

Department of Physics
Condensed Matter Theory

MASTER THESIS

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

Author:
Rene-Marcel Lehner

Supervisors:
Prof. Dr. Doris Reiter
Dr. Moritz Cygorek

Submitted on March 27, 2026
Second edition, revised September 2026

Imprint

Project: Master Thesis
Title: Photonic Band Theory of Moire Crystals: A Two-Scale Approach
Author: Rene-Marcel Lehner
Date: March 27, 2026 (first edition); September 2026 (second edition)
Keywords: photonic crystal, moire lattice, magic angle, flat bands, pwe solver, mpb, fdfd

Study program:
Master of Science in Physics, M.Sc.
TU Dortmund University

Supervisor 1:
Prof. Dr. Doris Reiter
TU Dortmund University
doris.reiter@tu-dortmund.de

Supervisor 2:
Dr. Moritz Cygorek
TU Dortmund University
moritz.cygorek@tu-dortmund.de

Preface

Before we explore the physics of moire lattices and their accompanying computational models, a few brief notes concerning terminology, reproducible software, and formatting are in order.

A Note on Orthography and Etymology



Throughout this thesis, the word “moire” is written without its technically correct acute accent (**moiré**). This deliberate choice declutters the text amidst dense mathematical notations and prevents encoding artifacts in script bindings, plot formats, and automated text pipelines.

Interestingly, contrary to ubiquitous naming conventions in physics, moire does not refer to a person. It stems from the French verb *moirer*, meaning “to give a watered or wavy finish to.” This term elegantly reflects the wavelike visual effect produced by these mesmerizing structures.

Visualizing Moire Structures

Most figures in this thesis are rendered as Scalable Vector Graphics (SVGs). Visualizing moire superlattices is challenging, as intricate spatial details easily get averaged out by standard raster image formats like PNG or WebP. However, because moire patterns can consist of thousands of individual lattice elements, these usually lightweight SVG files can become unusually large.

To find a reliable compromise, the most complex structures were converted to raster formats. Nonetheless, minor scrolling microstutters on certain devices and a slightly larger document size are natural consequences of preserving the high-fidelity visualizations required for these structures.

Reproducibility and Software



In the spirit of open science, the entire software ecosystem developed for this thesis is publicly available on GitHub, organized into two distinct repositories:

- **MSL (Moire SuperLattice)**: The central research repository. It hosts the procedural logic for 2D moire lattices, explicit Finite-Difference Frequency-Domain (FDFD) solvers, and the Envelope Approximation (EA) models utilized in these chapters. Performance is driven by Rust backends with seamless Python bindings.
- **Blaze2D**: A custom Plane-Wave Expansion (PWE) Maxwell solver engineered specifically for the dense data demands of EA. Written from scratch in Rust to provide explicit operator matrices, it features Python and WebAssembly bindings, and is published globally on PyPI (`pip install blaze2d`).

Both repositories are supported by dedicated GitHub Pages: the MSL documentation and the Blaze2D technical report serve as central platforms for deep exploration, transparent FDFD benchmarks, and comprehensive convergence validations against MPB.

Hardware Specifications



All workstation-specific measurements, including compute times and runtime analyses, were executed natively on a single isolated Desktop PC to guarantee consistent execution environments. The exact hardware specifications are detailed in Appendix C.

A Note on the Second Edition

This second edition revises the thesis submitted on March 27, 2026. It refines the derivation of the multi-band envelope approximation, reworks the second half of the validation chapter, and extends the story with results obtained after submission: an eigenvalue-exact comparison of the envelope model against two independent full-Maxwell solvers on a crystal built to the requirements such a comparison demands, and the completed model applied to the thesis crystal at angles no brute-force solver reaches.

Nothing in the first edition was silently overwritten. Every corrected statement is listed with its original in the errata appendix (Appendix E), every figure of the second edition regenerates from a script and a data snapshot kept in the thesis repository, and the two fully expanded effective Hamiltonians, TE and TM, open the appendix as full pages. The core conclusion stands; its evidence is now of a different quality.

Contents

Reproducibility and Software	iii
1 Introduction	1
1.1 Achievements in Photonic Moire Systems	2
1.2 Scope and Objective: Developing a New Framework	3
1.3 Structure of the Thesis	3
2 Photonic Moire Crystals	4
2.1 From Periodic Dielectrics to Photonic Bands	4
2.2 Building a Photonic Moire Crystal	6
2.3 Incompatibility of Standard Solvers with Moire Crystals	9
3 The Multi-Band Envelope Approximation	12
3.1 Local Periodicity and the Two-Atomic Crystal Approximation	12
3.2 The Two-Scale Lift	16
3.3 From Local Bloch Problems to a Multiscale Ansatz	18
3.4 A Primer on Bloch-Cell Projection	20
3.5 TE Expansion in Orders of η	21
3.6 The TM Case: Generalized and Hermitized Expansions	26
3.7 The Resummed Limit	29
3.8 From Effective Hamiltonian to Computable Data	30
4 Blaze2D: A Custom Plane-Wave Solver	32
4.1 Design Choices	32
4.2 Geometry and the Permittivity Matrix	32
4.3 Eigenvalue Operators and Their Application	33
4.4 Preconditioning	33
4.5 The LOBPCG Solver	34
4.6 Mixed Precision	35
4.7 Validation	35
4.8 Benchmarks	38
4.9 From Solver to Pipeline	38
5 The Envelope Framework in Practice	40
5.1 The Envelope Approximation Pipeline	40
5.2 The Need for Independent Validation	42
5.3 Reference Solvers: MPB and FDFD	43
5.4 What a Faithful Comparison Requires	49
5.5 The Thesis Crystal Revisited	50
5.6 Where the Envelope Approximation Is Exact	53
5.7 Internal Consistency Tests	58
5.8 Dirac Physics of the Honeycomb Crystal	60
5.9 Bandwidth Scaling and the Search for Magic Angles	62
6 Conclusion	64
Appendix A: The Effective Hamiltonians at a Glance	66
Appendix B: Downfolding and Coefficient Identities	68
Appendix C: Computational Hardware	71
Appendix D: Additional Figures	72
Appendix E: Errata to the First Edition	77
References	79

Glossary, Symbols & Abbreviations	82
Index	84
Acknowledgements	85

Abstract

Twisting two photonic crystals against each other produces an emergent moire lattice whose period far exceeds that of the crystals it is built from. Standard solvers cannot treat this system: the moire unit cell grows as the inverse of the twist angle, making direct computation infeasible precisely where the physics is richest. At generic angles the problem is even more fundamental: the bilayer is incommensurate and no periodic unit cell exists for any solver to operate on.

This thesis develops a multiband envelope approximation that, starting from the local Bloch modes of the twisted bilayer, yields an effective Hamiltonian whose components (band energies, group velocities, effective masses, Berry connections, and Born-Huang potentials) are all defined on the registry domain and independent of the twist angle. Because this approximation demands full Bloch eigenvector data across thousands of configurations, we developed Blaze2D, a plane-wave eigensolver written in Rust, purpose-built for the throughput and data transparency the envelope framework requires.

The pipeline is validated against an independent finite-difference frequency-domain solver checked against MPB. On a smooth single-valley crystal built to the requirements of an eigenvalue-exact comparison, the envelope model, the plane-wave reference and FDFD agree on the moire manifold state to below 10^{-6} in frequency with a measured convergence law, and the resummed-frame model matches every state of a declared domain on a supercell of 8911 cells within the reference's own discretisation error. On the strongly coupled square bilayer of the thesis the model reproduces the manifold floor within MPB's error and runs at angles no brute-force solver reaches. The geometric data, including Berry curvature, Born-Huang potential, velocity and mass fields, provide a spatially resolved decomposition of moire physics that no conventional supercell calculation can offer. The result is an open-source pipeline that takes a crystal specification and a twist angle as input and produces moire eigenvalues, miniband dispersions, and the full effective Hamiltonian data as output.

Zusammenfassung

Werden zwei photonische Kristalle gegeneinander verdreht, entsteht ein Moire-Gitter, dessen Periode die der erzeugenden Kristalle weit übersteigt. Konventionelle Solver können dieses System nicht behandeln: die Moire-Einheitszelle wächst invers mit dem Drehwinkel, sodass direkte Rechnungen gerade dort versagen, wo die Physik am reichhaltigsten ist. Bei allgemeinen Winkeln ist das Problem noch grundlegender: die Doppelschicht ist inkommensurabel und es existiert keine periodische Einheitszelle, auf der ein Löser operieren könnte.

Diese Arbeit entwickelt eine Multiband envelope approximation, die ausgehend von den lokalen Bloch-Moden der verdrehten Doppelschicht einen effektiven Hamiltonoperator liefert, dessen Bestandteile (Bandenergien, Gruppengeschwindigkeiten, effektive Massen, Berry-Zusammenhänge und Born-Huang-Potentiale) auf der registry domain definiert sind und nicht vom Drehwinkel abhängen. Da diese Näherung vollständige Bloch-Eigenvektordaten über Tausende von Konfigurationen erfordert, wurde eigens Blaze2D entwickelt, ein open-source PWE solver in Rust.

Die Validierung gegen einen unabhängigen FDFD solver, der seinerseits gegen MPB geprüft wurde, wird bis zur Eigenwert-Genauigkeit geführt: Auf einem glatten Einzeltal-Kristall stimmen envelope approximation, Ebene-Wellen-Referenz und FDFD im Moire-Zustand bis unter 10^{-6} in der Frequenz überein, mit gemessenem Konvergenzgesetz, und das resummierte Modell reproduziert jeden Zustand eines vorab festgelegten Bereichs auf einer Superzelle aus 8911 Zellen innerhalb des Diskretisierungsfehlers der Referenz. Auf der stark gekoppelten quadratischen Doppelschicht der Arbeit reproduziert das Modell den Boden der Mannigfaltigkeit innerhalb des MPB-Fehlers und rechnet bei Winkeln, die kein Superzellen-Löser mehr erreicht. Die geometrischen Daten, darunter Berry-Krümmung, Born-Huang-Potential, Geschwindigkeits- und Massefelder, liefern eine räumlich aufgelöste Zerlegung der Moire-Physik, die keine direkte Rechnung bieten kann. Die resultierende open-source Pipeline erzeugt aus einer Kristallspezifikation und einem Drehwinkel Moire-Eigenwerte, Miniband-Dispersionen und die vollständigen effektiven Hamiltonoperator-Daten.

1 Introduction

When two periodic structures are laid on top of one another with a slight mismatch in angle or spacing, a new pattern appears on a scale much larger than either of the originals. This is the *moire effect*: a geometric interference phenomenon that does not require any special material platform, only the superposition of regular structures. This effect was familiar long before it became a scientific object. It shows up in photographs of striped fabrics, on digital displays, and in many other situations where two grids almost agree (see Figure 1).



Figure 1: Moire fringes produced by the interference between the camera's pixel grid and a periodic subject: a striped shirt (left, from [1]) and a computer monitor (right, from [2]).

The scientific usefulness of this effect was recognized early. In 1874, Lord Rayleigh proposed superimposing two diffraction gratings to reveal imperfections in manufactured rulings [3]. Figure 2 demonstrates the application of Rayleigh's method on a pair of ruled gratings. The large moire fringes make minute deviations from perfect periodicity visible, turning small defects into easily readable distortions. In that sense, moire patterns are not merely visual curiosities. They amplify otherwise

difficult-to-detect deviations from periodicity.

The same geometric usefulness also appears in the *Inogon leading light* shown in Figure 3, a Swedish navigational aid developed in the 1980s. There, overlapping periodic grids generate a large moire pattern resembling an arrow whose orientation, as seen by an approaching vessel, indicates necessary course corrections for safe passage through shallow waters, entirely without electronics, despite the device's name.

Since any two superimposed periodic structures can produce moire patterns, the extension to crystalline matter is straightforward. A crystal lattice is itself a periodic structure. If two lattices are overlaid with a small relative twist or mismatch, the same geometric mechanism produces a new long-wavelength pattern: a *moire lattice*. The phenomenon is still geometric, but now it acts on a system whose waves, symmetries, and spectra already carry physical meaning.

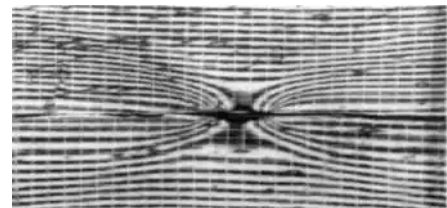


Figure 2: Superimposing two ruled gratings reveals manufacturing defects as distortions in the moire fringes, following Rayleigh's 1874 proposal. Image from [4].

