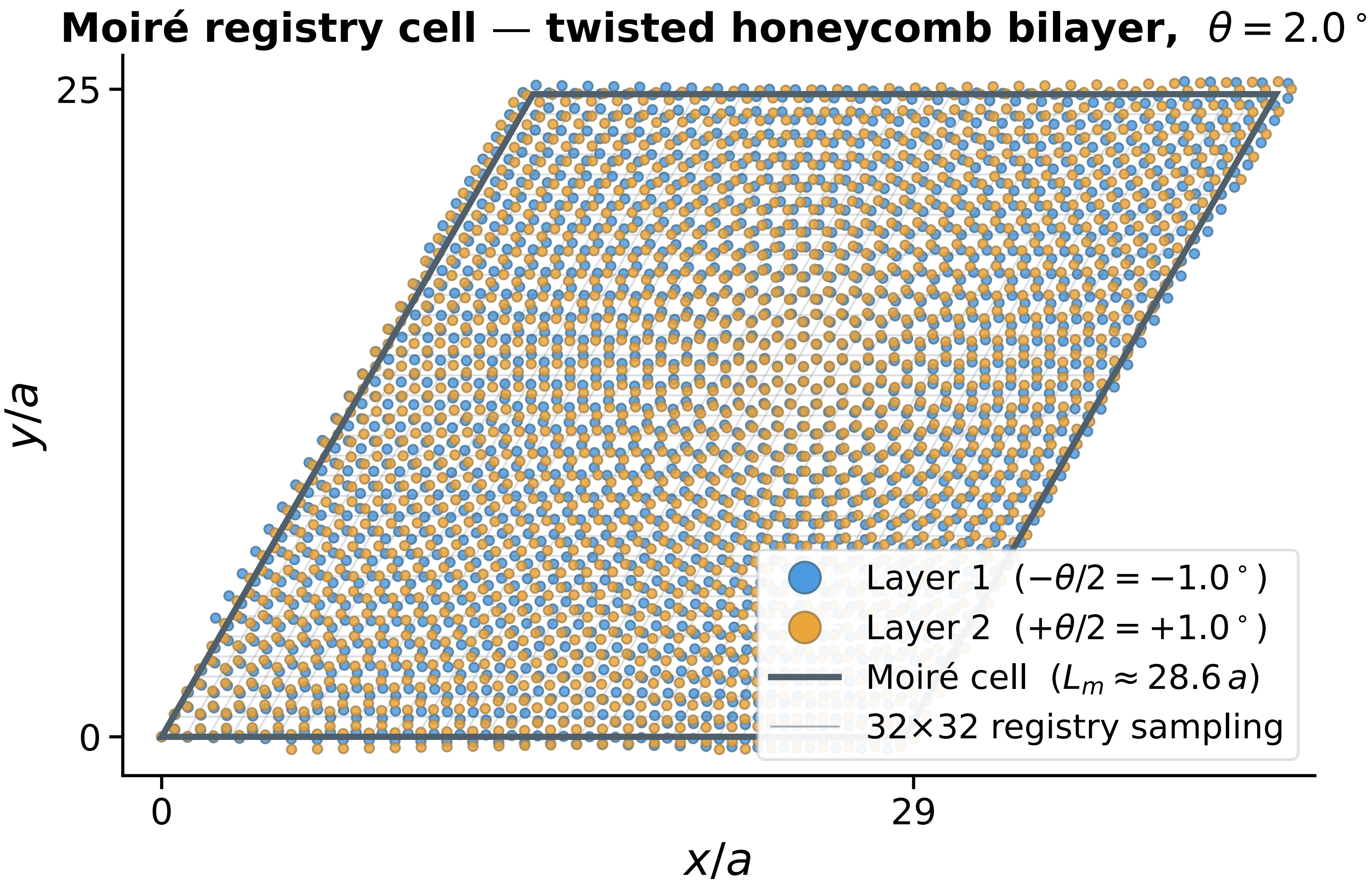
The Hunt for Magic Angles

One Concrete Example

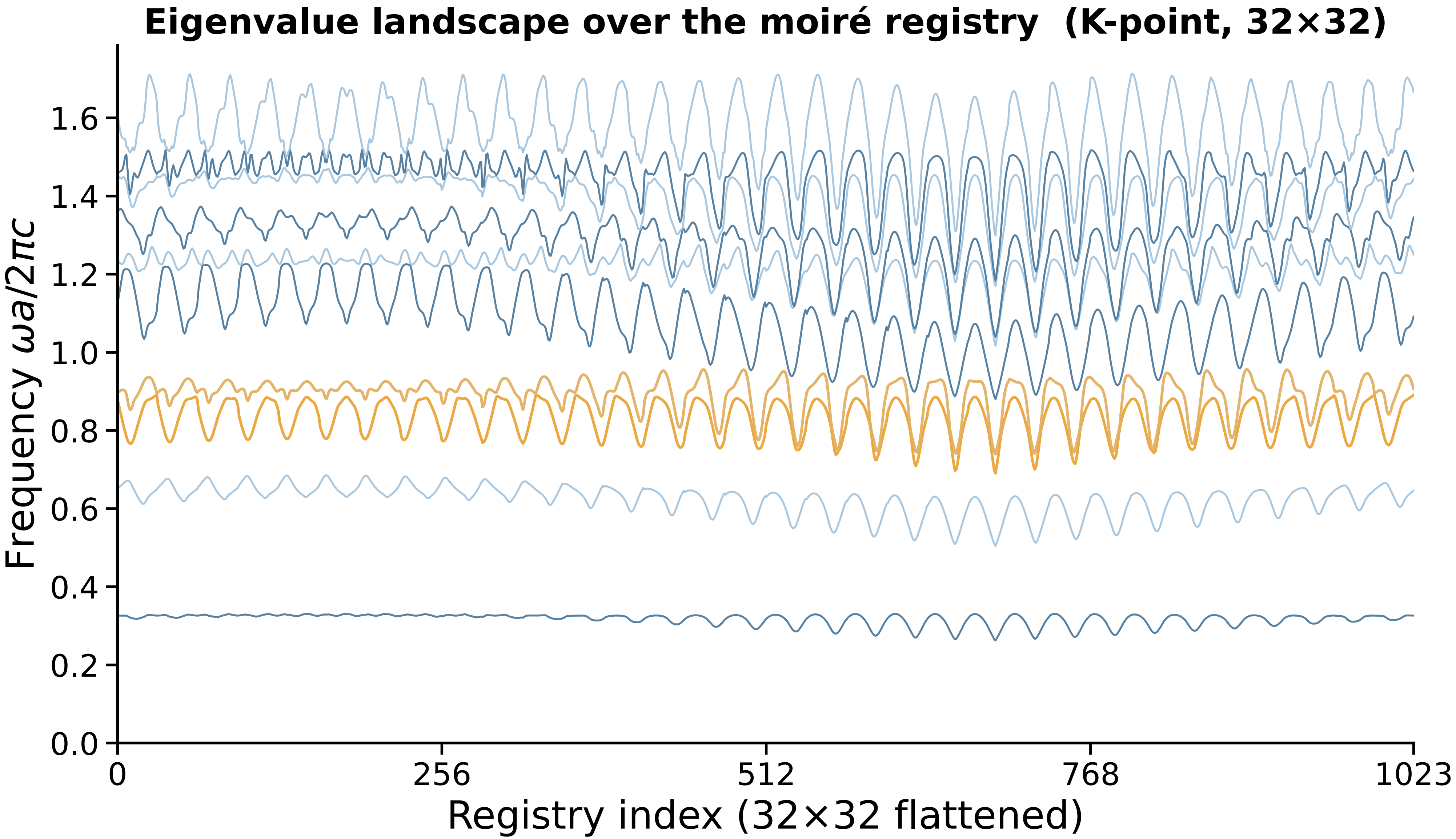




One Concrete Example



One Concrete Example



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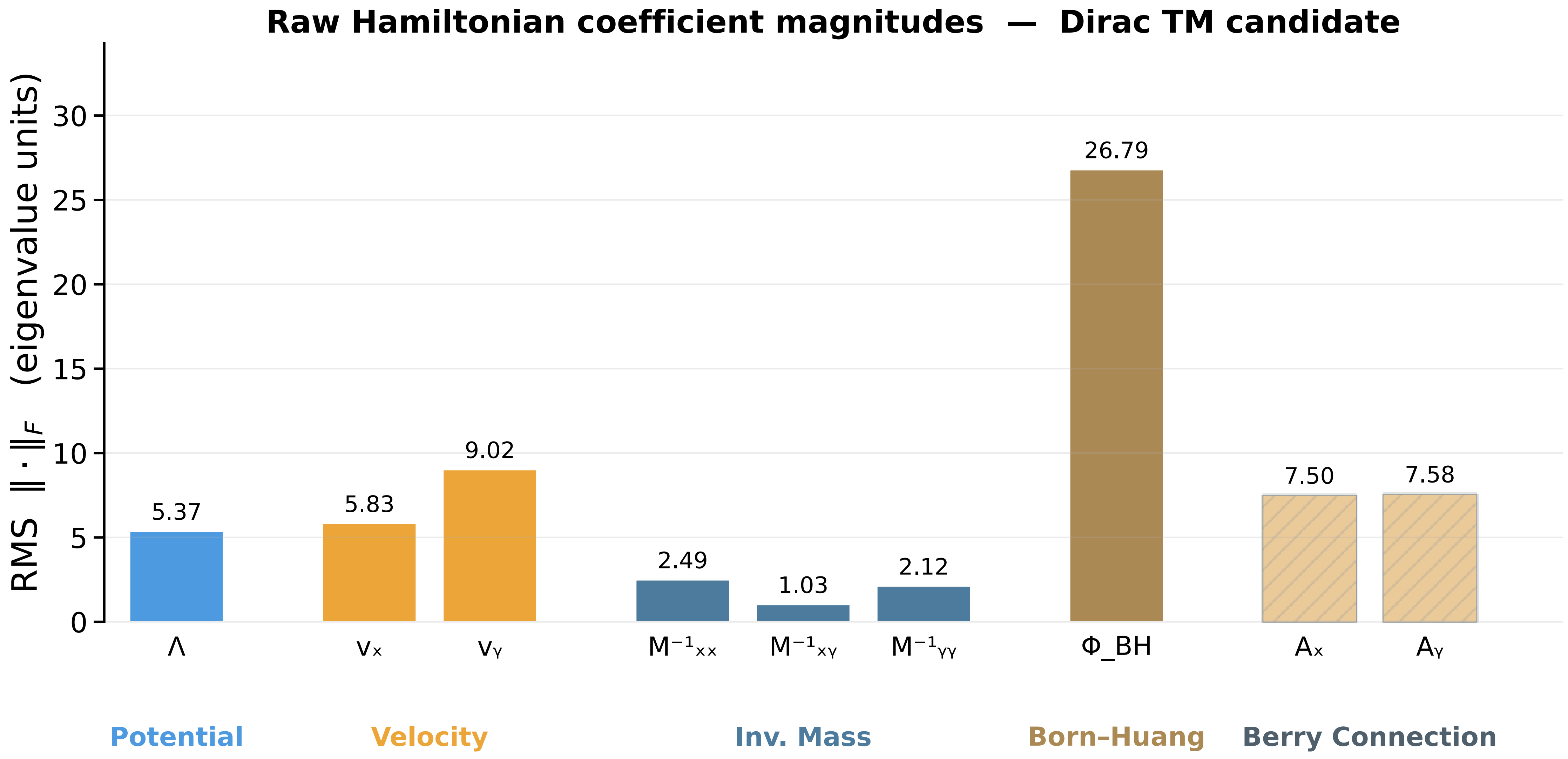
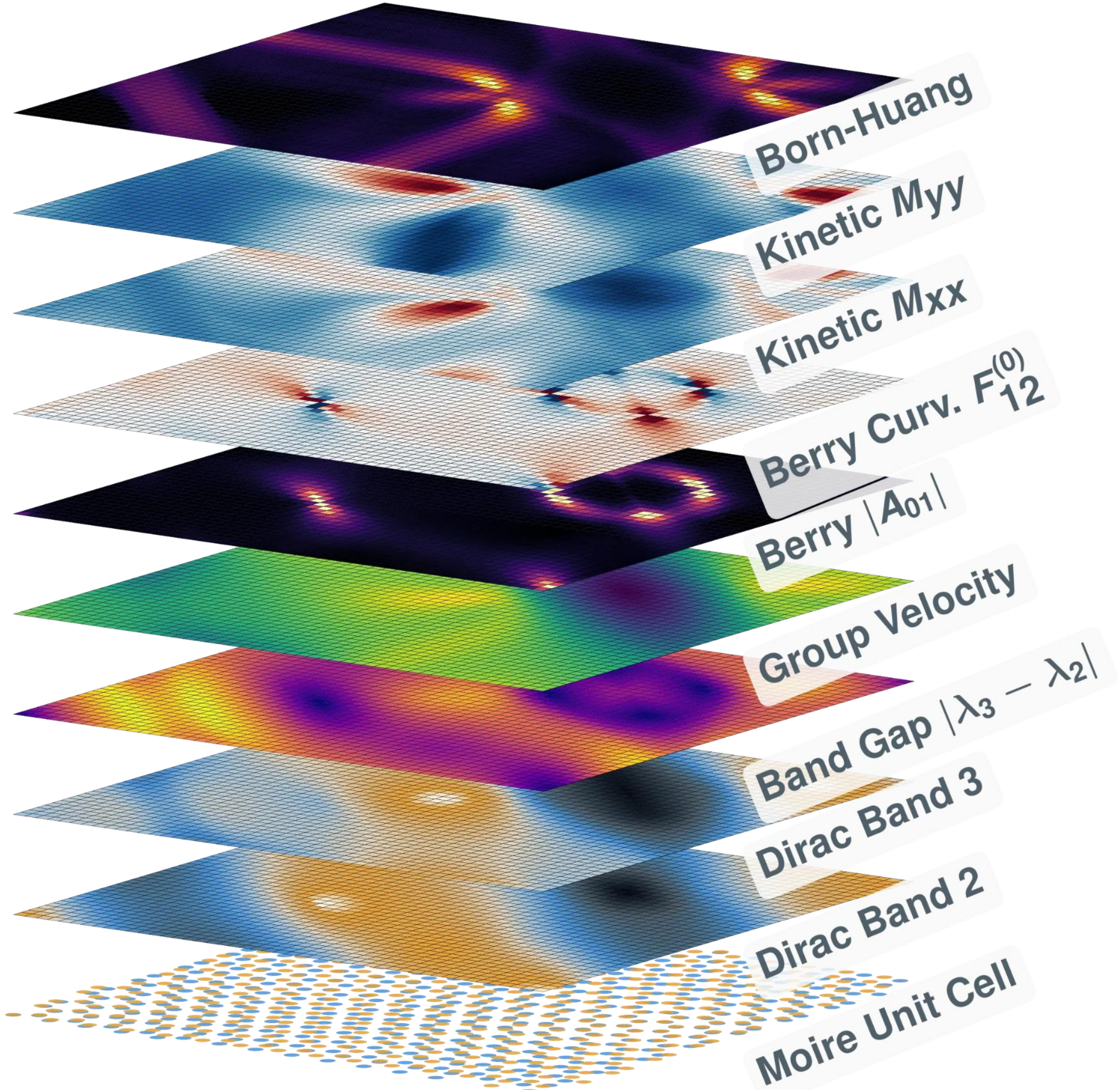
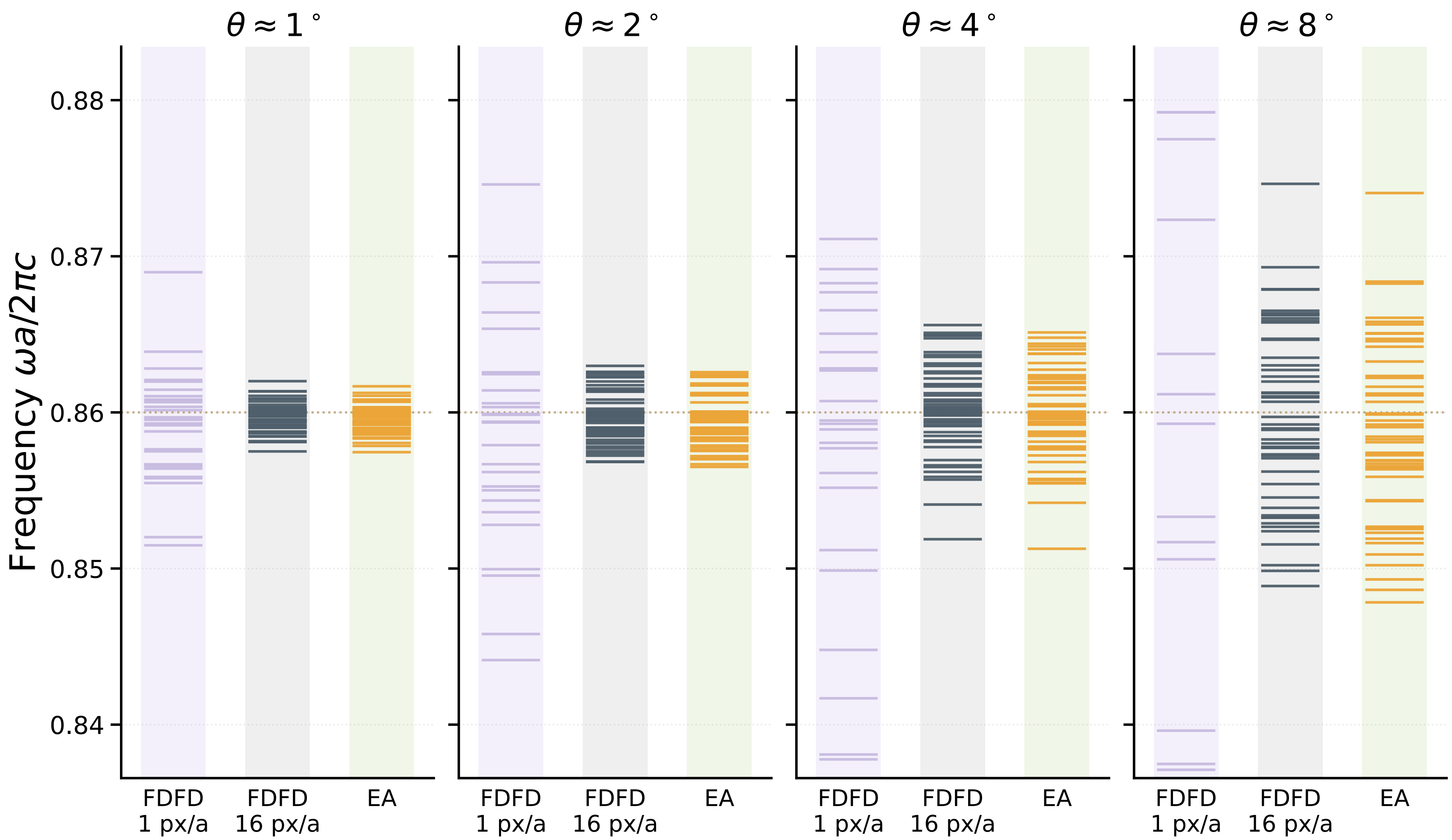


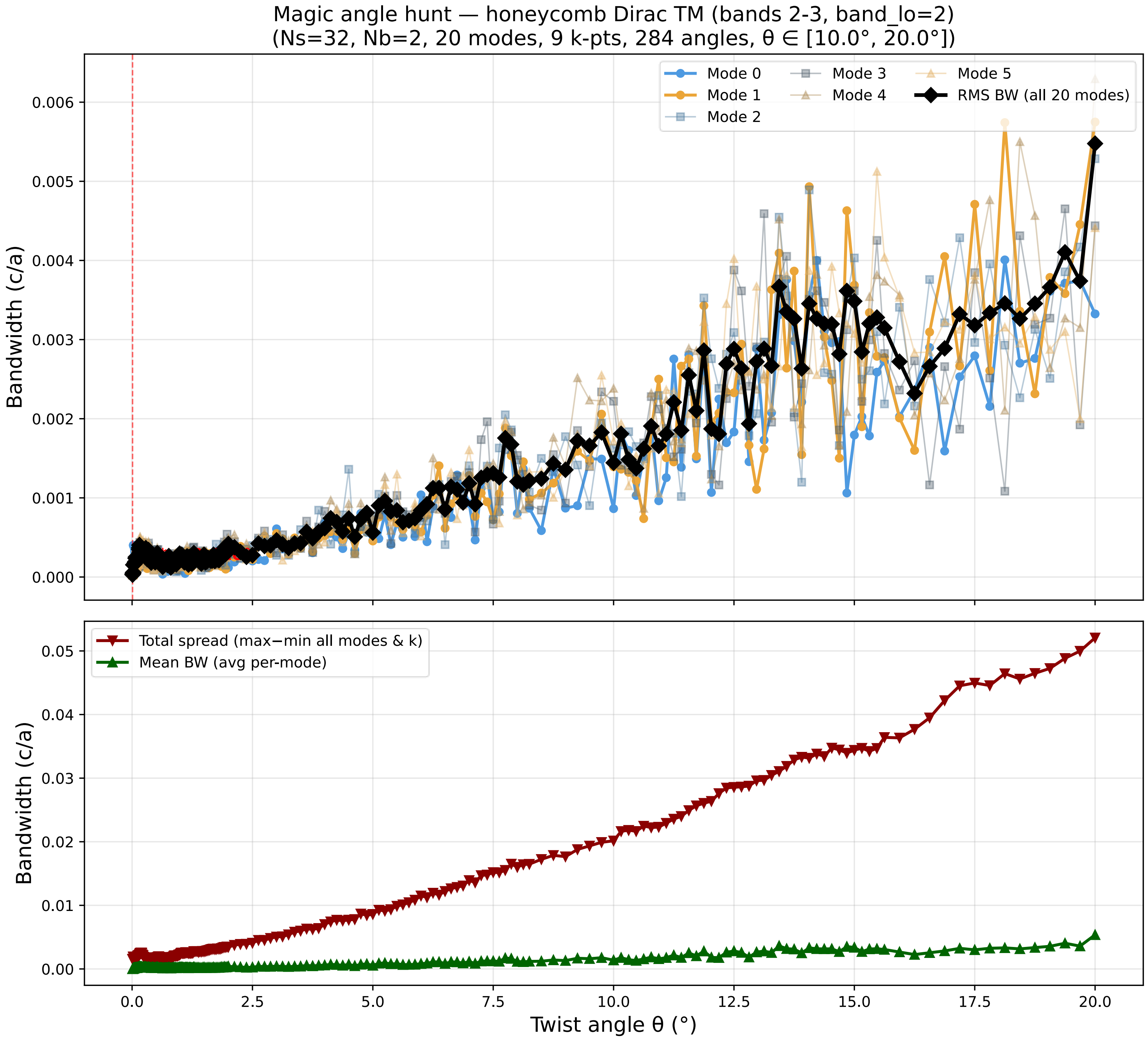


Born-Huang
Kinetic M_{yy}
Kinetic M_{xx}
Berry Curv. $F_{12}^{(0)}$
Berry $|A_{01}|$
Group Velocity
Band Gap $|\lambda_3 - \lambda_2|$
Dirac Band 3
Dirac Band 2
Moire Unit Cell

One Concrete Example