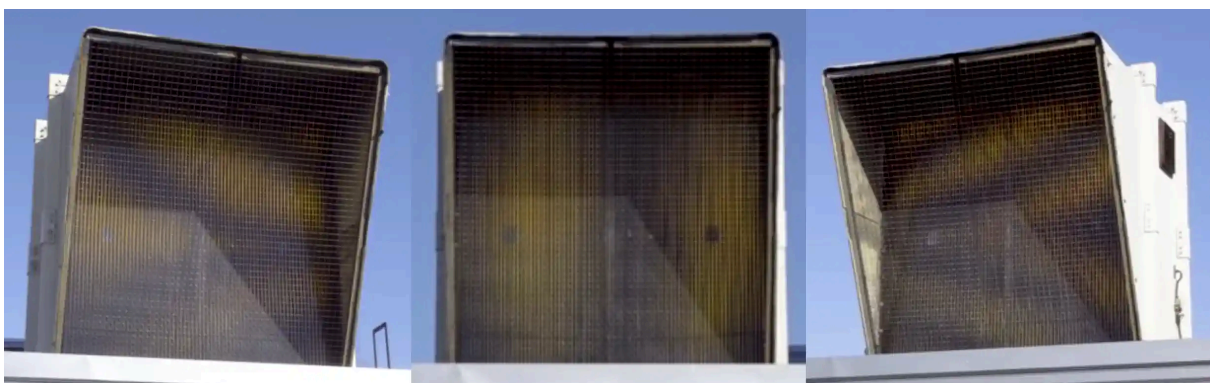


Figure 3: The Inogon leading light, a Swedish navigational aid based on overlapping periodic grids. The resulting moire arrow points left or right for course corrections and aligns vertically on the safe centerline. Image from [5].

The realization that geometric moire patterns could manipulate physical behavior opened a new direction in condensed matter research. In 2011, Bistrizter and MacDonald predicted that twisted bilayer graphene possesses what they termed *magic angles*: a discrete set of twist angles at which the Dirac velocity is strongly suppressed and the lowest moire minibands become extremely flat [6]. Seven years later, in 2018, Jarillo-Herrero's group at

MIT experimentally validated this prediction in two landmark papers, reporting correlated insulating behavior [7] and unconventional superconductivity [8] near the first magic angle at 1.05° . These publications founded the field of *twistronics*: the idea that geometry can serve as a tuning knob for electronic material behavior.

Photonic crystals are the optical analogue of this setting: periodic dielectric media whose band structures govern the propagation of electromagnetic waves, in the same way that electronic band structures govern the motion of electrons [9]. Twisting one photonic lattice against another should therefore also create a moire superstructure, and that superstructure should modify how light propagates. This prospect is the starting point of *photonic moire crystals*. Figure 4 illustrates such a construction for two hexagonal lattices with a small relative twist.

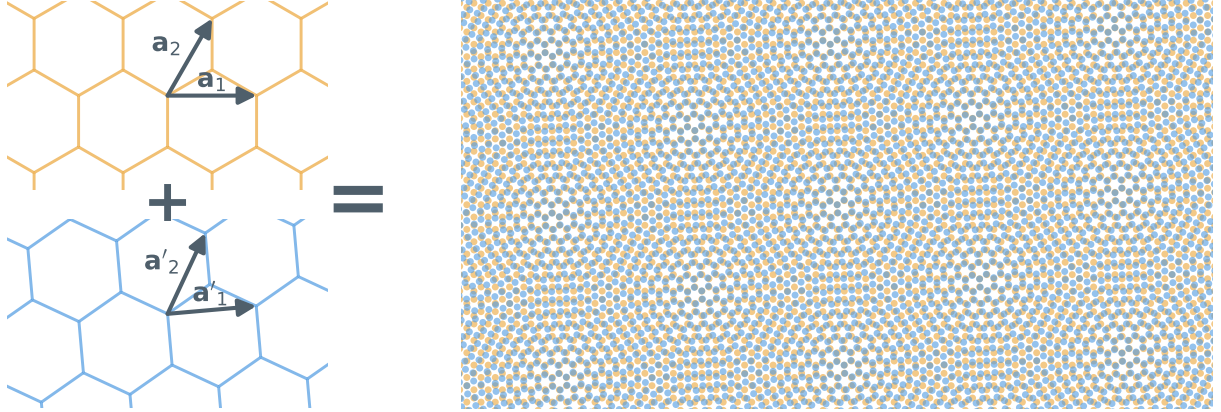


Figure 4: Construction of a moire pattern from two hexagonal lattices twisted by $\theta = 5^\circ$. **Left:** the two monolayers with lattice vectors $\mathbf{a}_1, \mathbf{a}_2$ (orange, fixed) and $\mathbf{a}'_1, \mathbf{a}'_2$ (blue, rotated). **Right:** the resulting bilayer, showing the emergent long-range moire periodicity.

1.1 Achievements in Photonic Moire Systems

In photonics, moire lattices are attractive for the same reason as in electronic systems: the twist introduces a second, much larger length scale that reshapes the underlying band structure in a tunable way. The natural expectation is that tuning the twist can flatten photonic bands, localize light, enhance the density of optical states, or open routes toward unusual dispersion and confinement, much as it does in the electronic case.

Several groups have already demonstrated this. Wang *et al.* demonstrated localization and delocalization of light in two-dimensional photonic moire lattices [10], making the geometric control of optical modes directly visible. Tang *et al.* modeled magic-angle flat bands and slow-light behavior in twisted bilayer silicon photonic crystal slabs [11], while Dong *et al.* developed a coupled-mode description for low-angle twisted bilayer honeycomb photonic crystals that closely parallels continuum models from graphene [12]. Lou *et al.* formulated a plane-wave treatment of twisted bilayer photonic crystal slabs valid beyond the strict small-angle limit [13]. Together, these works established that photonic moire systems exhibit much of the same phenomenology as their electronic counterparts.

The field then broadened quickly. Mao *et al.* connected flat-band enhancement to lasing in moire nanostructures, marking the first shift toward practical photonic engineering [14]. Yi *et al.* showed that strong interlayer coupling can support topological flat bands even at comparatively large twist angles [15]. Huang *et al.* related moire physics to quasi-bound states in the continuum [16], and Tang *et al.* later provided an on-chip experimental probe of twist-angle-dependent photonic band structure [17]. More recently, Qin *et al.* demonstrated optical moire bound states in the continuum in a merged one-dimensional photonic crystal slab [18], and Yan *et al.* reported Purcell-enhanced quantum-dot emission in moire photonic crystal nanocavities [19]. A broader overview of this rapidly developing area is given in the review by Oudich *et al.* [20].

This body of work shows that moire photonic systems can host minibands, spectral reshaping, localization, slow-light effects, and flat-band regimes. At the same time, it reveals what is still missing. Most successful descriptions in the literature are either highly capable full-wave calculations for specific geometries, or reduced models tailored to particular settings such as bilayer honeycomb structures, weak coupling, or Dirac-point physics. These

approaches are valuable, but they do not yet amount to a general and transparent framework for photonic moire crystals across different lattices and for arbitrary frequency ranges or reciprocal-space points.

1.2 Scope and Objective: Developing a New Framework

The lack of such a description sets the motivation for this thesis. The central question is whether we can derive a reduced theory directly from the photonic eigenproblem that remains tied to local Bloch physics, yet is flexible enough to describe moire-scale behavior beyond a single special model class.

This thesis approaches that question through a multiband *envelope approximation* inspired by the $\mathbf{k} \cdot \mathbf{p}$ method of semiconductor theory [21]. The guiding idea is to separate the fast periodic physics of the underlying crystal from the slow variation introduced by the moire superlattice, and to do so in a way that keeps the structure of the effective description transparent. In such a formulation, Berry connections [22,23] and Born-Huang-type corrections [24] appear as intrinsic contributions to the effective moire-scale dynamics, shifting band energies and coupling channels in ways that have no counterpart in the single-crystal problem.

The purpose of the thesis is to construct, implement, and validate such a first-principles description. Because the envelope approximation requires physical data not readily available from existing solvers, a dedicated two-dimensional plane-wave eigensolver, Blaze2D, was developed in Rust as part of this work.

1.3 Structure of the Thesis

The remainder of this thesis is organized as follows.

Section 2 introduces photonic moire crystals. It reviews photonic crystal band structure, constructs the twisted bilayer, and identifies the two length scales, monolayer and moire, that make direct numerical treatment expensive and even prohibitive.

Section 3 introduces the two-atomic crystal approximation that enables the envelope theory, together with a quality parameter for judging when this approximation is reliable. It then derives the multiband envelope approximation. Starting from the local Bloch modes of the two-atomic crystal, a two-scale expansion separates fast and slow degrees of freedom and yields an effective Hamiltonian whose components, band energies, velocities, mass tensors, Berry connections, and Born-Huang potentials, live on the moire scale alone. The chapter ends with the limit the expansion converges to, a model in which the local Bloch frame is taken exactly at every moire harmonic.

Section 4 presents Blaze2D, a plane-wave eigensolver written in Rust. The envelope approximation requires full Bloch eigenvector data at every point of a dense registry sweep, and Blaze2D was built specifically to provide this data efficiently.

Section 5 assembles the pipeline end-to-end and tests it. It establishes two independent reference solvers, an FDFD eigensolver and MPB, states what an eigenvalue-by-eigenvalue comparison between the envelope model and a supercell solver must satisfy, and carries such a comparison through: first on the thesis crystal, a strongly coupled square bilayer where the completed model reproduces the manifold floor and runs at angles no brute-force solver reaches, then on a smooth single-valley crystal built to the requirements, where the envelope model, the plane-wave reference and FDFD agree on every state of a declared domain to within the reference's own discretisation error. The chapter closes with the internal consistency of the pipeline, the geometric Hamiltonian data of a honeycomb Dirac crystal, and the search for magic angles.

Section 6 summarises the contributions and discusses open questions.

2 Photonic Moire Crystals

To apply the moire idea to light requires a concrete physical system. We begin by reviewing the photonic crystal and its band structure, then construct the twisted bilayer and identify the two-scale problem that will drive the rest of the thesis.

The construction itself is simple: duplicate a periodic dielectric medium and introduce a small relative twist. The resulting structure contains two very different length scales at once, and that coexistence produces rich new behavior while placing the system beyond the reach of conventional computational approaches.

2.1 From Periodic Dielectrics to Photonic Bands

A photonic crystal is a dielectric structure whose material parameters repeat periodically in space (see Figure 5). This periodicity reorganizes the allowed electromagnetic modes into bands, in close analogy with how a periodic potential reorganizes electronic wave functions in a solid. The terminology of lattices, Brillouin zones, Bloch waves, dispersion relations, density of states, and band gaps transfers almost unchanged from electronic crystals to photonic crystals [9].

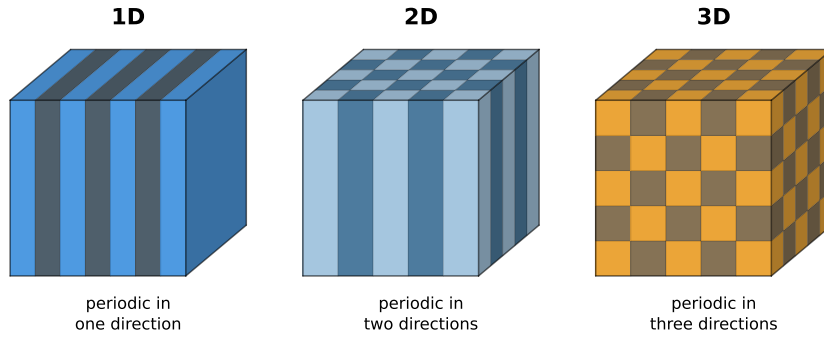


Figure 5: Examples of one-, two-, and three-dimensional photonic crystals. In each case, the defining ingredient is the periodic arrangement of dielectric material.

This analogy is powerful because both electrons and photons obey wave equations in periodic media. The difference is not in the existence of bands, but in the operator that generates them. For electrons, the starting point is the Schrödinger equation. For photons, it is Maxwell's equations.

2.1.1 The Governing Equations of Photonic Crystals

For linear, lossless, non-magnetic, nondispersive media, the electromagnetic field is governed by Maxwell's equations. Assuming time-harmonic fields $\mathbf{H}(\mathbf{x}, t) = \mathbf{H}(\mathbf{x})e^{-i\omega t}$ with angular frequency ω , we can eliminate the electric field and write the problem as an eigenvalue equation for the magnetic field. The central photonic-crystal equation is then

Photonic Master Equation

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

where $\varepsilon(\mathbf{x})$ is the spatially varying dielectric function at the physical position $\mathbf{x}$. For $\omega \neq 0$, taking the divergence of both sides implies $\nabla \cdot \mathbf{H} = 0$, so the transversality constraint is automatically satisfied by the eigenstates. This equation is the foundation on which the theory of later sections is built.