Honeycomb air rods $\varepsilon_{\mathrm{bg}} = 3.78$**,** $r/a = 0.41$**, TM at K — 50 lowest modes**





Magic angle hunt — honeycomb Dirac TM (bands 2-3, band_lo=2)
(Ns=32, Nb=2, 20 modes, 9 k-pts, 284 angles, θ ∈ [10.0°, 20.0°])
Mode 0
Mode 1
Mode 2
Mode 3
Mode 4
Mode 5
RMS BW (all 20 modes)
Bandwidth (c/a)
0.000
0.001
0.002
0.003
0.004
0.005
0.006
Total spread (max−min all modes & k)
Mean BW (avg per-mode)
0.00
0.01
0.02
0.03
0.04
0.05
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Twist angle θ (°)

Conclusion & Outlook

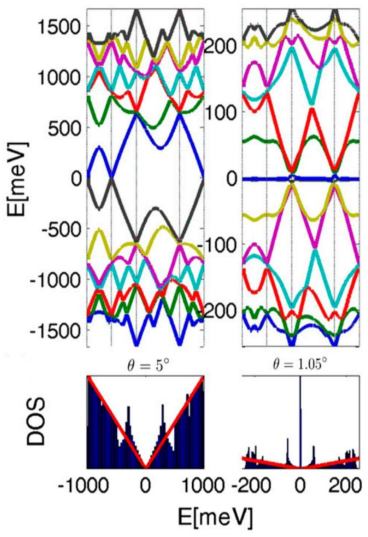
- New framework is **hard** to compare
  - No experimental data