For the two-dimensional systems studied here, translational invariance along the out-of-plane direction reduces the vector problem to two scalar polarizations. This decoupling requires that the permittivity is a scalar function of in-plane position only, $\varepsilon = \varepsilon(x, y)$, i.e. a spatially local, isotropic permittivity with no z -dependence. In the 2D photonic-crystal convention used here (and by MPB [25]), TE denotes $H_z \neq 0$ with in-plane electric field, while TM denotes $E_z \neq 0$ with in-plane magnetic field. It is convenient to write both polarizations in the generalized form

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

with the operator pair (A, B) depending on the polarization (Table 1).

Polarization	Field	A	B
TE	H_z	$-\nabla \cdot (\varepsilon^{-1}(\mathbf{x}) \nabla)$	$\mathbb{1}$
TM	E_z	$-\nabla^2$	$\varepsilon(\mathbf{x})$

Table 1: Operator pairs for the two scalar polarizations of the 2D photonic eigenproblem.

The TE problem is especially convenient because it is already a standard Hermitian eigenvalue problem:

$$-\nabla \cdot \left(\frac{1}{\varepsilon(\mathbf{x})} \nabla H_z(\mathbf{x}) \right) = \frac{\omega^2}{c^2} H_z(\mathbf{x}). \quad (3)$$

The TM sector is most naturally obtained from the dual electric-field formulation of Maxwell's equations, yielding the generalized eigenproblem

$$-\nabla^2 E_z(\mathbf{x}) = \frac{\omega^2}{c^2} \varepsilon(\mathbf{x}) E_z(\mathbf{x}), \quad (4)$$

but conceptually the consequence is the same: once the dielectric geometry is fixed, the photonic crystal becomes an *eigenvalue problem*. This thesis works in the two-dimensional scalar setting and focuses predominantly on the TE formulation, because it is the cleanest environment in which to isolate the moire-scale physics.

From this point onward, non-bold H and E denote the scalar polarization components H_z and E_z . Bold notation is reserved for the full vector fields in the three-dimensional Maxwell formulation.

2.1.2 Bloch Waves and Photonic Bands

Bloch's theorem is most naturally stated for the full vector field before specializing to either scalar polarization. For an ordinary photonic crystal, the dielectric function satisfies lattice periodicity, $\varepsilon(\mathbf{x} + \mathbf{T}) = \varepsilon(\mathbf{x})$ for every lattice vector $\mathbf{T}$. Bloch's theorem therefore applies directly:

$$\mathbf{H}_{n\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} \mathbf{u}_{n\mathbf{k}}(\mathbf{x}), \quad (5)$$

where the periodic part $\mathbf{u}_{n\mathbf{k}}$ has the periodicity of the primitive cell. Substituting the Bloch form into the master equation yields the Bloch-periodic eigenproblem

Photonic Band Equation

$$(\nabla + i\mathbf{k}) \times \left[\frac{1}{\varepsilon(\mathbf{x})} (\nabla + i\mathbf{k}) \times \mathbf{u}_{n\mathbf{k}}(\mathbf{x}) \right] = \frac{\omega_{n\mathbf{k}}^2}{c^2} \mathbf{u}_{n\mathbf{k}}(\mathbf{x}), \quad (6)$$

and from it the photonic band structure $\omega_n(\mathbf{k})$.

With the band structure $\omega_n(\mathbf{k})$ in hand, the condensed-matter analogy becomes operational. Band gaps are frequency windows without propagating modes. Flat bands imply small group velocity and enhanced density of states. High-symmetry points such as Γ , X , M , or K organize the discussion exactly as they do in electronic crystals. Figure 6 illustrates this analogy for two canonical lattices, displaying bands and band gaps along the standard high-symmetry path.

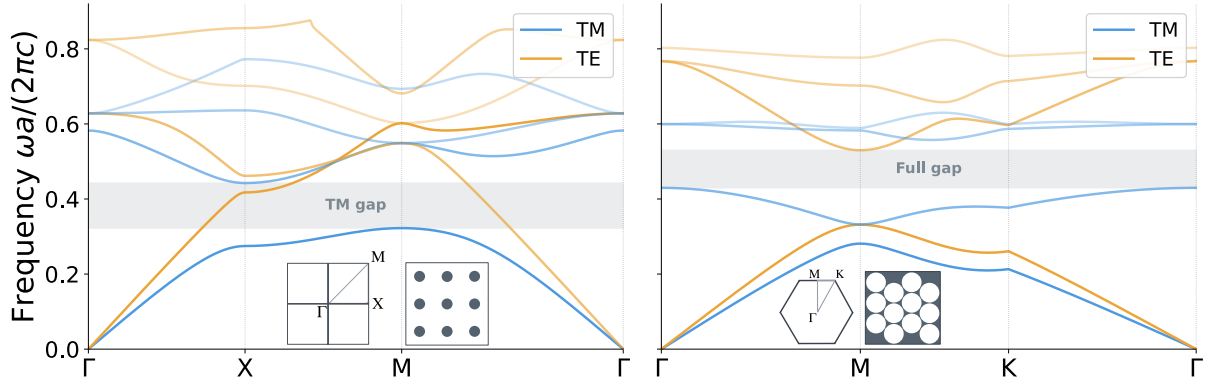


Figure 6: Photonic band diagrams for two canonical two-dimensional lattices. **Left:** square lattice of dielectric rods in air. **Right:** triangular lattice of air holes in dielectric. The band-structure terminology familiar from electronic crystals carries over directly to these photonic systems. After Joannopoulos et al. [26].

2.1.3 Computationally Solving a Photonic Crystal

Once Bloch's theorem has reduced the problem to a primitive cell, several mature numerical methods are available. The most relevant method in this thesis is the plane-wave expansion (PWE), implemented for example in MIT's *Photonic Bands* solver MPB [25]. There, the dielectric function and the Bloch-periodic field are expanded in reciprocal-lattice Fourier modes, and the wave equation becomes a matrix eigenproblem at fixed $\mathbf{k}$. For ordinary photonic crystals, this is an efficient and physically transparent route: it yields both eigenfrequencies and Bloch functions.

Real-space methods provide a complementary route. Finite-difference frequency-domain (FDFD) discretizations turn the same eigenproblem into a sparse matrix problem on a grid. Many full-vector formulations use Yee-type staggered layouts [27,28], while scalar 2D TE/TM formulations can also be discretized directly. These methods are often more flexible for complex geometries. With Bloch-periodic boundary conditions they can also compute Bloch modes, although the band structure is not exposed as directly as in plane-wave calculations.

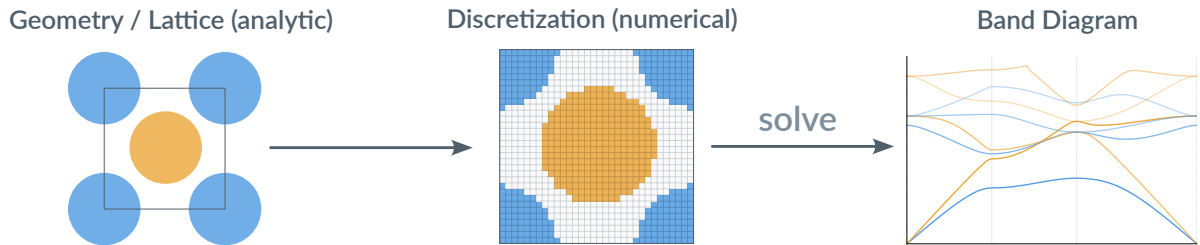


Figure 7: Standard pipeline for computing photonic bands. The analytic geometry is exact, but a computer cannot operate on it directly. Discretization converts materials and operators into finite numerical matrices whose eigenproblem yields the band diagram.

For a single periodic crystal, the standard pipeline is clear (Figure 7): define the geometry, discretize and solve the eigenproblem, and retrieve the eigenvalues for chosen $\mathbf{k}$ -points. Established solver frameworks handle all of these steps automatically. For moiré crystals, however, this pipeline begins to break down. To understand why, we first look at how a moiré crystal is constructed.

2.2 Building a Photonic Moiré Crystal

Stacking two copies of a photonic crystal lattice produces a *bilayer*. Rotating one copy by a small angle θ produces a *twisted bilayer*, which is also the standard moiré platform in both condensed matter [7,8] and photonics [11–13,15].

2.2.1 The Moiré Period and Its Inherited Symmetry

As discussed, creating a moiré crystal by superimposing two identical lattices with a small relative twist produces long-range periodic modulations. The crucial observation is that this modulation defines an *effective moiré lattice*, even when the full decorated bilayer is not exactly periodic. We identify the moiré lattice vectors $\mathbf{L}_1$ and $\mathbf{L}_2$, and denote the shortest of the two as the moiré period L_m . Figure 8 shows four bilayer types, each twisted by

5°: in every case, the moire pattern forms a regular lattice that inherits the symmetry of its parent monolayers. A square bilayer produces a square moire lattice, a triangular bilayer a triangular one, and so on.

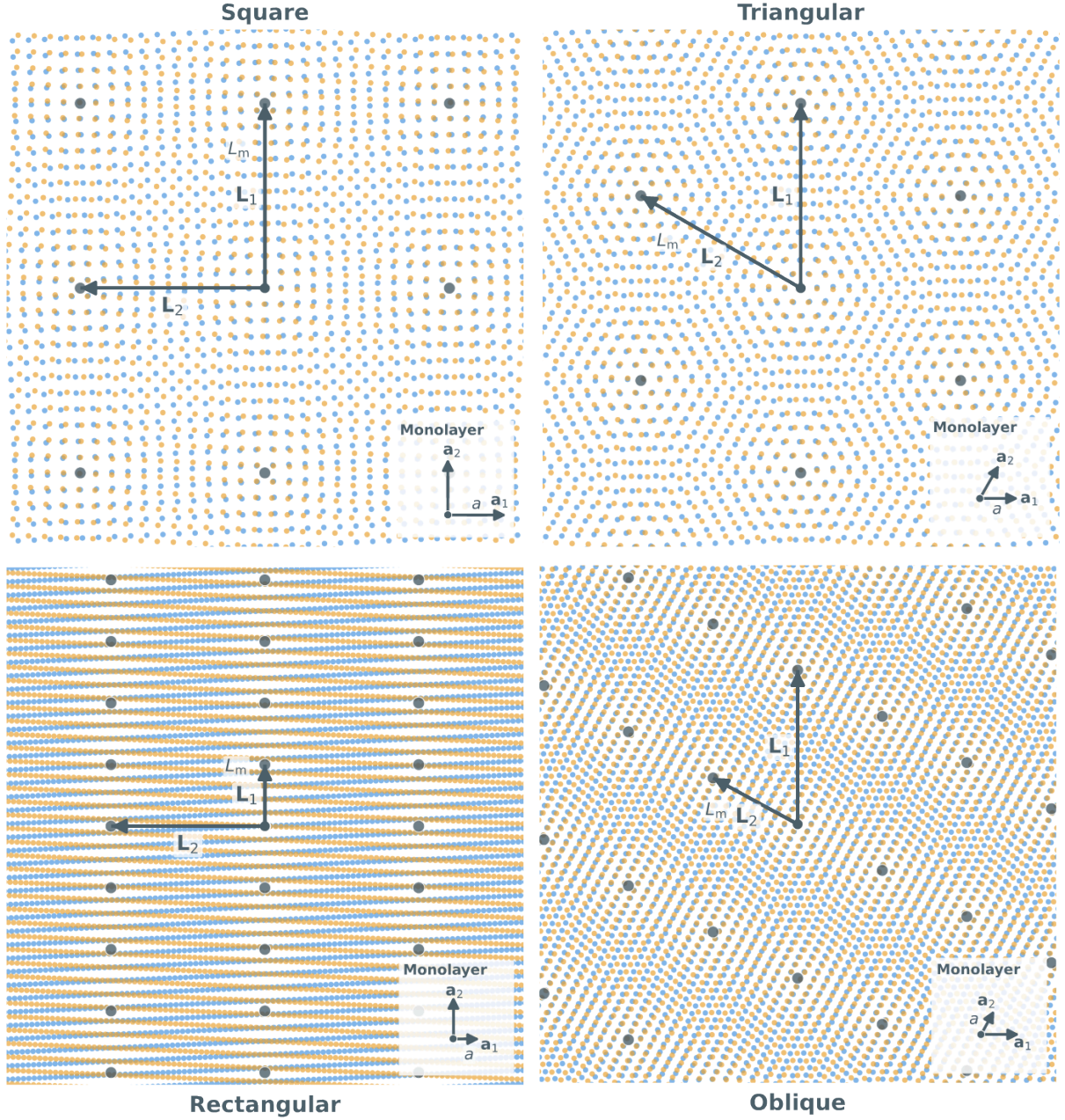


Figure 8: Twisted bilayers for four lattice types at $\theta = 5^\circ$. Dark arrows mark the moire lattice vectors L_1 , L_2 ; L_m labels the shortest. Each moire pattern inherits the symmetry of its parent monolayer.