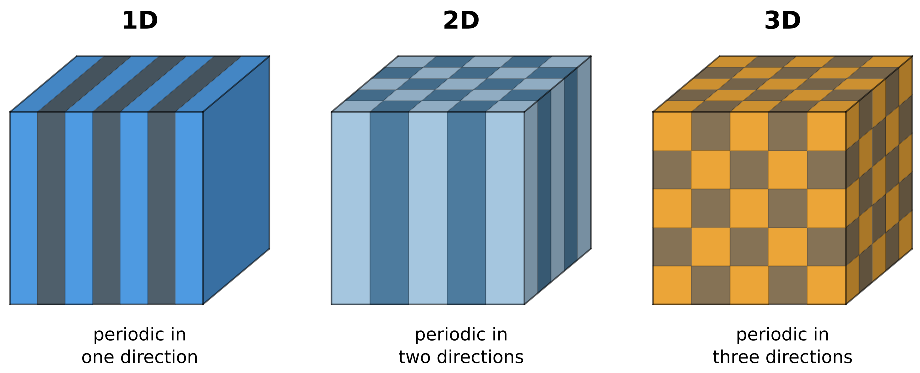
- **Accuracy** regimes must be tested
- Subspace selection might be too restrictive

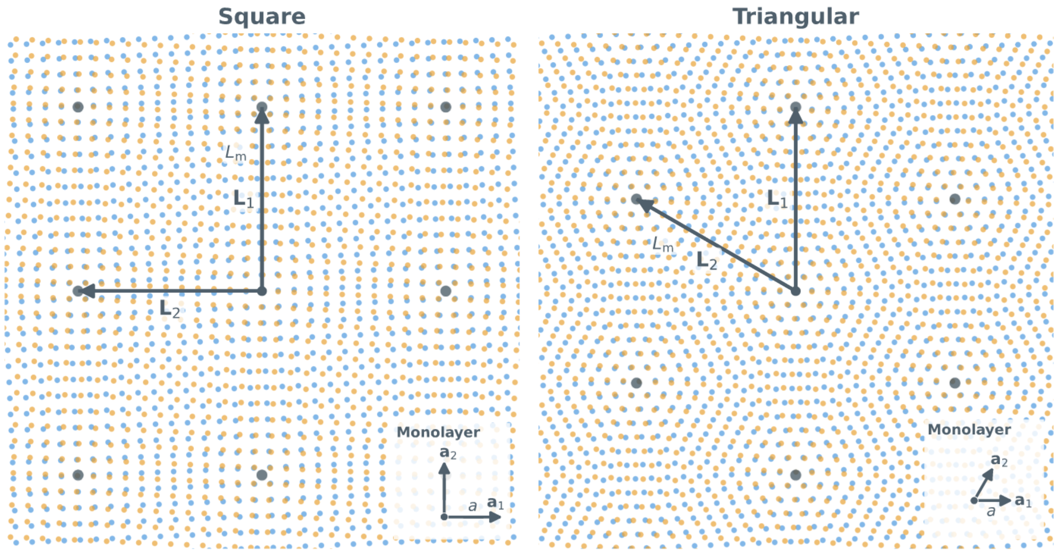
- Novel framework with rich exposure of **physical quantities**
  - **Arbitrary** k-points, bands, angles*, lattice types

- New 2D Maxwell Solver

Summary







Photonic Master Equation

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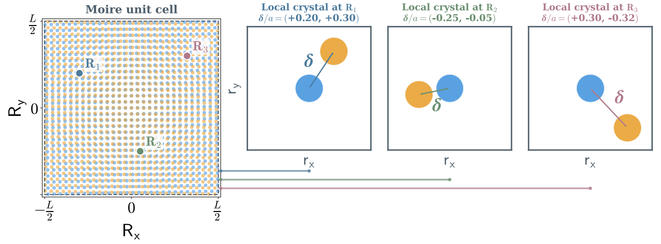
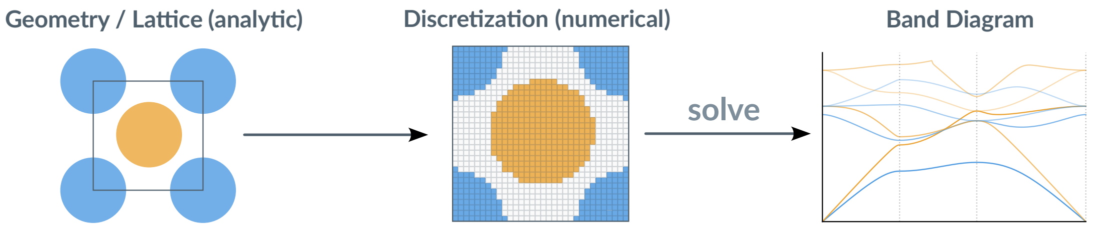
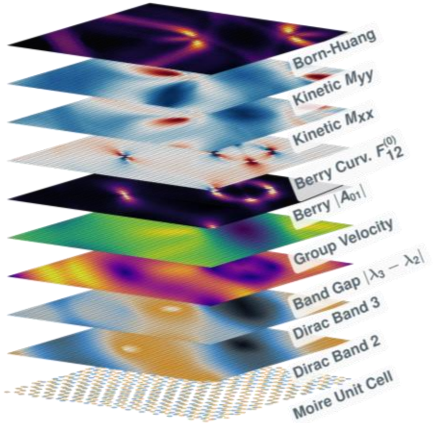
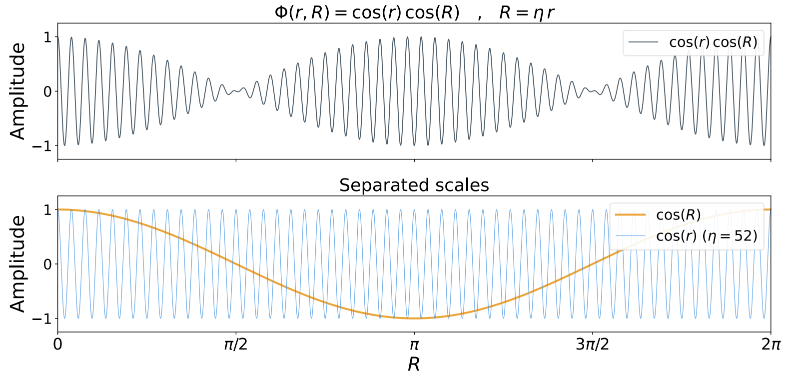


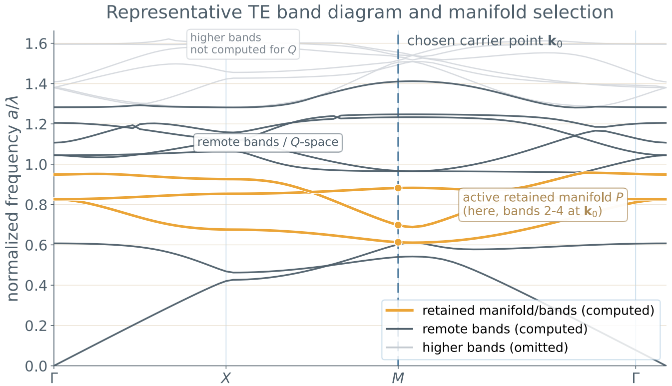


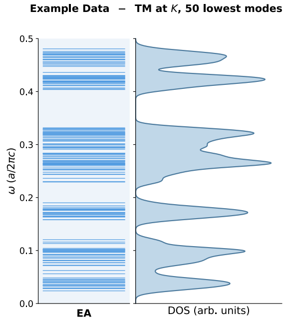
Effective Hamiltonian

$$\mathcal{H}_{\text{eff}} \approx \Lambda + \eta \mathcal{H}_1 + \eta^2 \mathcal{H}_2$$





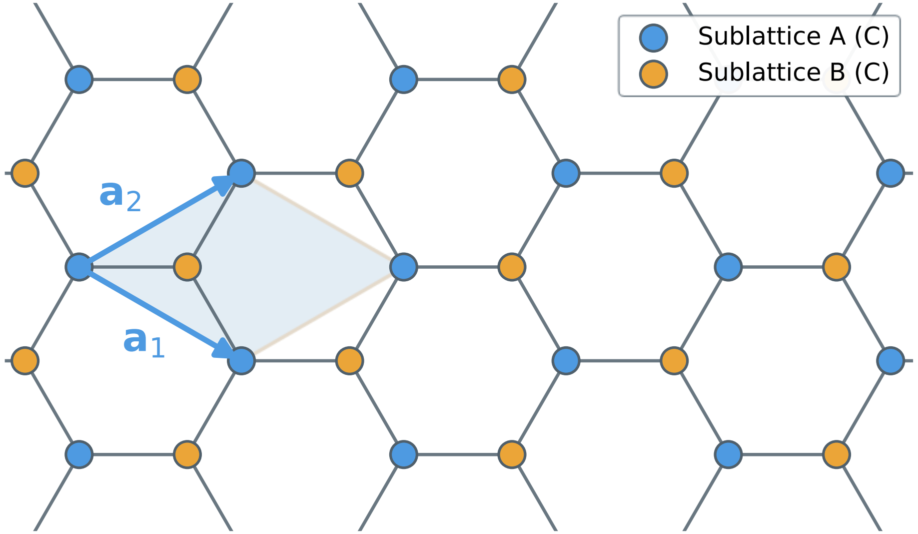




Appendix

Electronic Crystal vs. Photonic Crystal

Graphene

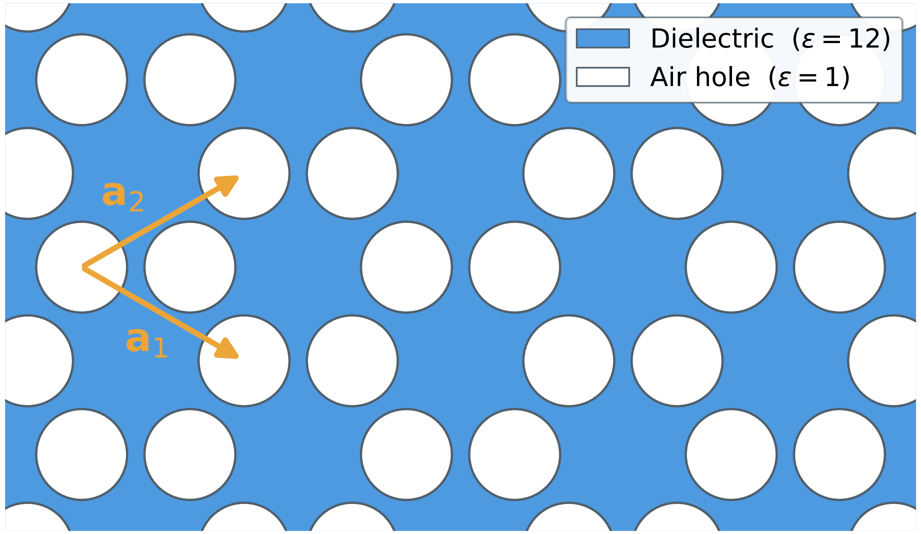


Schrödinger Equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{x})\right]\psi(\boldsymbol{x}) = E\,\psi(\boldsymbol{x}),$$

"**Micro**scopic"