The length of the moire period L_m depends on the twist angle θ . For a monolayer with lattice constant a (defined by the shortest lattice vector),

$$L_m = \frac{a}{2 \sin(\theta/2)} \approx \frac{a}{\theta} \quad \text{for small } \theta. \quad (7)$$

Because of the inverse dependence on θ , small twist angles produce large moire periods. A 2° twist already gives $L_m \approx 29a$.

2.2.2 Commensurability and Quasi-Periodicity

Independently of exact commensurability, the relative rotation produces a long-wavelength moire modulation of local stacking. This modulation can be described by a moire reciprocal lattice built from differences of monolayer

reciprocal vectors. The associated effective moire length L_m introduced in Equation 7 should not be identified with the exact commensurate supercell length except in special families.

An arbitrary twist angle generally produces an *incommensurate* (quasiperiodic) structure in which the two lattices never perfectly realign. Let Γ be the monolayer Bravais lattice and $\Gamma_\theta = R_\theta \Gamma$ its rotated copy. The two lattices are *commensurate* if and only if $\Gamma \cap \Gamma_\theta$ has finite index in both lattices. Equivalently, if A is a basis matrix of Γ , the commensurability condition is

$$A^{-1}R(\theta)A \in GL(2, \mathbb{Q}). \quad (8)$$

In that case, the *coincidence-site lattice* $\Gamma_{\text{CSL}} = \Gamma \cap \Gamma_\theta$ defines an exact supercell of the decorated bilayer, which we call the *commensurate moire lattice* (CML). For the square lattice with coprime (p, q) , $p > q \geq 1$, the rotation angle $\theta_{pq} = 2 \arctan(\frac{q}{p})$ gives $L_{\text{CML}} = a\sqrt{p^2 + q^2}$. At small angles the dominant family has $q = 1$, for which $L_{\text{CML}} = 2L_m$. The CML cell then contains four moire lattice points, which is the situation illustrated in Figure 9. For higher- q families the ratio $\frac{L_{\text{CML}}}{L_m}$ can differ.

At generic twist angles the commensurability condition fails, and no nonzero translation leaves the full decorated bilayer invariant.

Whether a clean family of commensurate angles exists depends on the parent lattice symmetry; Table 2 summarizes the situation for all 2D Bravais lattice types.

Lattice	Commensurate angles	L_{CML}
Square	Dense family. Coprime (p, q) , $\theta_{pq} = 2 \arctan(q/p)$, $p > q \geq 1$: $L_{\text{CML}} = a\sqrt{p^2 + q^2}$	e.g. $29a$ at $\approx 4^\circ$
Triangular	Dense family. Coprime (m, r) : $\theta_{mr} = \arccos((2m^2 + 2mr + r^2)/(2(m^2 + mr + r^2)))$	analogous
Rectangular / Rhombic	Exist iff the aspect ratio satisfies $\rho^2 = b^2/a^2 \in \mathbb{Q}$; the commensurate set is then countably dense but absent for generic ρ .	case-specific
Oblique	Nontrivial commensurate rotations can occur when the lattice metric satisfies specific arithmetic conditions; for generic metric parameters, only $\theta = 0$ is commensurate [29].	case-specific

Table 2: Commensurate twist angles for all 2D Bravais lattice types. In each case the commensurability condition Equation 8 specializes to the parametrizations shown, yielding CML cells whose side length L_{CML} depends on the specific integer family [29].

This thesis works exclusively with square and triangular lattices, whose dense commensurate families allow easier numerical validation. Figure 9 shows CML cells at three accessible commensurate angles for the square lattice.

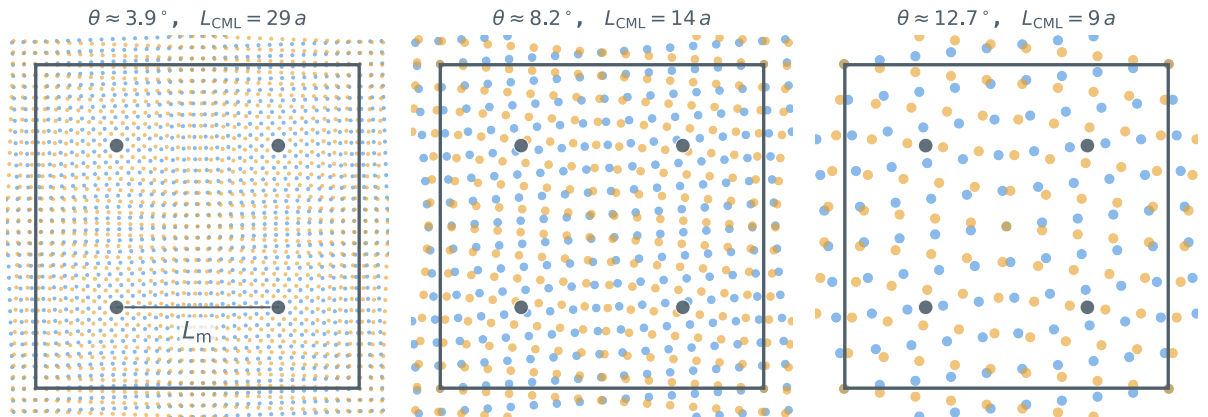


Figure 9: Commensurate supercells for the square lattice at three twist angles (all from the $q = 1$ family). Each panel shows one CML cell with blue (lattice 1) and orange (lattice 2) lattice sites. Both layers coincide *exactly* at the cell corners. The underlying moire lattice points (dark) are drawn for comparison; for this family $L_{\text{CML}} = 2L_m$.

2.2.3 Relevance of Commensurability

Exact periodicity is required for numerical calculations like plane-wave expansion or FDFD, but at small twist angles, continuum descriptions of low-energy moire physics are often largely insensitive to exact commensurability, even though the exact decorated bilayer is periodic only at commensurate angles. The canonical magic angles discussed earlier in twisted bilayer graphene are generically incommensurate, and continuum models reproduce their physics without any periodicity assumption [6]. The same approach extends to photonic crystals [11,12]: all these models parametrize the system with a continuous angle, producing flat bands and magic angles as continuous functions of the twist. Commensurate structures systematically approximate the continuous incommensurate limit [30].

Consequently, this thesis treats θ as a continuous parameter in the analytical envelope framework. Commensurate approximants are only employed when rigorous exact periodicity is required for numerical validation.

2.3 Incompatibility of Standard Solvers with Moire Crystals

Using standard photonic-crystal solvers on a moire structure raises two independent obstacles, one rooted in the loss of exact periodicity and one in the large size of the resulting computational domain.

2.3.1 The Periodicity Problem

Standard photonic-crystal solvers require strict translational periodicity. We input a lattice's unit cell, and the solver tiles it into an infinite crystal and computes Bloch modes. For a moire crystal at a generic (incommensurate) twist angle, no finite cell tiles the structure exactly.

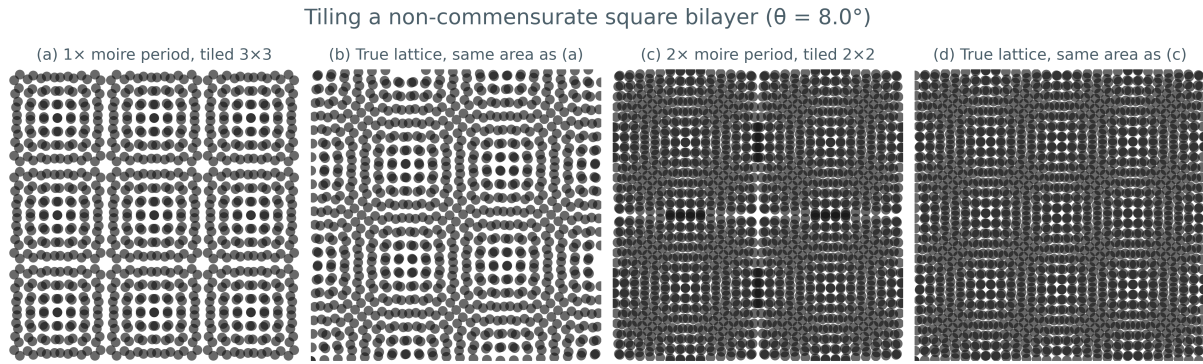


Figure 10: Tiling a non-commensurate moire bilayer versus the true lattice. **(a)** One moire unit cell tiled 3×3 . **(b)** The true (non-tiled) bilayer over the same area as (a). **(c)** A cell twice as large as (a), tiled 2×2 . **(d)** The true bilayer over the same area as (c). Comparing tiled and true panels reveals visible seams at every cell boundary in the tiled versions, while the true lattice is seamless. No finite cell tiling can recover exact periodicity for this incommensurate angle.

Figure 10 illustrates the problem directly. When we take a patch of the moire pattern (e.g. one moire period or a forced periodic supercell) and tile it, the atoms at opposite edges do not match. Seams appear at every cell boundary. Doubling the cell does not help: the mismatch shifts but does not vanish, because at an incommensurate angle no nonzero translation leaves the full structure invariant. This is not a numerical artifact; it is the defining property of an incommensurate lattice.

The consequence is significant for conventional pipelines: any solver or framework built on the assumption of exact periodicity cannot represent the structure faithfully. Plane-wave expansion, FDFD with periodic boundary conditions, transfer-matrix methods; all require a unit cell that tiles without seams. For a quasi-periodic moire crystal, that cell does not exist.

The CML from the previous section offers a partial workaround: at a discrete set of special angles, exact periodicity is restored and the CML cell can be fed to a standard solver. But the interesting moire physics varies continuously with θ . Being restricted to commensurate angles means sampling only a sparse, isolated set of twist angles while the physics of interest varies continuously between them.

2.3.2 The Resolution Problem

Even at commensurate angles where a valid CML cell exists, a second obstacle appears: as the twist angle decreases, the supercells become orders of magnitude larger than the constituent monolayer cells.

A single moire cell already contains monolayer unit cells on the order of $(L_m/a)^2$. Because $L_m \approx a/\theta$ for small angles, the cell count scales as $1/\theta^2$. A 2° twist already packs roughly 800 monolayer cells into one moire period. At 1° , the count exceeds 3000. The CML cell required by exact-periodicity solvers is even larger; for the dominant $q = 1$ family it is four times the moire cell area.

A photonic-crystal solver must resolve the internal structure of every one of these cells. The dielectric function contains sharp material boundaries at the monolayer scale, and accurate eigenfrequencies require that this fine structure is captured on the computational grid.

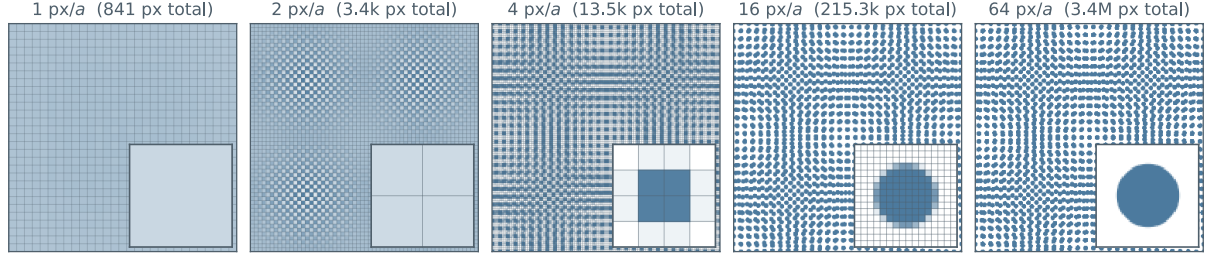


Figure 11: Discretization of a 2° twisted square bilayer CML cell at five resolutions: 1, 2, 4, 16, and 64 pixels per monolayer lattice constant a . The dielectric function is rendered with subpixel smoothing on the full cell. Each title shows the total pixel count. At 1–2 px/a the rod geometry is unrecognizable; 4 px/a shows only coarse pixel clusters; 16 px/a begins to resolve individual rods; 64 px/a is needed for quantitatively reliable eigenfrequencies.

Figure 11 shows the effect of grid resolution on a single CML cell. At 1 or 2 pixels per lattice constant, no structural information survives. At 4, pixels individual rods appear as coarse blobs without clear boundaries. Only at 16 pixels does the rod geometry become recognizable, and quantitatively reliable band structures require 64 pixels per monolayer cell.

The total grid size is therefore

$$N_{\text{grid}} = \left(\frac{N_{\text{px}}}{a}\right)^2 \times \left(\frac{L_m}{a}\right)^2 \approx \frac{N_{\text{px}}^2}{\theta^2}, \quad (9)$$

where N_{px} is the number of pixels per lattice constant. For a 2° twist at 64 px/a resolution, a single side of the grid has $64 \times 29 \approx 1856$ points, giving roughly 3.4×10^6 grid points total. CML calculations at the same resolution require a grid four times as large. The memory and compute cost of the eigenproblem scales with these numbers.