Photonic Honeycomb Crystal

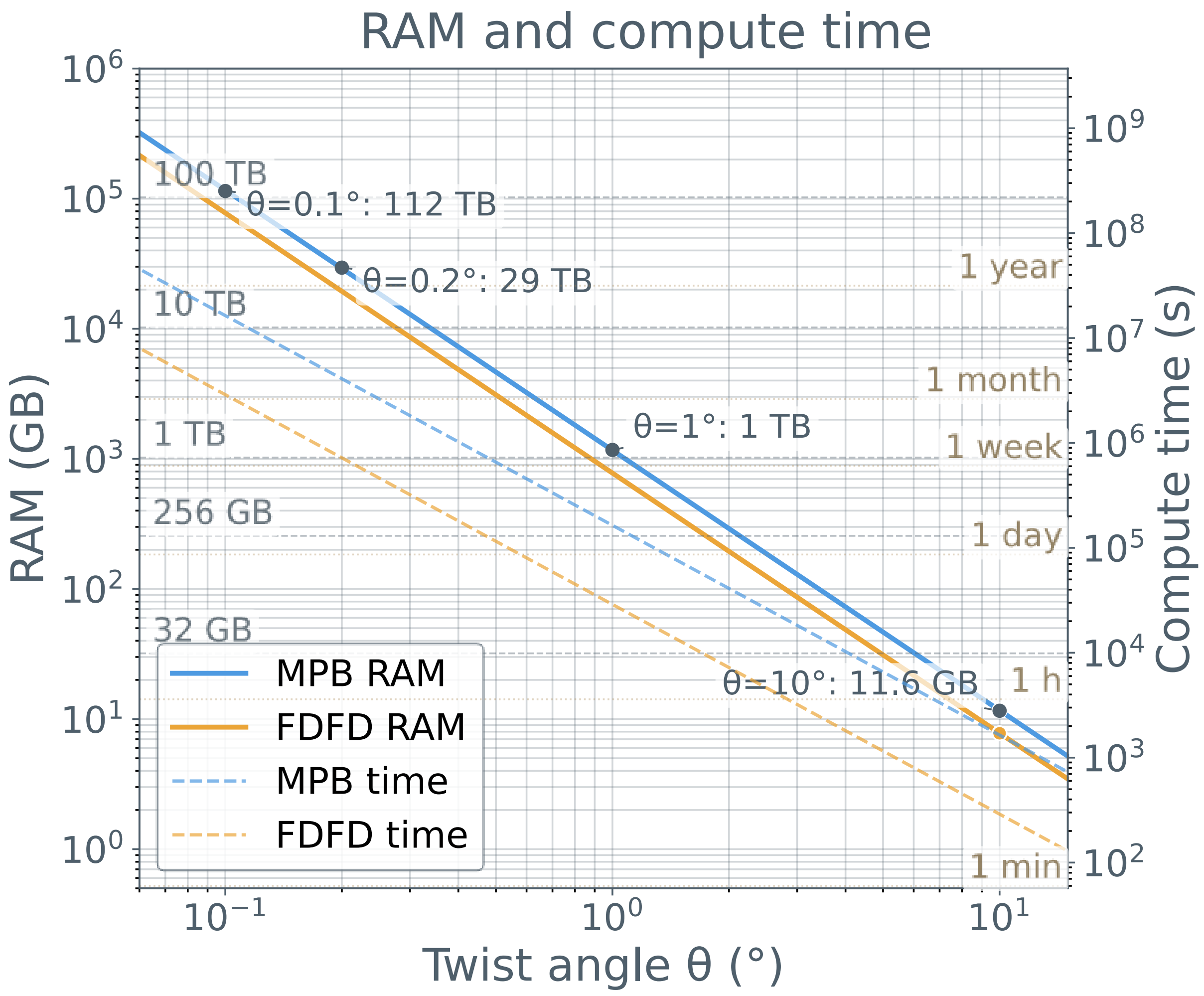


Photonic Master Equation

$$\nabla \times \left(\frac{1}{\varepsilon(\boldsymbol{x})}\nabla \times \boldsymbol{H}(\boldsymbol{x})\right) = \frac{\omega^2}{c^2}\boldsymbol{H}(\boldsymbol{x}),$$

"**Macro**scopic"

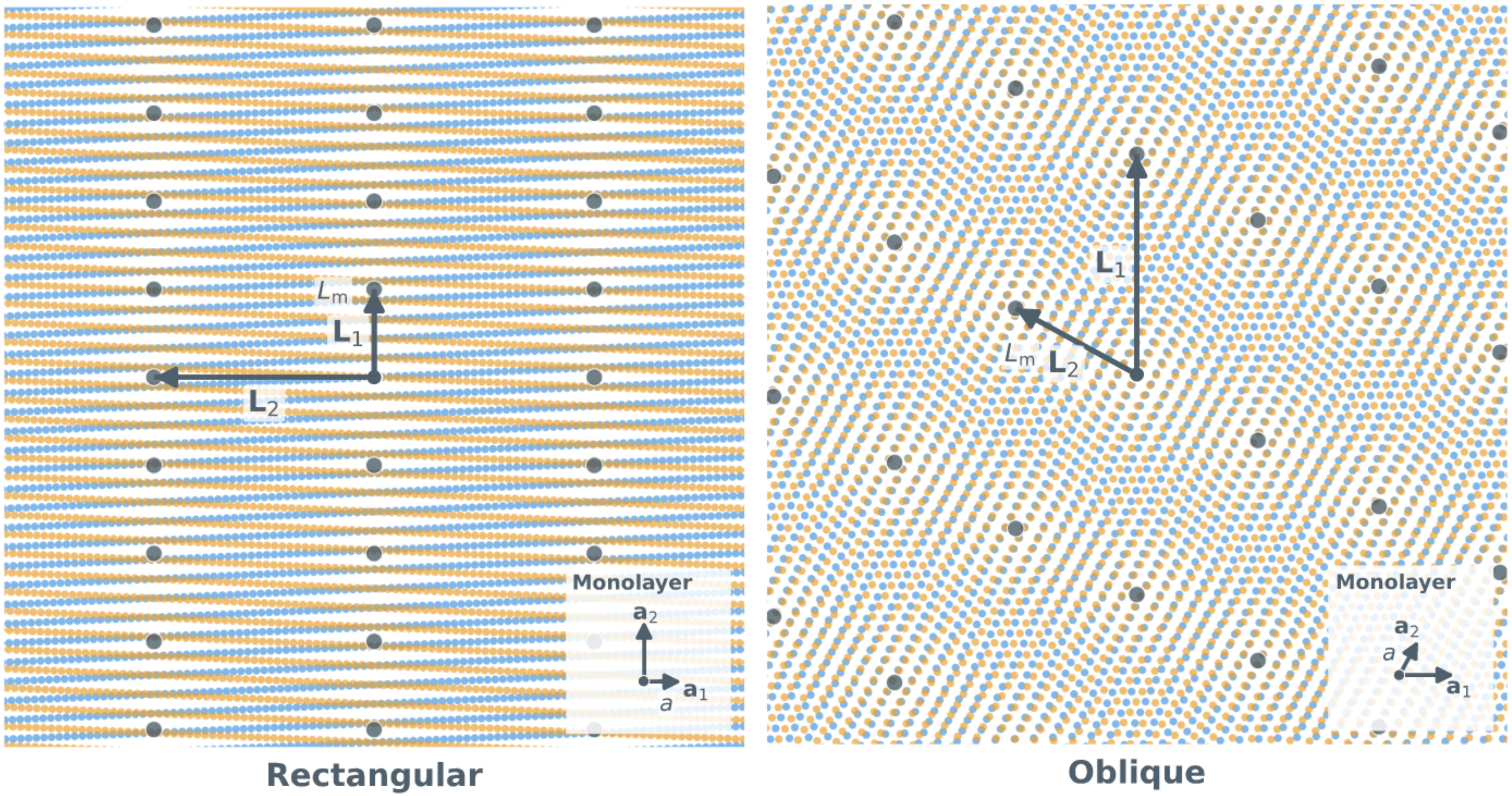
Computational Bottleneck



Reference Solvers: **MPB** (MIT Photonic Bands) & **FDFD** (Finite-Difference Frequency-Domain)

Twisted Bilayer

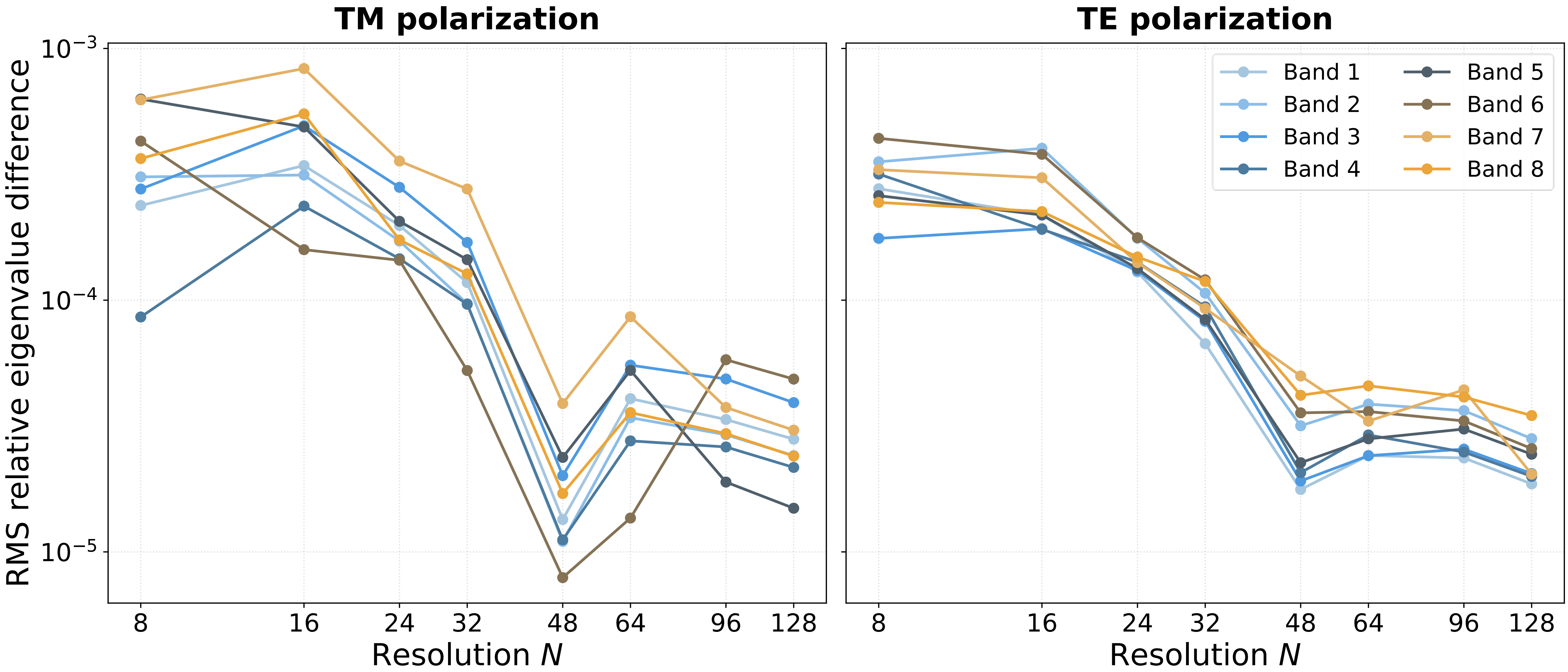
$\Theta = 5°$ Twist



Moiré Period Length

$$L_m = \frac{a}{2\sin(\theta/2)} \approx \frac{a}{\theta} \quad \text{for small}\,\theta.$$

Validating Blaze with MPB



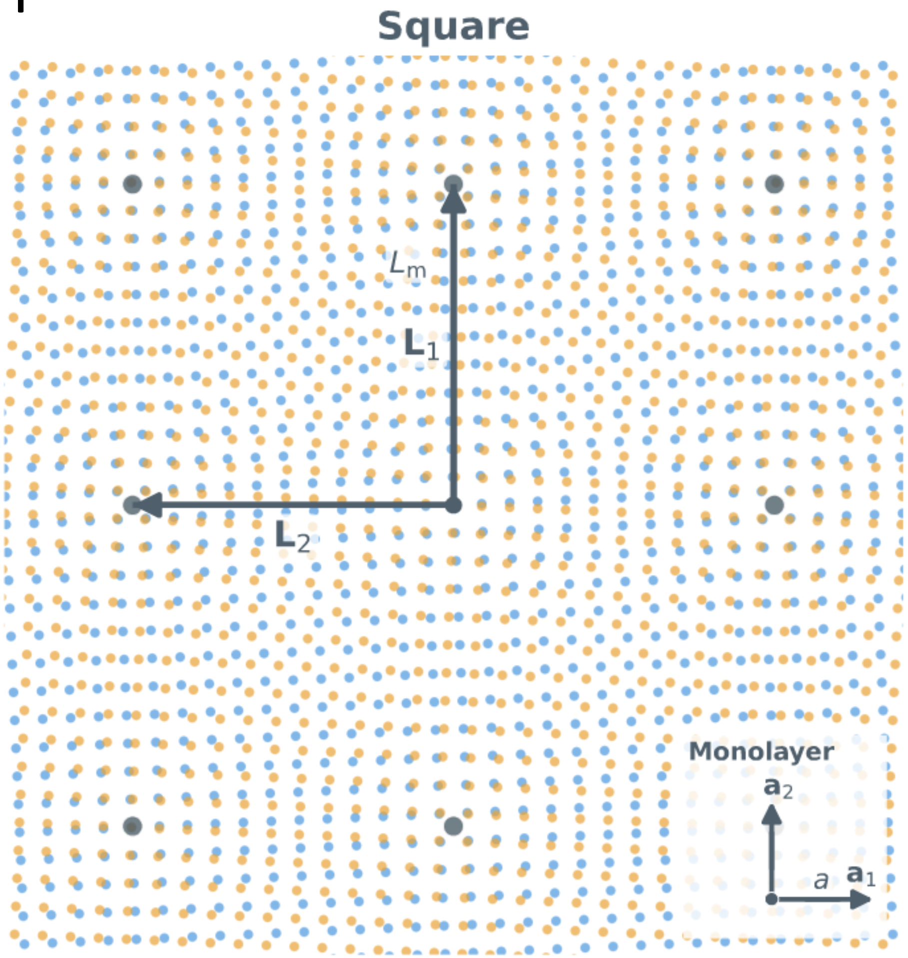
Ansatz for a New Description

Periodic Media: $\varepsilon(\boldsymbol{x}+\boldsymbol{T}) = \varepsilon(\boldsymbol{x})$