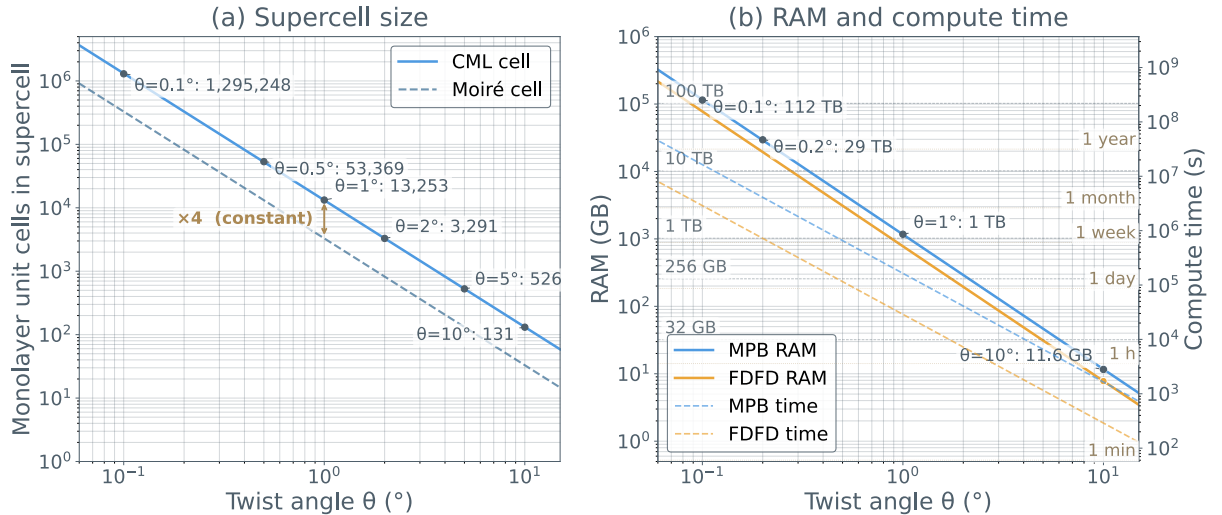


Figure 12: **Left:** Number of monolayer unit cells inside the CML cell (solid) and moire cell (dashed) as a function of twist angle θ . The $1/\theta^2$ scaling makes the cell count diverge rapidly at small angles. **Right:** Estimated RAM usage for a single band-structure calculation at 64 px/a resolution, comparing MPB (plane-wave expansion) and FDFD (finite-difference frequency-domain). Both methods become infeasible below $2\text{--}3^\circ$ for typical workstations.

Figure 12 quantifies the scaling wall. The left panel shows the raw cell count inside the CML and, for reference, the moire cell (which is four times smaller). The right panel translates the CML grid into RAM estimates for two standard solvers at the representative 64 px/ a resolution used throughout this section. For these estimates and workstation-scale memory budgets, MPB, which stores the dielectric tensor in the Fourier domain, crosses the 1 TB line around 1° . FDFD works with sparse matrices and uses roughly five times less memory per grid point, but even the sparse approach exceeds typical workstation memory below $2\text{--}3^\circ$. Running parameter sweeps at these angles is out of reach with current hardware.

2.3.3 Consequences for Moire Simulations

The challenges of quasi-periodicity and resolution cost reinforce each other. The first restricts standard solvers to the sparse set of commensurate angles. At those angles, the CML cell is four times the area of the moire cell, adding to the already steep resolution cost. Even at moderate angles ($\theta \gtrsim 4^\circ\text{--}5^\circ$), accurate CML calculations challenge modern workstation memory limits; below that, both moire and CML cells become infeasible.

But even unlimited computational resources would not help: at generic twist angles the structure is incommensurate, and no periodic unit cell exists at all. The barrier is not one of scale but of principle.

With the limits of conventional solvers explained, we turn to a reformulation that directly addresses these constraints. Rather than treating the moire crystal at a single scale, the next section introduces an ansatz that recognizes and separates the two vastly different length scales inherent to moire structures.

3 The Multi-Band Envelope Approximation

A general theory of moire-scale physics requires reformulating the geometry so that the monolayer scale and the moire scale separate cleanly. The present section carries out that separation by identifying the local periodicity of a twisted bilayer, lifting the problem into a two-scale framework, and expanding the effective operator order by order. Projecting the expanded operator onto a chosen band subspace then yields a reduced eigenproblem whose degrees of freedom are moire-scale envelope functions alone.

3.1 Local Periodicity and the Two-Atomic Crystal Approximation

For small twist angles, a moire bilayer exhibits a distinct structural property: any sufficiently small patch closely resembles a periodic crystal with a two-atom basis. Figure 13 illustrates this for a square-lattice bilayer. Zooming in at different positions across the moire pattern reveals local patches that each look like an ordinary periodic lattice, but with two distinct sites per unit cell, one from each layer. The relative shift between them varies smoothly from patch to patch, so the local two-atomic crystal changes continuously across the moire period.

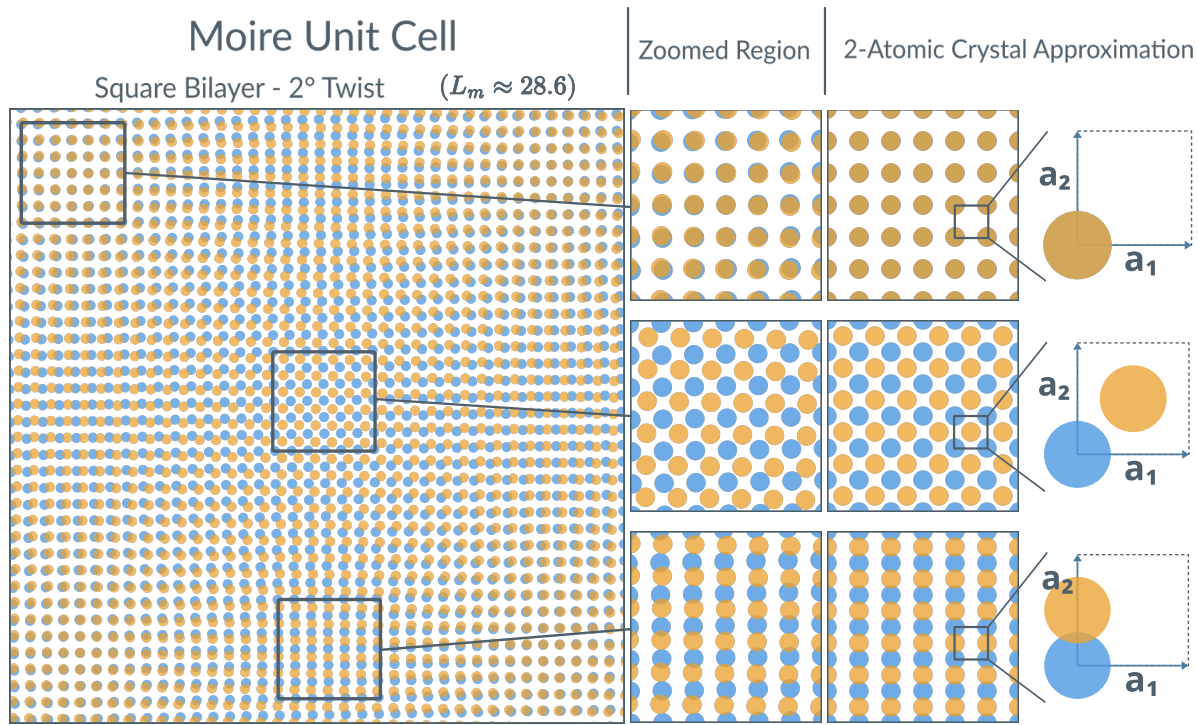


Figure 13: Local periodicity in a square-lattice moire bilayer. Each zoomed patch from the full twisted structure is approximated by a periodic two-atomic crystal with a continuously assigned local shift $\delta(\mathbf{R})$. Neighboring moire positions correspond to neighboring two-atomic crystals; the shift varies continuously rather than snapping between discrete cell representatives.

This observation is the crucial first step toward identifying and separating the two length scales inherent in a moire structure. Rather than treating the full bilayer permittivity as a single complicated function of the physical coordinate $\mathbf{x}$, we can describe it locally as a periodic dielectric that depends on a fast lattice coordinate $\mathbf{r}$ and is parametrized by a slowly varying inter-layer shift δ . The fast coordinate captures the internal structure of the local unit cell; the shift encodes which member of the two-atomic crystal family applies at a given moire position $\mathbf{R}$. Making this decomposition precise is the task of the present section.

Concretely, the local configuration is parameterized by the relative shift δ between the two layers. For each fixed shift, we define the corresponding periodic two-atomic crystal permittivity

$$\varepsilon_{\text{loc}}(\mathbf{r}; \delta) := \varepsilon_1(\mathbf{r}) + \varepsilon_2(\mathbf{r} + \delta). \quad (10)$$

Here ε_1 and ε_2 are understood as the layer contributions entering the local proxy; any common background is absorbed into this definition rather than counted twice. The resulting field is periodic in the fast coordinate $\mathbf{r}$ on the monolayer unit cell. The moire pattern then enters through a slowly varying registry map

$$\delta = \delta(\mathbf{R}), \quad (11)$$

so that different moire positions correspond to different members of this periodic family.

For a twisted bilayer formed by rotating the two layers by $\pm \frac{\theta}{2}$, the unwrapped relative displacement between the layers at the physical point $\mathbf{x}$ is $(R_{-\frac{\theta}{2}} - R_{+\frac{\theta}{2}})\mathbf{x}$, where $R_{\pm \frac{\theta}{2}}$ denotes the planar rotation matrix. The exact identity $R_{-\frac{\theta}{2}} - R_{+\frac{\theta}{2}} = -2 \sin(\theta/2) J$, with J the rotation by 90° , shows that this displacement grows linearly with $\mathbf{x}$ at the rate $2 \sin(\theta/2)$. Measured in units of the lattice constant and expressed through the slow coordinate $\mathbf{R} = \mathbf{x}/L$ of the two-scale lift (Section 3.2), with $L = a/(2 \sin(\theta/2))$ from Equation 7, the two small factors cancel exactly:

$$\delta_{\text{raw}}(\mathbf{R}) := (R_{-\frac{\theta}{2}} - R_{+\frac{\theta}{2}}) \frac{\mathbf{x}}{a} = -J\mathbf{R}. \quad (12)$$

The raw registry shift is therefore an order-one function of the slow coordinate: it advances by one lattice constant per moire period, which is exactly what makes the moire pattern periodic on the scale L . Its slow gradient is the constant matrix $\partial_{\mathbf{R}} \delta_{\text{raw}} = -J$, with no remaining factor of the twist angle. The actual registry map $\delta(\mathbf{R})$ is obtained by reducing this displacement modulo the monolayer Bravais lattice, so its precise representative depends on the lattice type. In the present thesis, only the square and hexagonal cases are needed:

Bilayer type	Monolayer Bravais lattice	Registry map $\delta(\mathbf{R})$
Square	$\Lambda_{\text{sq}} = \{m\mathbf{a}_1 + n\mathbf{a}_2 : m, n \in \mathbb{Z}\}$ $\mathbf{a}_1 = a(1, 0), \quad \mathbf{a}_2 = a(0, 1)$	$\delta(\mathbf{R}) \equiv \delta_{\text{raw}}(\mathbf{R}) \bmod \Lambda_{\text{sq}}$ $\delta(\mathbf{R}) = d_1\mathbf{a}_1 + d_2\mathbf{a}_2 \quad d_1, d_2 \in [-\frac{1}{2}, \frac{1}{2})$
Hexagonal	$\Lambda_{\text{hex}} = \{m\mathbf{a}_1 + n\mathbf{a}_2 : m, n \in \mathbb{Z}\}$ $\mathbf{a}_1 = a(1, 0), \quad \mathbf{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2})$	$\delta(\mathbf{R}) \equiv \delta_{\text{raw}}(\mathbf{R}) \bmod \Lambda_{\text{hex}}$ $\delta(\mathbf{R}) = d_1\mathbf{a}_1 + d_2\mathbf{a}_2 \quad d_1, d_2 \in [-\frac{1}{2}, \frac{1}{2})$

Table 3: Registry map definitions for the square and hexagonal bilayer lattices. The displacement $\delta(\mathbf{R})$ is reduced modulo the respective Bravais lattice Λ into the fundamental domain $d_1, d_2 \in [-\frac{1}{2}, \frac{1}{2})$.