Bloch's Theorem: $\boldsymbol{H}_{n\boldsymbol{k}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\boldsymbol{u}_{n\boldsymbol{k}}(\boldsymbol{x})$

$$\varepsilon(\boldsymbol{r}, \boldsymbol{R}+\boldsymbol{L}) = \varepsilon(\boldsymbol{r}, \boldsymbol{R})$$

$$F_{n\boldsymbol{q}}(\boldsymbol{R}) = \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}} f_{n\boldsymbol{q}}(\boldsymbol{R})$$



Full TE Effective Hamiltonian

η^0 zeroth order η^1 first order η^2 second order **band energies** **group velocity** **Berry connection** **inverse mass tensor** **Born-Huang potential** **Löwdin remote-band pieces**

$$\mathcal{H}_{\text{eff}} = \left[\underbrace{\Lambda}_{\textbf{band energies}} \right] + \eta \left[\underbrace{\frac{1}{2}\left(v^{(i)}\,\Pi_i + \Pi_i\,v^{(i)}\right)}_{\textbf{group velocity}\,\cdot\,\textbf{covariant momentum}} + \underbrace{\Xi^{(1)}_{\text{sc}} + \frac{\mathrm{i}}{2}\,\partial_{R_i} v^{(i)} + \frac{1}{2}\left(A_i\,v^{(i)} + v^{(i)}\,A_i\right)}_{\textbf{first-order remainder}\ \ +U^{(1)}_{\text{rem}}} \right]$$

$$+\,\eta^2 \left[\underbrace{\frac{1}{2}\,\Pi_i\,M^{-1}_{ij}\,\Pi_j}_{\textbf{inverse mass tensor}\,+\,\text{(Löwdin downfolded)}} + \underbrace{\Xi_i^\dagger\,\varepsilon^{-1}\,\Xi_i}_{\textbf{Born-Huang}} + \underbrace{\left(K_i^\dagger - K_i\right)\mathcal{D}_i - \mathcal{D}_i\,K_i}_{\textbf{direct 1-deriv. remainder}} - \underbrace{\mathcal{T}_i^\dagger\,R_Q\,\mathcal{R} + \mathcal{R}^\dagger\,R_Q\,\mathcal{T}_i}_{\textbf{Löwdin 1-deriv. cross}} - \underbrace{\mathcal{R}^\dagger\,R_Q\,\mathcal{R}}_{\textbf{Löwdin scalar}} + \underbrace{\Gamma^{(2)}}_{\textbf{slow-coefficient scalar}} \right] + O(\eta^3)$$

where

gauge-covariant slow momentum, slow covariant derivative, and Berry connection (in P-space)

$$\Pi_i = -\mathrm{i}\,\mathcal{D}_i\,, \quad \mathcal{D}_i = D_{R_i} - \mathrm{i}\,A_i\,, \quad A_i = \mathrm{i}\,U^\dagger\,\partial_{R_i} U$$

velocity matrix elements and TE velocity operator (action on a test field φ)

$$v^{(i)}_{mn} = \langle u_m, \mathcal{V}_i\,u_n\rangle_\Omega\,, \quad \mathcal{V}_i\,\varphi = -\mathrm{i}\left[D_{r_i}(\varepsilon^{-1}\varphi) + \varepsilon^{-1} D_{r_i}\varphi\right]$$

Löwdin-corrected inverse mass tensor; bare metric $G_{mn} = \langle u_m, \varepsilon^{-1} u_n\rangle_\Omega$

$$\left(M^{-1}_{ij}\right)_{mn} = 2\,\delta_{ij}\,G_{mn} + \sum_{\ell\notin P}\left[\frac{v^{(i)}_{m\ell} v^{(j)}_{\ell n}}{\lambda_n - \lambda_\ell} + \frac{v^{(j)}_{m\ell} v^{(i)}_{\ell n}}{\lambda_m - \lambda_\ell}\right]$$

out-of-subspace frame leakage and first-order scalar remainder

$$\Xi_i = Q\,\partial_{R_i} U\,, \quad \Xi^{(1)}_{\text{sc}} = -\sum_i \left[\mathrm{i}\,U^\dagger\,\mathcal{V}_i\,\Xi_i + U^\dagger\left(\partial_{R_i}\varepsilon^{-1}\right) D_{r_i}\,U\right]$$

direct second-order scalar (no Löwdin); slow-dielectric variation of the basis

$$\Gamma^{(2)}_{mn} = -\sum_{i=x,y} \langle u_m, \partial_{R_i}\left(\varepsilon^{-1}\,\partial_{R_i} u_n\right)\rangle_\Omega$$

Löwdin coupling operators (P–Q channels) and reduced resolvent

$$K_i = U^\dagger\,\varepsilon^{-1}\,\Xi_i\,, \quad \mathcal{T}_i = -\mathrm{i}\,Q\,\mathcal{V}_i\,U\,, \quad R_Q = \left[Q\left(\mathcal{L}^{(0)}_{\text{TE}} - \lambda_{\text{ref}}\right)Q\right]^{-1}$$

Löwdin scalar feed (drives the $R_Q\mathcal{R}$ corrections)

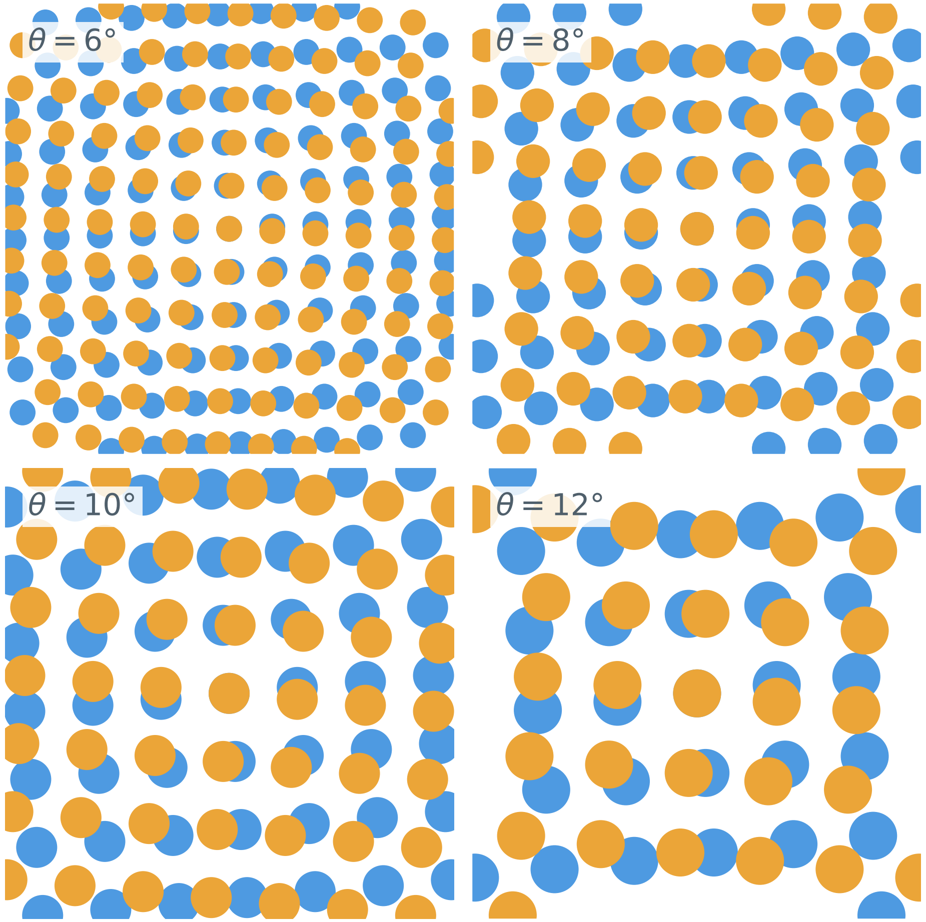
$$\mathcal{R} = -Q\left[\mathrm{i}\,\mathcal{V}_i\,\Xi_i + \left(\partial_{R_i}\varepsilon^{-1}\right) D_{r_i}\,U\right]$$

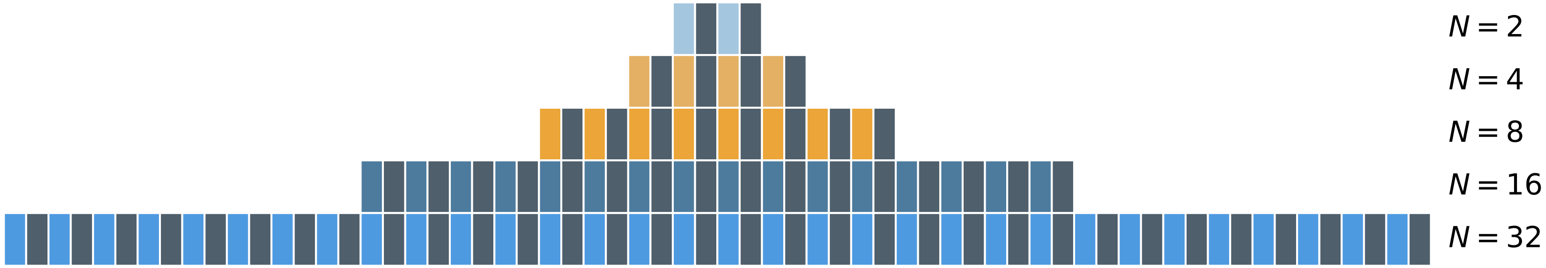
Born-Huang leakage potential (ε^{-1}-weighted form is exact)

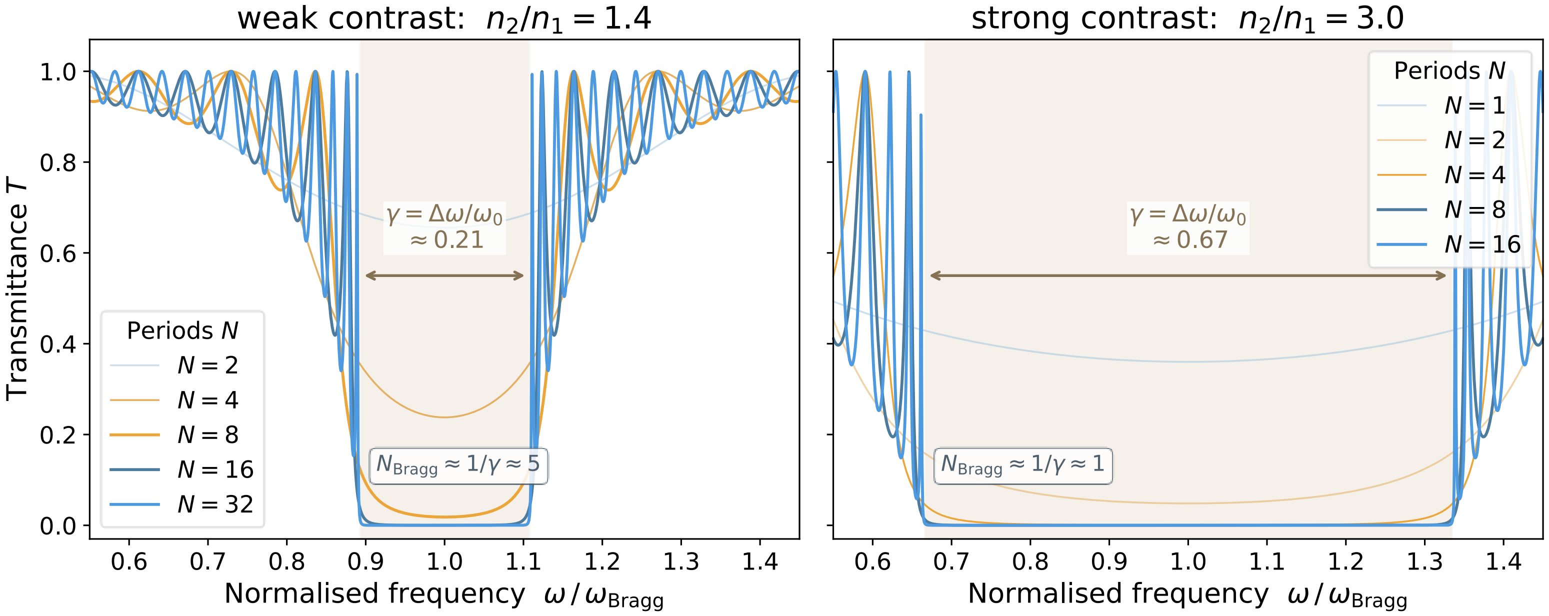
$$U_{\text{BH,exact}} = \Xi_i^\dagger\,\varepsilon^{-1}\,\Xi_i\,, \quad U_{\text{BH}} \approx \Xi_i^\dagger\,\Xi_i \quad \text{(unweighted approximation)}$$

$P = U\,U^\dagger$ (retained-band projector) | $Q = 1 - P$ (remote complement) | $U(\boldsymbol{R})$: retained Bloch frame, columns u_n | $D_{r_i} = \partial_{r_i} + \mathrm{i}\,k_{0,i}$ (fast cov. deriv.) | $D_{R_i} = \partial_{R_i} + \mathrm{i}\,q_i$ (slow cov. deriv.) | φ: smooth test field | $\langle\cdot,\cdot\rangle_\Omega$: fast-cell inner product

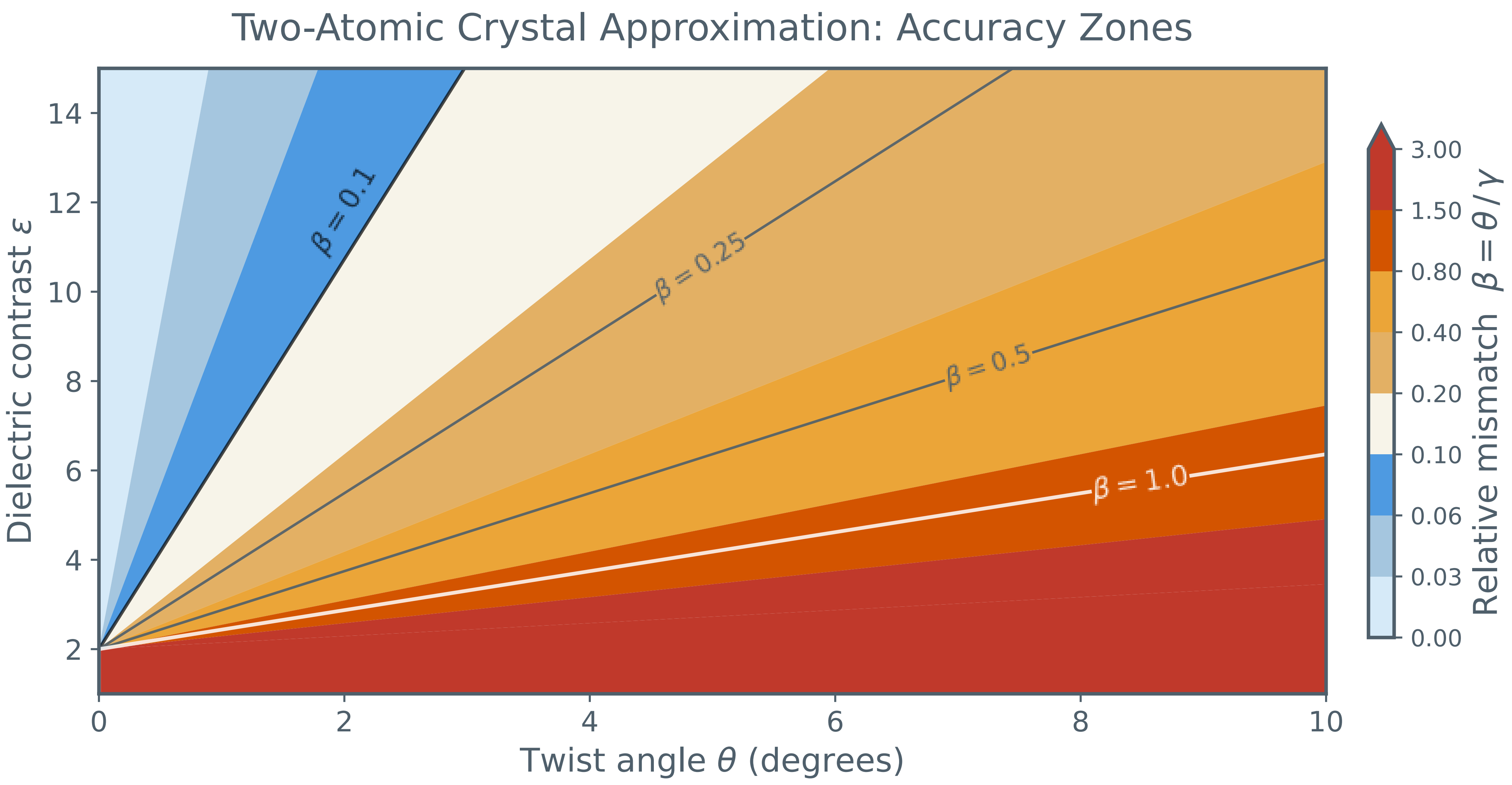
Limits of the Two-Atomic Crystal Approximation