Because $\delta_{\text{raw}}(\mathbf{R})$ is linear in $\mathbf{R}$, the registry map is globally smooth *before* reduction. Reducing modulo the Bravais lattice means that $\delta(\mathbf{R})$ takes values in the torus $\frac{\mathbb{R}^2}{\Lambda}$. Any choice of fundamental-domain representative, such as the half-open cell $d_1, d_2 \in [-\frac{1}{2}, \frac{1}{2})$ used in Table 3, necessarily introduces branch cuts at the cell boundary where the representative jumps. This is a coordinate artifact: the torus-valued map itself is continuous, and the periodicity of $\varepsilon_{\text{loc}}(\mathbf{r}; \delta)$ in δ makes the composed field independent of which representative is chosen. For the derivation below we assume that the family $\delta \mapsto \varepsilon_{\text{loc}}(\cdot; \delta)$ is sufficiently smooth, so that the induced $\mathbf{R}$ -dependence can be differentiated classically; for sharp-interface structures the same formulas should instead be understood as a formal limit or handled in a weak formulation. Under this regularity assumption, the slow derivatives $\partial_{R_j} \varepsilon_{\text{loc}}$ are well defined and continuous. Figure 14 illustrates this by sampling three arbitrary points $\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3$ and displaying the resulting unit cells; the shift vector δ (colored arrows) changes direction and magnitude continuously with $\mathbf{R}$. Each sample point $\mathbf{R}$ disregards the actual bilayer configuration and instead assumes a two-atomic crystal centered at that position; the resulting local permittivity therefore varies smoothly with $\mathbf{R}$. This smoothness, once assumed for the local family, facilitates the algebraic manipulations that follow.

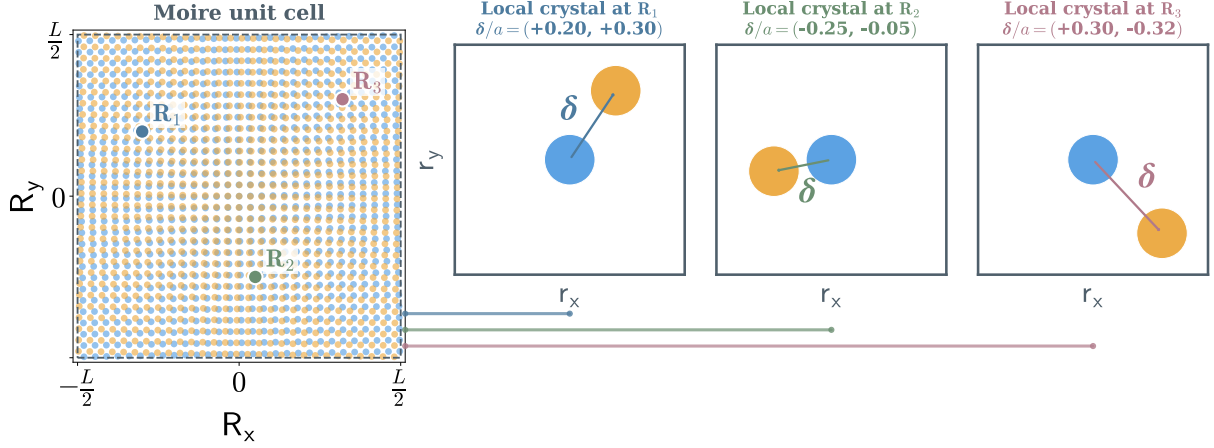


Figure 14: Any continuous position $\mathbf{R}$ inside the moire cell determines a local two-atomic crystal via the registry map $\delta(\mathbf{R})$. The colored arrows show δ for three sample positions; the shift varies smoothly with $\mathbf{R}$. Each local cell spans $r_x, r_y \in [-\frac{a}{2}, \frac{a}{2}]$.

A note on coordinates: the physical position is always $\mathbf{x}$. Neither $\mathbf{R}$ nor $\mathbf{r}$ is a second physical position. Here, $\mathbf{R}$ is the slow moire-scale label attached to $\mathbf{x}$, while $\mathbf{r}$ is the internal fast coordinate of the local unit cell used to represent the neighborhood of that point. The formal meaning of these two scales will be made precise in the two-scale lift (Section 3.2); for now, $\mathbf{R}$ simply indexes which member of the two-atomic crystal family applies locally.

3.1.1 Limits of the Two-Atomic Crystal Approximation

The two-atomic crystal approximation is visibly a good description for small angles, but it clearly breaks down for increasing twist angles. Figure 15 demonstrates this break-down. Before building an entire effective theory on this approximation, we should therefore obtain a quantitative estimate of its validity range and, in particular, identify what it depends on. A useful such estimate emerges from combining a geometric and a spectral perspective.

The two-atomic crystal approximation freezes the inter-layer shift at the value $\delta(\mathbf{R}_0)$ and tiles that local crystal everywhere. For any point at distance N monolayer periods from $\mathbf{R}_0$, the true shift has drifted by

$$\Delta \frac{\delta}{a} \approx N \cdot 2 \sin(\theta/2) \approx N\theta \quad (13)$$

in units of the lattice constant a (θ in radians). The mismatch grows linearly with distance and is controlled by the twist angle alone. The degradation is clearly visible already at moderate angles (Figure 15); for each orange atom we move along one direction ($N = 1, 2, \dots$), the geometric overlap-mismatch grows larger.

To understand how severe this mismatch is, we first need to know how many periods a photonic crystal requires to develop its spectral identity at all. The relevant scale is the Bragg penetration depth N_{Bragg} : the number of periods over which coherent scattering builds up a directional stop-band [31]. A stop-band is a frequency window in which light cannot propagate through the crystal and is instead reflected. A stop-band with relative width γ (gap-to-midgap ratio) requires roughly $N_{\text{Bragg}} \sim \frac{1}{\gamma}$ periods to form. Evaluating the geometric mismatch Equation 13 at $N = N_{\text{Bragg}}$ yields a single dimensionless quality parameter

Quality Parameter

$$\beta := \frac{\theta}{\gamma}, \quad (14)$$

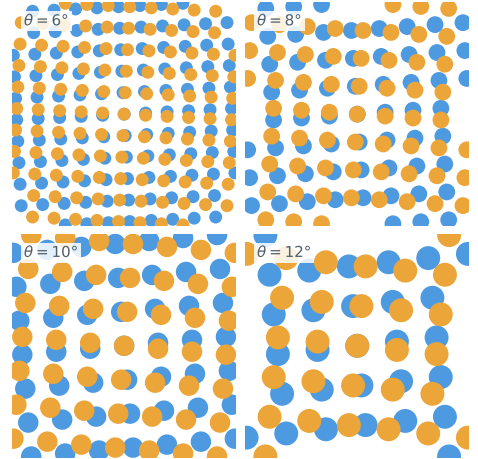


Figure 15: Moire unit cells at various twist angles. Local periodicity degrades rapidly with increasing twist.

(θ in radians). This is the accumulated registry shift, in units of the lattice constant, at the distance where the stop-band is fully established. When $\beta \ll 1$ the local crystal barely changes over that formation length; when $\beta \gtrsim 1$ the shift exceeds a full lattice constant within that range, and the local-periodicity picture breaks down.

To see concretely why $N_{\text{Bragg}} \sim \frac{1}{\gamma}$ holds, we consider the simplest periodic photonic structure: a 1D quarter-wave stack of alternating refractive indices n_1 and n_2 , with each layer having the thickness of one optical quarter-wavelength. Figure 16 shows these photonic structures for various period lengths. We compute the transmittance T as a function of the normalised probe frequency $\frac{\omega}{\omega_{\text{Bragg}}}$ for stacks of increasing period count N using the transfer-matrix method, where ω_{Bragg} is the Bragg frequency (stop-band center) and $\gamma = \frac{\Delta\omega}{\omega_{\text{Bragg}}}$ is the relative stop-band width (gap-to-midgap ratio).

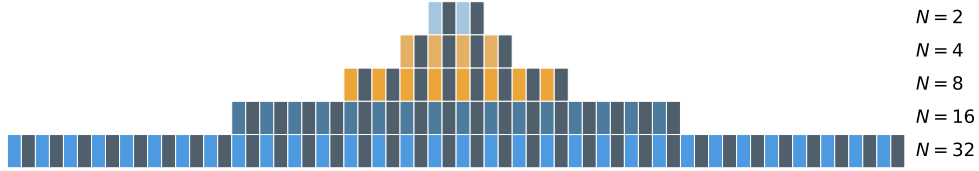


Figure 16: 1D photonic crystals with $N = 2, 4, 8, 16, 32$ periods. Colors match the transmission curves in Figure 17.

Figure 17 shows the result for two contrast values. When only a few periods N are present, the transmission dip is shallow: the crystal has not yet developed its spectral identity. As N increases past $N_{\text{Bragg}} \sim \frac{1}{\gamma}$, the stop-band saturates to the infinite-crystal limit and additional periods no longer change the spectrum. The stop-band is not an instantaneous property. It requires a minimum spatial extent to form.

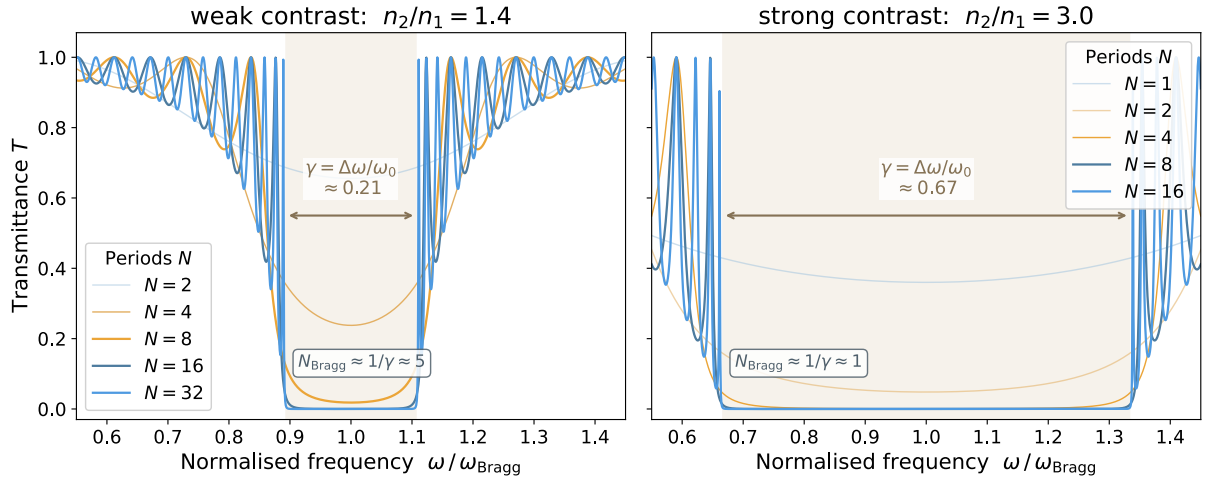


Figure 17: Transmittance of a 1D quarter-wave stack (air | $[n_1 | n_2]^N$ | air) for increasing period count N . **Left:** weak contrast ($n_2/n_1 = 1.4$, $\gamma \approx 0.21$). **Right:** strong contrast ($n_2/n_1 = 3.0$, $\gamma \approx 0.67$). The shaded region marks the infinite-crystal stop-band. The stop-band is fully established after $N_{\text{Bragg}} \sim 1/\gamma$ periods; stronger contrast yields a wider stop-band that forms in fewer periods.

This spectral formation-length requirement limits the two-atomic crystal approximation. At each position $\mathbf{R}_0$, the frozen two-atomic crystal has a well-defined band structure, but that band structure materialises only if the crystal extends over roughly N_{Bragg} periods without significant structural change. If the twist causes the registry to drift by a full lattice constant within those N_{Bragg} periods, the band structure never forms and the two-atomic crystal approximation is expected to become unreliable at that position. The quality parameter $\beta = \frac{\theta}{\gamma}$ therefore provides a heuristic diagnostic of the accumulated drift, in lattice constants, over the spectral formation length.

Figure 18 maps β across the (θ, ε) plane, using the approximate dependence $\gamma(\varepsilon)$ for TE-polarized square-lattice rods in air. Blue regions indicate $\beta < 0.1$ (mismatch below 10% of a lattice constant at Bragg depth); red regions indicate $\beta > 1$.