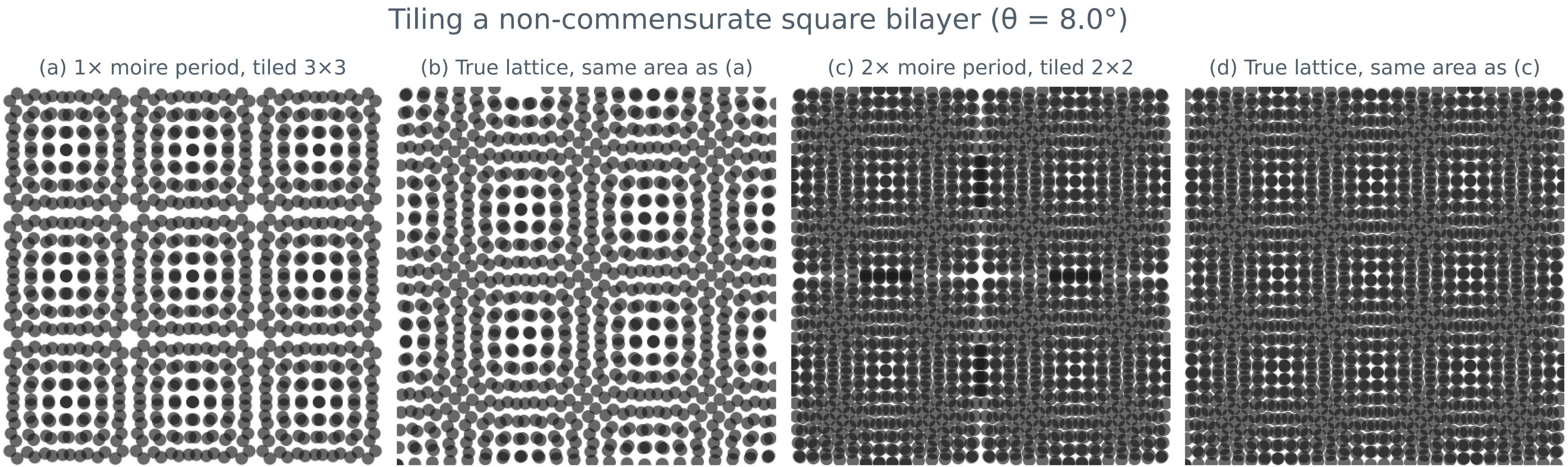




Limits of the Two-Atomic Crystal Approximation

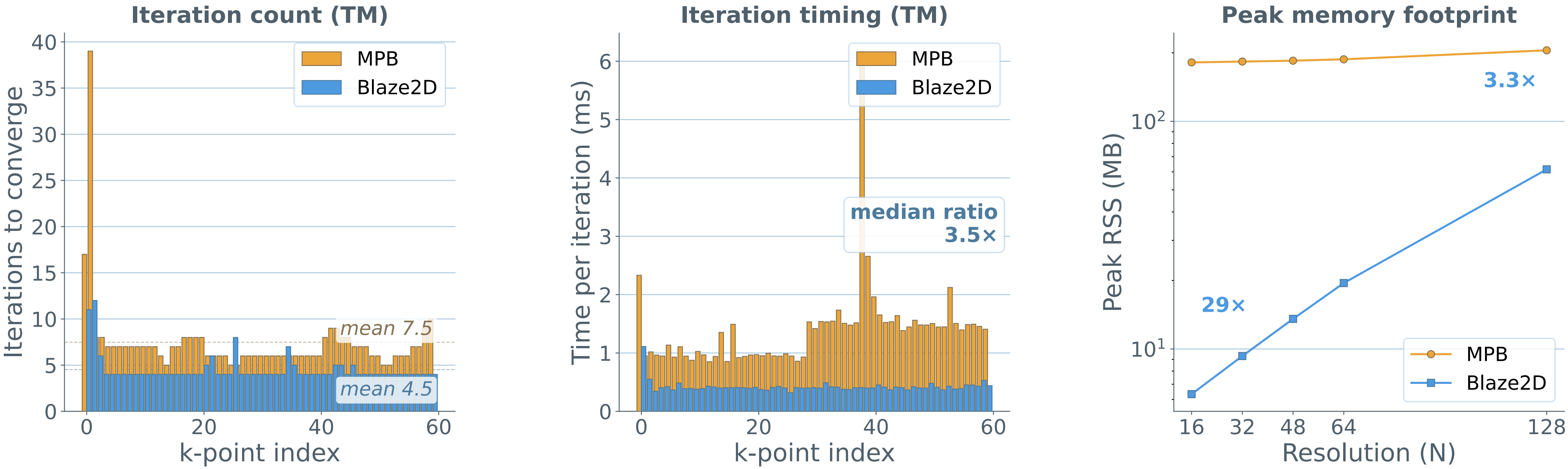


Conceptual Mismatch

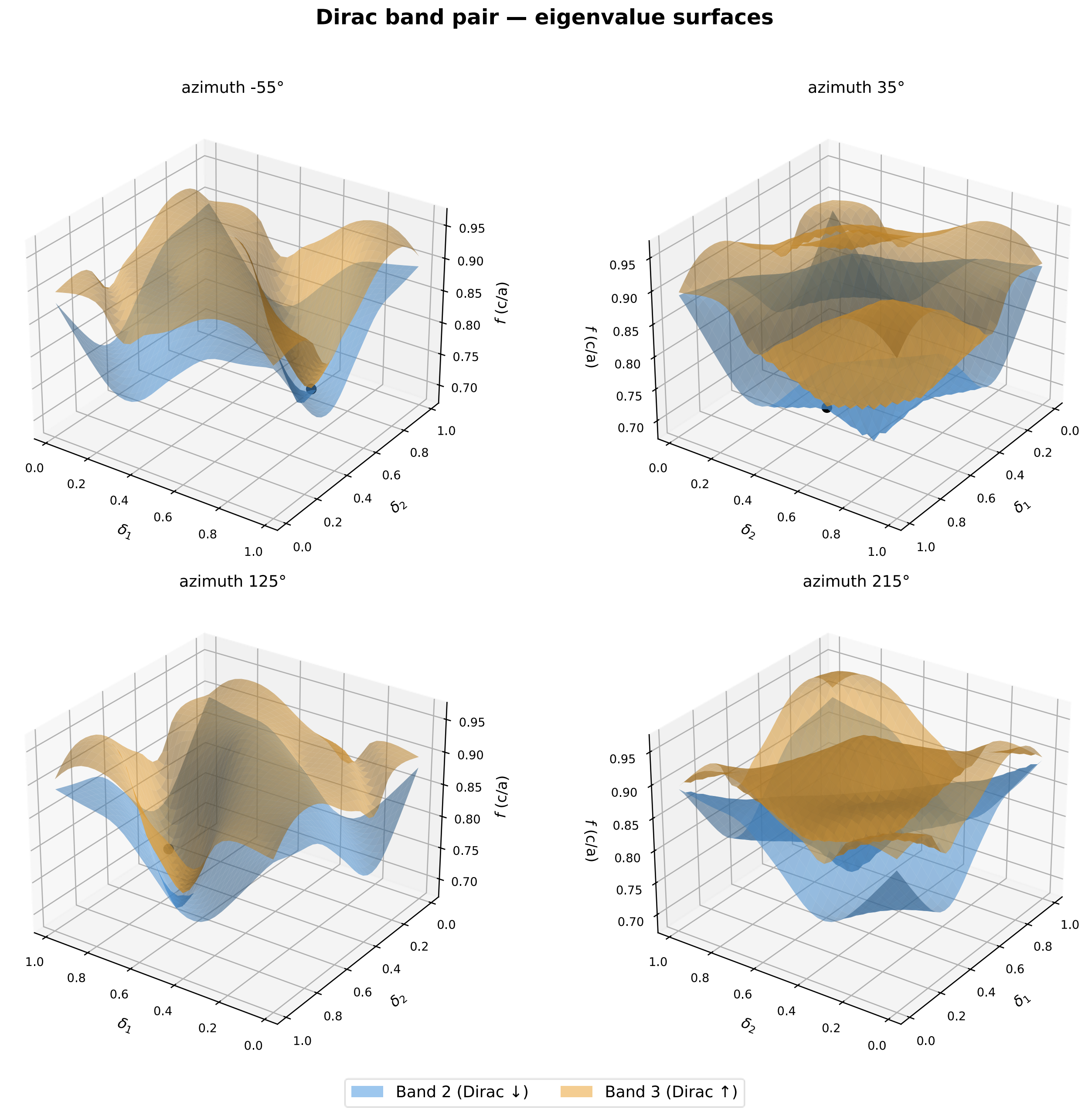


Solvers *need* Commensurability

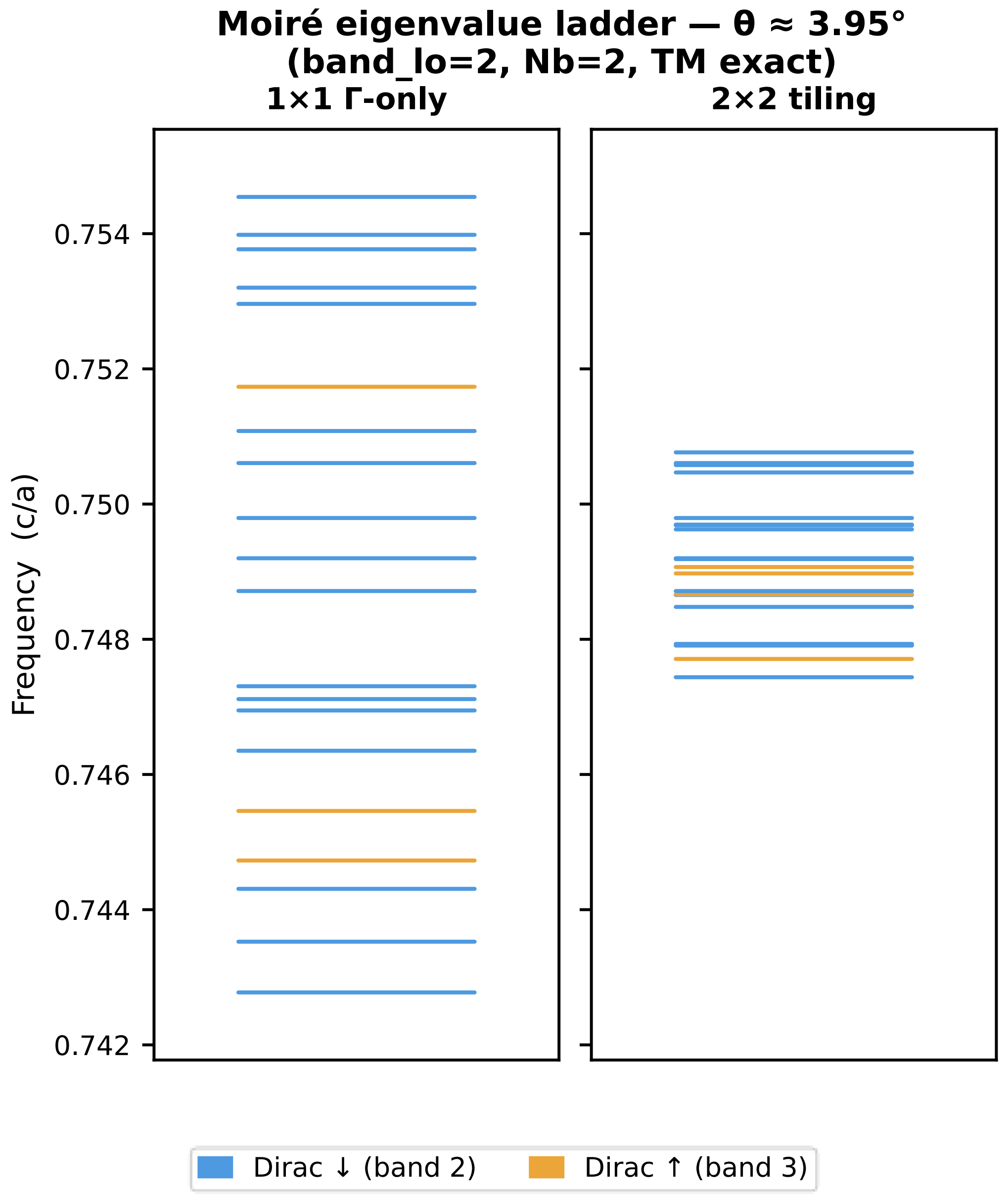
Benchmarking Blaze against MPB



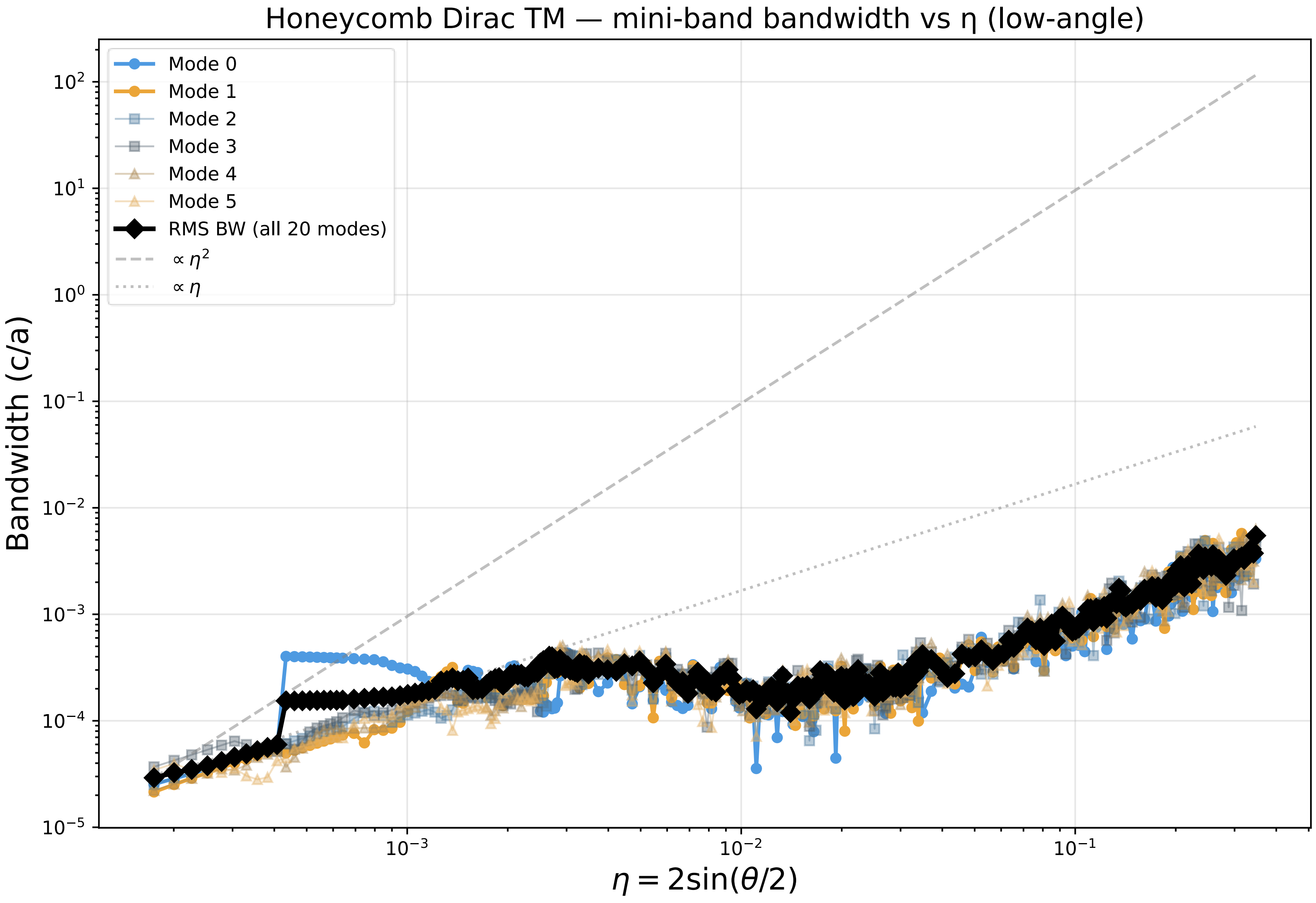
Dirac K-point, TM **Eigenvalue Surface**



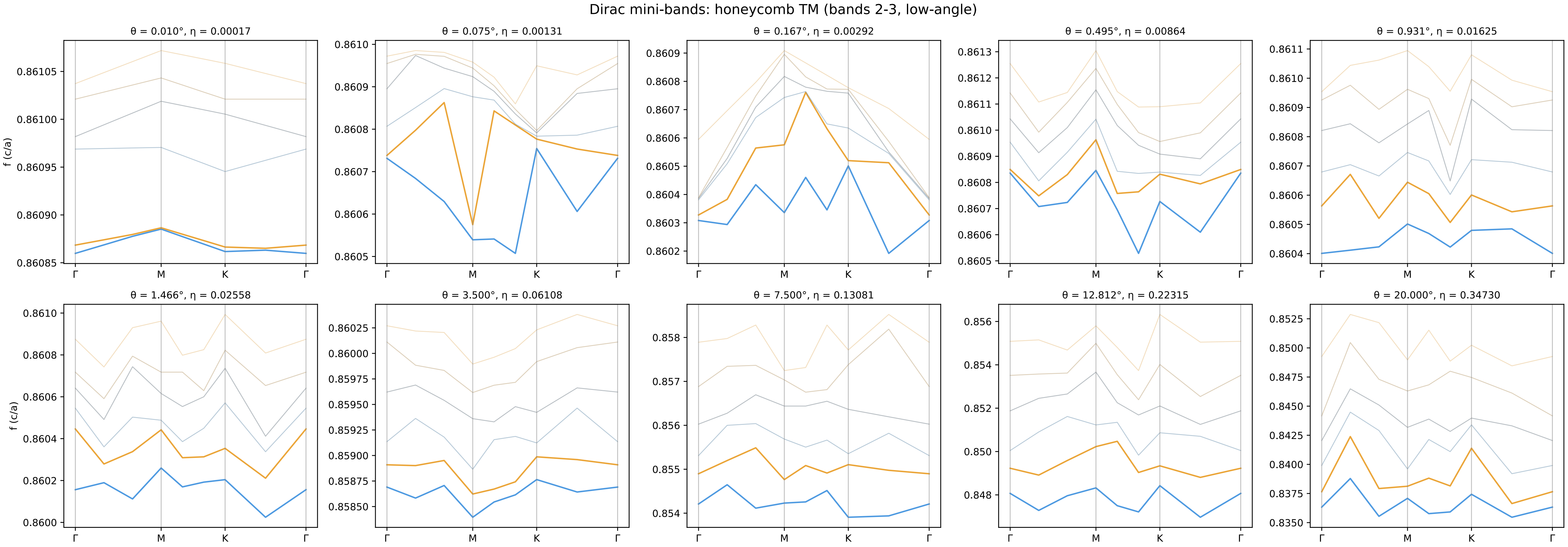
Dirac K-point, TM **Band Contribution**



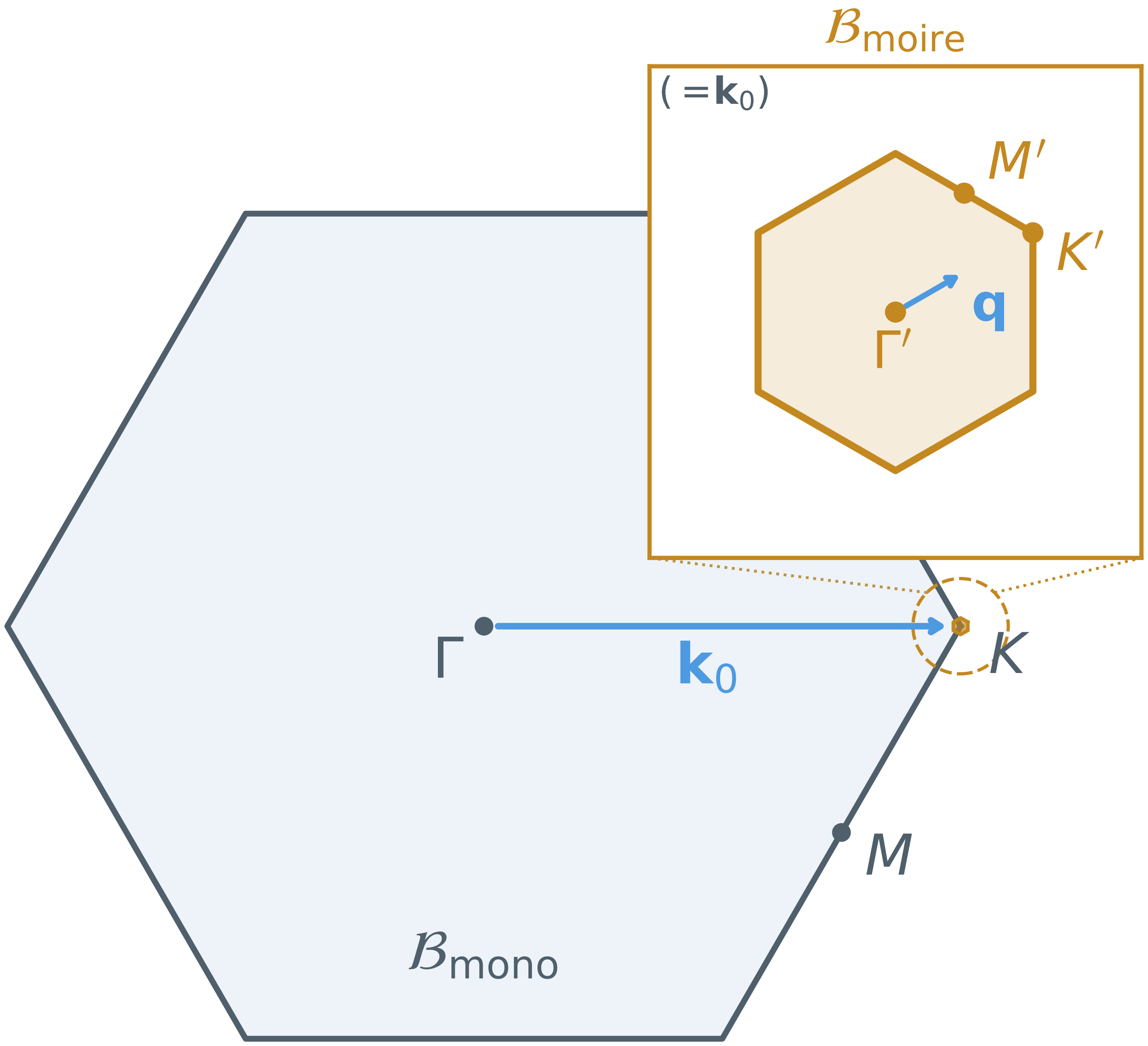
Dirac K-point, TM **Angle Scan**



Dirac K-point, TM **Minibands**

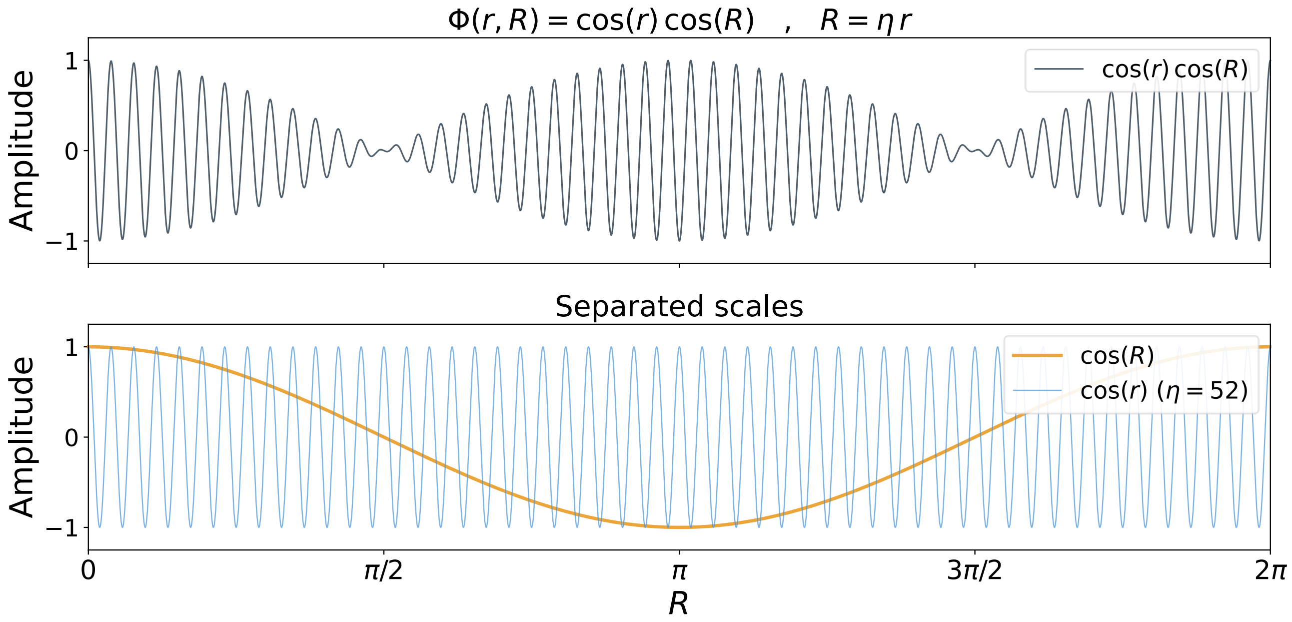


Envelope Approximation: Two Scales in $\boldsymbol{k}$-Space



How to *Separate* Two Scales: **Projection**

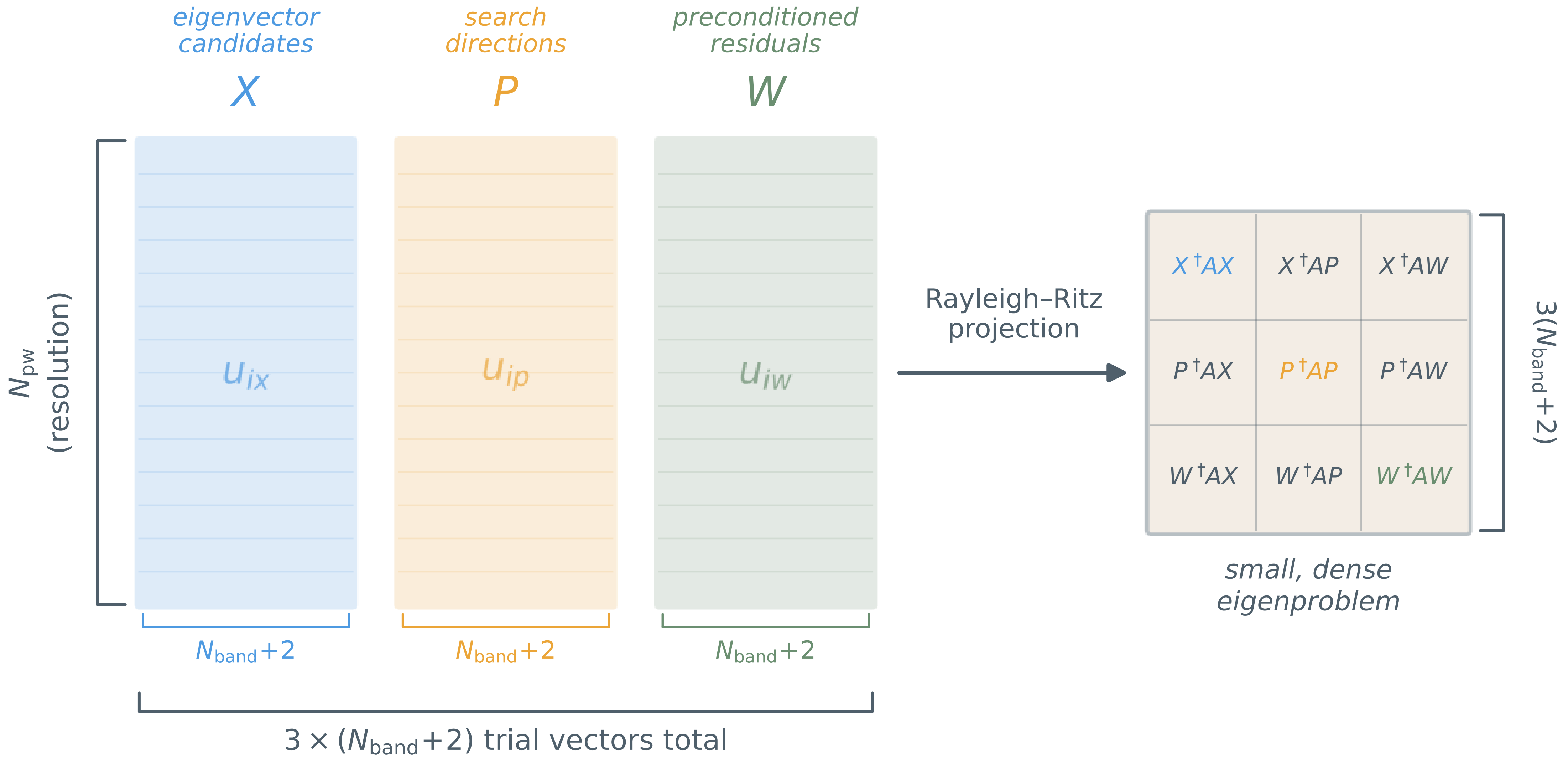
$$\langle \cos(r), \Phi \rangle_{[0,2\pi]} := \frac{1}{2\pi} \int_0^{2\pi} \cos(r)\Phi(r, R)\mathrm{d}r = \frac{\cos(R)}{2\pi} \int_0^{2\pi} \cos^2(r)\mathrm{d}r = \frac{1}{2}\cos(R)$$



Generally

$$\langle g, h \rangle_\Omega := \frac{1}{|\Omega|} \int_\Omega g^*(\boldsymbol{r}; \boldsymbol{R}) h(\boldsymbol{r}; \boldsymbol{R}) \mathrm{d}\boldsymbol{r}$$

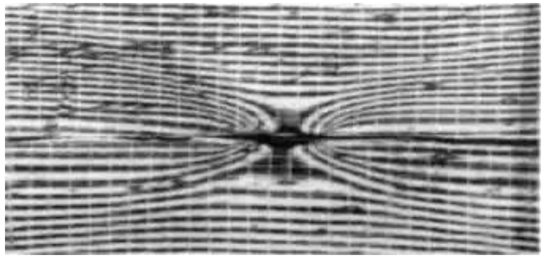
LOBPCG Search Subspace



Effective Hamiltonian – What's inside?

Term	Order	Physical meaning
Λ band energies	η^0	Local photonic band energies of the two-atomic crystal at each moire position.
$\frac{1}{2}\left(v^{(i)}\Pi_i + \Pi_i v^{(i)}\right)$ group-velocity drift	η^1	Band slope at $\boldsymbol{k}_0$: how fast modes propagate across the moire cell.
A_i non-Abelian Berry connection	η^1–η^2	Geometric gauge field from the Bloch frame rotating as registry varies.
$\frac{1}{2}\Pi_i M_{ij}^{-1}\Pi_j$ inverse mass tensor	η^2	Band curvature at $\boldsymbol{k}_0$, dressed by virtual transitions into remote bands.
$\Xi_i^\dagger \varepsilon^{-1}\Xi_i$ Born-Huang potential	η^2	Energy cost of the active Bloch frame leaking into remote bands as $\boldsymbol{R}$ varies.

Moiré Effect – Scientific Use



Strutt (Rayleigh) et al., *Philosophical Magazine* ***47****, 81 (1874)*

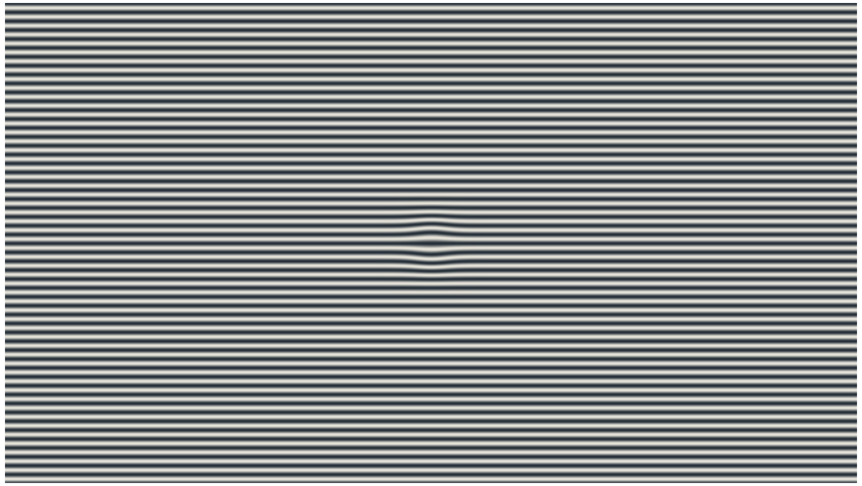


Image References

[1] C. Tuggle, Moiré Effect, https://www.callitugglephotography.com/post/moir%C3%A9-effect.
[2] u/Cyb3r3xp3rt, Why does any picture I take of my screen do this?, https://www.reddit.com/r/computers/comments/p5k4yz/why_does_any_picture_i_take_of_my_screen_do_this/.
[3] S. Dufresne, Using Moiré Patterns To Guide Ships, https://hackaday.com/2018/04/07/using-moire-patterns-to-guide-ships/.