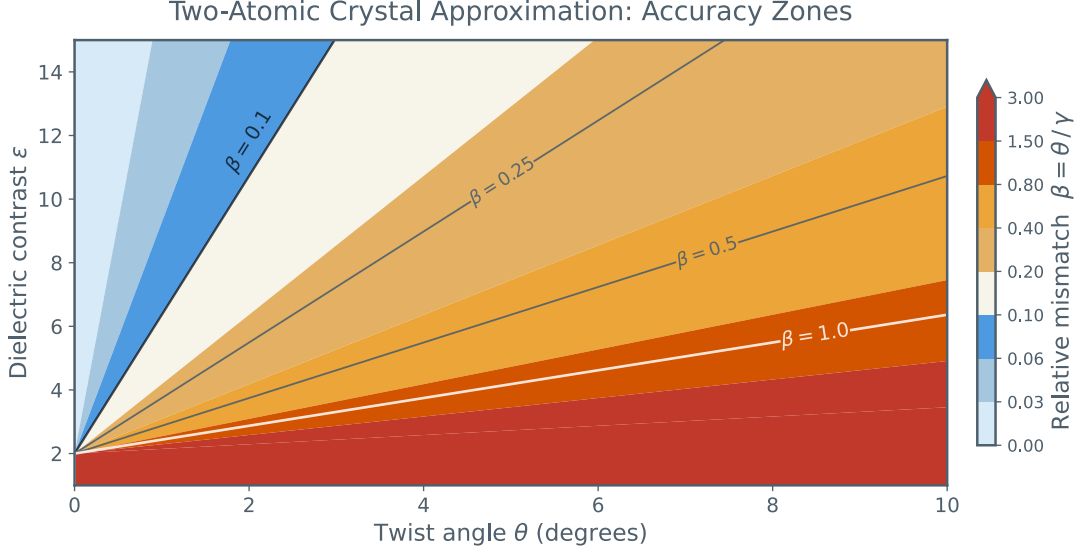


Figure 18: Accuracy zones for the two-atomic crystal approximation. Color encodes the quality parameter $\beta = \theta/\gamma$, the accumulated registry mismatch at the Bragg penetration depth. The zone boundaries and color thresholds are conventional; the β contour values themselves provide the quantitative criterion.

The zone boundaries in Figure 18 are conventional choices. In practice, the relevant threshold depends on the observable of interest: eigenfrequency shifts require tighter control than spatially averaged quantities. The β contour values provide the relevant diagnostic reference; users of this approximation should select a mismatch threshold appropriate for their application.

3.2 The Two-Scale Lift

To apply a two-scale ansatz, we must rigorously define how the physical coordinate separates into a microscopic and a macroscopic scale. While this separation is intuitive, making it mathematically strict is essential because all subsequent derivatives and algebraic manipulations rely on it. Let a denote the monolayer lattice constant, L the moire period (denoted L_m in Section 2.2.1; we drop the subscript for readability in the mathematical framework), and

$$\eta := \frac{a}{L} \ll 1 \quad (15)$$

the small scale-separation parameter. Following the standard two-scale viewpoint of homogenization theory [32,33], we introduce the dimensionless variables

$$\mathbf{r} := \frac{\mathbf{x}}{a}, \quad \mathbf{R} := \frac{\mathbf{x}}{L}. \quad (16)$$

Both $\mathbf{r}$ and $\mathbf{R}$ are dimensionless, and so are their conjugate Bloch momenta $\mathbf{k}$ and $\mathbf{q}$ used throughout the lifted derivation. When both Brillouin zones are later drawn in a single physical reciprocal plane, the corresponding physical wavevectors are $\mathbf{k}_{\text{phys}} = \frac{\mathbf{k}}{a}$ and $\mathbf{q}_{\text{phys}} = \frac{\mathbf{q}}{L} = \eta \frac{\mathbf{q}}{a}$. We do *not* treat them as a literal change of variables on physical space. Instead, the two-scale method promotes $\mathbf{r}$ and $\mathbf{R}$ to independent variables on a product space. We will refer to the corresponding product-space representative as a *lifted* two-scale object: we lift the physical field from the single physical coordinate $\mathbf{x}$ to a function of the two independent variables $(\mathbf{r}, \mathbf{R})$. This label is standard descriptive multiscale language; the reference [33] supplies the rigorous two-scale framework, even though its focus is the terminology of two-scale convergence rather than the specific word “lifted”. A physical field is then recovered by evaluating the corresponding lifted object on the physical diagonal.

Concretely, if $\Phi(\mathbf{r}, \mathbf{R})$ is a lifted two-scale quantity, its physical realization is defined by

$$\Phi^\eta(\mathbf{x}) := \Phi\left(\frac{\mathbf{x}}{a}, \frac{\mathbf{x}}{L}\right). \quad (17)$$

The word diagonal simply refers to the subset of the independent $(\mathbf{r}, \mathbf{R})$ space obtained from one and the same physical point $\mathbf{x}$. This is the precise meaning behind expressions such as $\Phi(\mathbf{r}, \mathbf{R})$: the two variables are

independent in the lifted description, but the physical object is obtained only after the restriction Equation 17 is applied. Figure 19 illustrates this construction schematically.

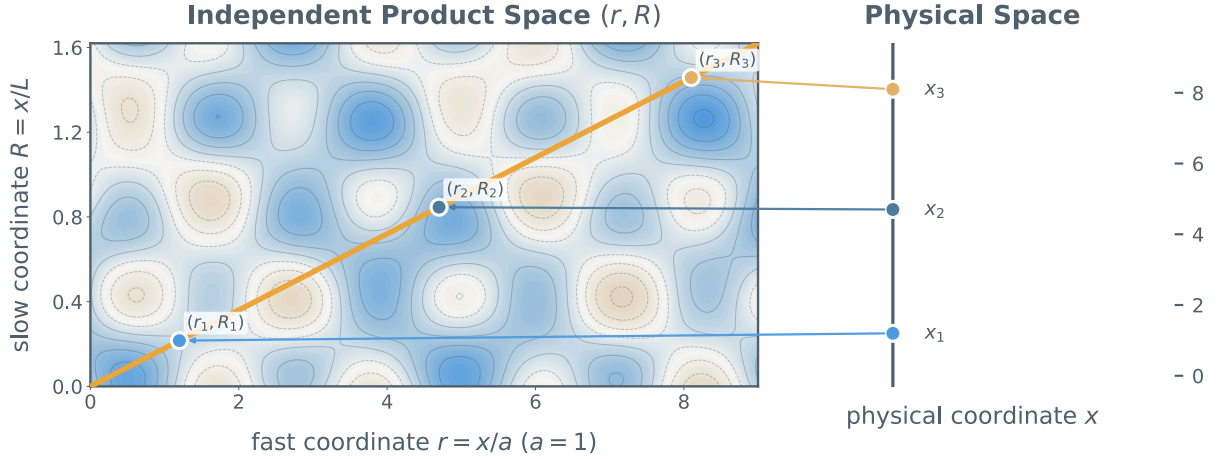


Figure 19: One-dimensional schematic of the two-scale lift. **Right:** the physical field depends on one coordinate x . **Left:** its lifted representative $\Phi(\mathbf{r}, \mathbf{R})$ is defined on the independent product space $(\mathbf{r}, \mathbf{R})$. The highlighted line is the physical slice $\mathbf{x} \mapsto (\frac{\mathbf{x}}{a}, \frac{\mathbf{x}}{L})$ along which we sample the lifted field to recover $\Phi^\eta(\mathbf{x})$. In the plotted scaled axes this set is the line $\mathbf{R} = \eta \mathbf{r}$, so the term *diagonal* refers to inserting the same physical $\mathbf{x}$ into both scale maps, not necessarily to a 45° line. Here $\eta = 0.18$.

The figure should be read only as a one-dimensional toy model of the construction. In the actual moire problem, $\mathbf{x}$, $\mathbf{r}$, and $\mathbf{R}$ are two-dimensional vectors, so the full lifted space $(\mathbf{r}, \mathbf{R})$ is four-dimensional and cannot be drawn directly in a comparably simple way. The colored region away from the highlighted line therefore does *not* represent additional physical parts of the moire crystal. It represents the mathematical extension of the field to the independent variables $(\mathbf{r}, \mathbf{R})$.

This extension is precisely what makes the two-scale method useful. For each physical point $\mathbf{x}$, the diagonal restriction still selects one unique pair $(\mathbf{r}, \mathbf{R}) = (\frac{\mathbf{x}}{a}, \frac{\mathbf{x}}{L})$. At the same time, once $\mathbf{r}$ and $\mathbf{R}$ have been promoted to independent variables, we can differentiate with respect to them separately. The lifted object thus provides two independent directions of variation around each point of the physical slice: a fast direction associated with the microscopic lattice scale and a slow direction associated with the moire scale. That is the mathematical reason the chain rule Equation 21 is well defined.

This resolves the apparent ambiguity in writing two-scale coefficients. The lifted permittivity is defined as

$$\varepsilon(\mathbf{r}, \mathbf{R}) := \varepsilon_{\text{loc}}(\mathbf{r}; \delta(\mathbf{R})), \quad (18)$$

and its diagonal restriction is the two-atomic proxy of the moire permittivity in physical space,

$$\varepsilon^\eta(\mathbf{x}) = \varepsilon\left(\frac{\mathbf{x}}{a}, \frac{\mathbf{x}}{L}\right) = \varepsilon_{\text{loc}}\left(\frac{\mathbf{x}}{a}; \delta\left(\frac{\mathbf{x}}{L}\right)\right). \quad (19)$$

How close is this proxy to the true bilayer? Written out, the two layers of the twisted structure are $\varepsilon_1(R_{+\frac{\theta}{2}}\mathbf{x}/a)$ and $\varepsilon_2(R_{-\frac{\theta}{2}}\mathbf{x}/a)$. Locking the fast coordinate to the first layer, $\mathbf{r}_1 := R_{+\frac{\theta}{2}}\mathbf{x}/a$, gives the exact representation

$$\varepsilon_{\text{bilayer}}(\mathbf{x}) = \varepsilon_1(\mathbf{r}_1) + \varepsilon_2(\mathbf{r}_1 - J\mathbf{R}), \quad (20)$$

with no approximation at all: the registry map Equation 12 enters exactly, and the only difference to Equation 19 is the rotation of the fast frame by $\theta/2$. Along the diagonal $\mathbf{R} = \eta \mathbf{r}$ one has $R_{\pm\frac{\theta}{2}}\mathbf{r} = \cos(\theta/2)\mathbf{r} \pm \frac{1}{2}J\mathbf{R}$, so the proxy differs from the exact bilayer by a dilation of the fast frame by $\cos(\theta/2) = 1 - \eta^2/8 + O(\eta^4)$. This is an $O(\eta^2)$ correction to the coefficient field, the same order as the highest terms retained in the effective operator derived below. It is uniform over the crystal (a rescaling of the lattice constant by a known factor) and is absorbed into the local band data of the two-atomic family; wherever a comparison at the 10^{-6} level is made in Section 5, the layer-locked lift Equation 20 is the object that all solvers share. The same logic applies to Bloch functions, envelope amplitudes, and all other two-scale objects used later in the derivation.

Because the lifted variables are independent, the chain rule is exact. If $\Phi^\eta(\mathbf{x}) = \Phi(\frac{\mathbf{x}}{a}, \frac{\mathbf{x}}{L})$, then

$$\nabla_x \Phi^\eta(x) = \frac{1}{a} (\nabla_r + \eta \nabla_R) \Phi(r, R) \big|_{r=\frac{x}{a}, R=\frac{x}{L}}. \quad (21)$$

This identity is the basis of the later asymptotic expansion. It is not a heuristic replacement rule; it follows directly from the lifted definition Equation 17.

Under the same smooth-family assumption, the R -dependence of the permittivity is equally well defined. Since R enters $\varepsilon(r, R)$ only through the registry map $\delta(R)$, slow derivatives act by the ordinary chain rule:

$$\partial_{R_j} \varepsilon(r, R) = (\nabla_{\delta \varepsilon_{\text{loc}}}(r; \delta(R))) \cdot \partial_{R_j} \delta(R), \quad \partial_{R_j} \delta = -J e_j, \quad (22)$$

and similarly for $\partial_{R_j} \varepsilon^{-1}$. The Jacobian of the registry map is the constant rotation $-J$ from Equation 12, so the slow-coefficient terms that appear later in the effective description are of order one in the twist angle; their smallness in the final operator comes entirely from the explicit powers of η in front of the slow derivatives.

3.3 From Local Bloch Problems to a Multiscale Ansatz

Once the lifted coefficient field Equation 18 is defined, each fixed moire position R defines an ordinary periodic Bloch problem in the fast variable r . For the TE polarization, we solve

$$-D_r(k) \cdot (\varepsilon^{-1}(r, R) D_r(k)) u_{nk}(r; R) = \lambda_n(R, k) u_{nk}(r; R), \quad (23)$$

with $D_r(k) := \nabla_r + i k$ and periodic boundary conditions in r . The dependence on R is parametric: for each slow position, we have a local Bloch basis and a local band structure.

At this point, two distinct reciprocal-space structures coexist. The local Bloch problem above lives in the reciprocal space of the underlying monolayer lattice, with crystal momentum k in the monolayer Brillouin zone $\mathcal{B}_{\text{mono}}$. The envelope problem, by contrast, lives on the moire lattice in the slow coordinate R , and therefore has its own reciprocal lattice and its own Brillouin zone $\mathcal{B}_{\text{moire}}$. Since the moire period scales as $L = \frac{a}{\eta}$, the characteristic linear size of $\mathcal{B}_{\text{moire}}$ scales as $\frac{1}{L} = \frac{\eta}{a}$: for comparable lattice geometry, the moire Brillouin zone is smaller than the monolayer Brillouin zone by the factor η in linear dimension and by η^2 in area. Equivalently, the lifted momentum q remains dimensionless and $O(1)$ on the moire torus, while its embedding into the physical reciprocal plane is the smaller vector $q_{\text{phys}} = \frac{q}{L}$.

This is the point where the ordinary Bloch ansatz must be extended. A single periodic part $u_{n\mathbf{k}}(\mathbf{x})$ is no longer enough, because the local crystal itself varies across the moire pattern. Figure 20 illustrates the scale separation: $\mathcal{B}_{\text{moire}}$ is drawn to scale for a 1° twist and is barely visible at the K point of $\mathcal{B}_{\text{mono}}$. Because $\mathbf{q}$ ranges over this tiny zone while $\mathbf{k}_0$ sits at a fixed point of the monolayer zone, the two momenta live on well-separated scales. In particular, sweeping $\mathbf{q}$ across $\mathcal{B}_{\text{moire}}$ produces negligible displacement in $\mathcal{B}_{\text{mono}}$, so that to the retained order in η the local Bloch data can be computed once at the fixed carrier momentum $\mathbf{k}_0$; the effect of small deviations away from $\mathbf{k}_0$ is encoded perturbatively by the velocity and mass-tensor terms derived below.

The extension of the Bloch ansatz is best stated in two explicit steps. In the first step, we attach a slow moire-scale envelope to a single local Bloch state,

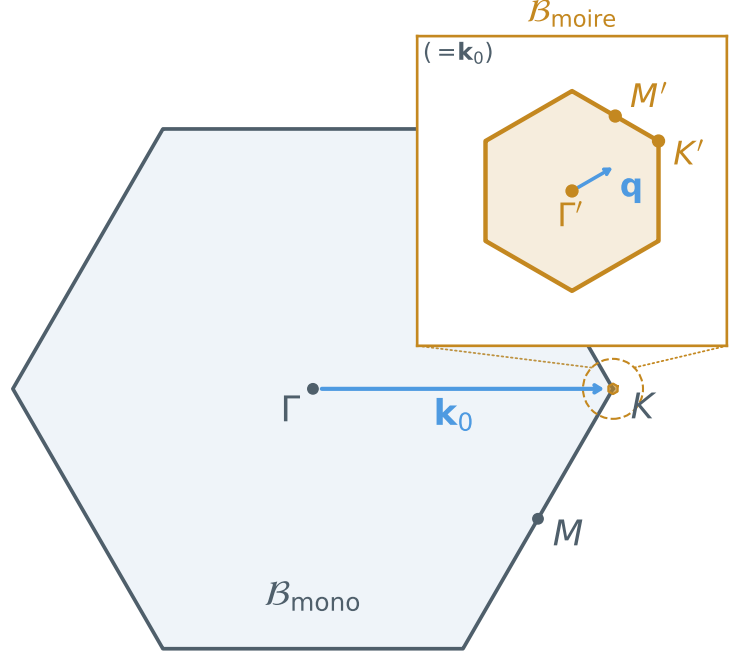


Figure 20: Monolayer Brillouin zone $\mathcal{B}_{\text{mono}}$ with the carrier momentum $\mathbf{k}_0$ pointing to K , where the moire Brillouin zone $\mathcal{B}_{\text{moire}}$ is drawn to scale for a 1° twist in the physical reciprocal plane. The inset magnifies $\mathcal{B}_{\text{moire}}$, showing its high-symmetry points and the dimensionless moire Bloch momentum $\mathbf{q}$ whose physical scale is $\frac{q}{L}$.

Single-Band Envelope Extension

$$e^{i\mathbf{k}_0 \cdot \mathbf{r}} u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R}) \rightarrow e^{i\mathbf{k}_0 \cdot \mathbf{r}} F_{n\mathbf{q}}(\mathbf{R}) u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R}), \quad (24)$$

where the envelope is itself a Bloch function on the moire lattice,

$$F_{n\mathbf{q}}(\mathbf{R} + \mathbf{L}) = e^{i\mathbf{q} \cdot \mathbf{L}} F_{n\mathbf{q}}(\mathbf{R}), \quad \mathbf{q} \in \mathcal{B}_{\text{moire}} \quad (25)$$

for every moire lattice vector $\mathbf{L}$. In this sense, the construction is a second Bloch-type decomposition performed on the slow scale. Only at the moire Γ' point, $\mathbf{q} = 0$, does this reduce to strict periodicity of the envelope.

It is convenient to factor out the moire Bloch phase and work with the periodic part instead:

$$F_{n\mathbf{q}}(\mathbf{R}) = e^{i\mathbf{q} \cdot \mathbf{R}} f_{n\mathbf{q}}(\mathbf{R}), \quad f_{n\mathbf{q}}(\mathbf{R} + \mathbf{L}) = f_{n\mathbf{q}}(\mathbf{R}). \quad (26)$$

This representation will later make it transparent that nonzero $\mathbf{q}$ enters the effective theory through a shift of the slow derivatives.

The components $F_{n\mathbf{q}}(\mathbf{R})$ and $f_{n\mathbf{q}}(\mathbf{R})$ assemble into N -component vectors on the retained manifold,

$$\mathbf{F}_{\mathbf{q}}(\mathbf{R}) := (F_{1\mathbf{q}}(\mathbf{R}), \dots, F_{N\mathbf{q}}(\mathbf{R}))^T, \quad \mathbf{f}_{\mathbf{q}}(\mathbf{R}) := (f_{1\mathbf{q}}(\mathbf{R}), \dots, f_{N\mathbf{q}}(\mathbf{R}))^T, \quad (27)$$

whereas the local Bloch states $u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R})$ remain scalar fields in the TE formulation used here. The same is true for the full TE field itself: $H_{\mathbf{k}_0\mathbf{q}}(\mathbf{r}, \mathbf{R})$ is scalar in physical space, even though its envelope coefficients form a vector in band space.

In the second step, we allow several local bands to participate and expand in that retained band manifold:

Multi-Band Envelope Ansatz

$$H_{\mathbf{k}_0\mathbf{q}}(\mathbf{r}, \mathbf{R}) \approx e^{i\mathbf{k}_0 \cdot \mathbf{r}} \sum_{n=1}^N F_{n\mathbf{q}}(\mathbf{R}) u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R}). \quad (28)$$

Here $\mathbf{k}_0$ is a chosen carrier momentum in $\mathcal{B}_{\text{mono}}$, the $u_{n\mathbf{k}_0}$ are local Bloch states at that momentum, and $\mathbf{q}$ is the moire Bloch momentum in $\mathcal{B}_{\text{moire}}$. The sum runs over an arbitrary number N of retained bands; choosing N is part of the approximation itself, since it specifies which monolayer bands are treated as active degrees of freedom in the reduced theory. The physical field is recovered as $H_{\mathbf{k}_0\mathbf{q}}^\eta(\mathbf{x}) = H_{\mathbf{k}_0\mathbf{q}}(\frac{\mathbf{x}}{a}, \frac{\mathbf{x}}{L})$.

3.4 A Primer on Bloch-Cell Projection

Before beginning the explicit derivation, it is useful to isolate the projection step in a minimal toy model. Consider the lifted two-scale function

$$\Phi(r, R) = \cos(r) \cos(R), \quad (29)$$

whose physical restriction is obtained along the slice $R = \eta r$. The resulting field oscillates rapidly in the fast variable r , but its amplitude varies only on the slow scale set by R (Figure 21).

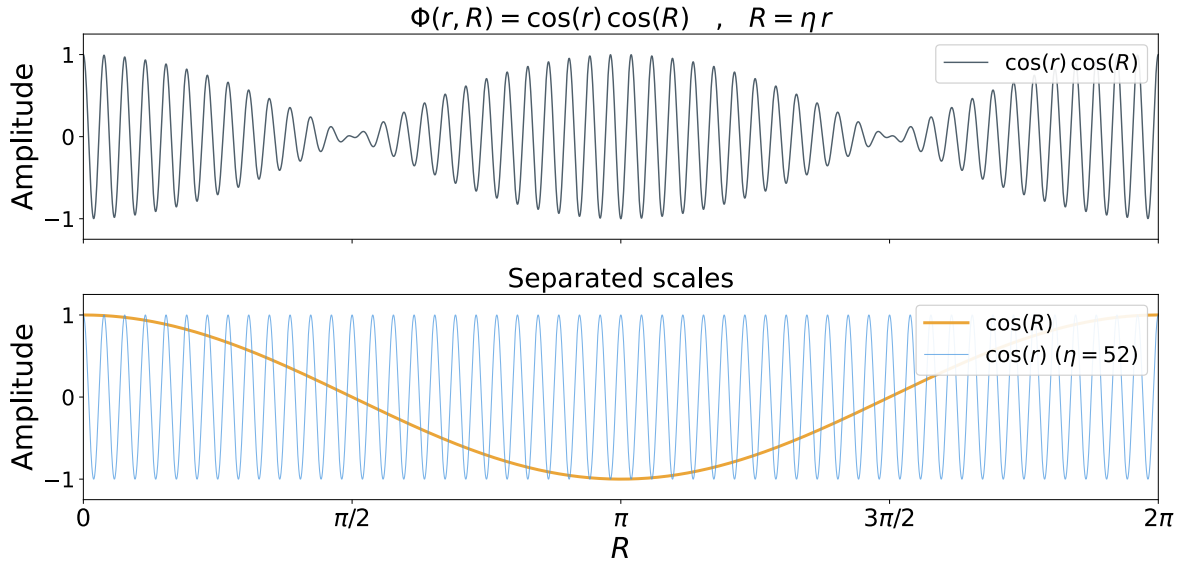


Figure 21: Two-scale structure of the toy function $\Phi(r, R) = \cos(r) \cos(R)$. The rapid oscillation in the fast variable is modulated by a slowly varying amplitude, which can be extracted by projection onto the appropriate fast basis function.

The slow factor cannot be recovered by a naive average, because $\cos(r)$ has zero mean over one fast period. Instead, we project onto the matching fast basis function:

$$\langle \cos(r), \Phi \rangle_{0, 2\pi} := \frac{1}{2\pi} \int_0^{2\pi} \cos(r) \Phi(r, R) dr = \frac{\cos(R)}{2\pi} \int_0^{2\pi} \cos^2(r) dr = \frac{1}{2} \cos(R). \quad (30)$$

This is exactly the mechanism used later in the Bloch-cell projection. The local Bloch states provide the fast basis, while the envelope coefficients are the slow amplitudes extracted by projection. For each fixed moire position $\mathbf{R}$, let Ω denote the primitive monolayer cell on which both $\varepsilon(\cdot, \mathbf{R})$ and $u_{n\mathbf{k}_0}(\cdot; \mathbf{R})$ are periodic in the fast variable. We then use the fast-cell inner product

$$\langle g, h \rangle_\Omega := \frac{1}{|\Omega|} \int_\Omega g^*(\mathbf{r}; \mathbf{R}) h(\mathbf{r}; \mathbf{R}) d\mathbf{r}, \quad (31)$$

with the orthonormality convention

$$\langle u_{m\mathbf{k}_0}, u_{n\mathbf{k}_0} \rangle_\Omega = \delta_{mn}, \quad m, n \in \{1, \dots, N\} \quad (32)$$

for the retained local Bloch states at the fixed carrier momentum $\mathbf{k}_0$. Here the index n labels the component being expanded, while the index m labels the basis state used for the projection.

From this point onward, the derivation is carried out explicitly for the TE polarization. The TM case follows the same two-scale logic and the same moire-Bloch factorization, but its operator remains a generalized eigenproblem and the formulas differ in detail. The derivation naturally separates into two stages: **Stage 1** expands the lifted operator in powers of η , while **Stage 2** writes those terms out explicitly and identifies the physical quantities they contain.

3.5 TE Expansion in Orders of η

The starting point is the TE master equation written in the lifted variables. Using the exact chain rule Equation 21 and multiplying the physical equation by a^2 , we obtain

$$-(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}}) \cdot [\varepsilon^{-1}(\mathbf{r}, \mathbf{R})(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}}) H_{\mathbf{k}_0 \mathbf{q}}(\mathbf{r}, \mathbf{R})] = \lambda H_{\mathbf{k}_0 \mathbf{q}}(\mathbf{r}, \mathbf{R}), \quad (33)$$

where, by a slight abuse of notation, the symbol λ now denotes the dimensionless eigenvalue after this rescaling. At this stage the equation is still exact at the level of the lifted TE problem.

To expose the moire Bloch momentum cleanly, it is convenient to factor both the fast carrier phase and the slow moire phase from the field. Using Equation 26, define the periodic core

$$\psi_{\mathbf{q}}(\mathbf{r}, \mathbf{R}) := \sum_{n=1}^N f_{n\mathbf{q}}(\mathbf{R}) u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R}), \quad (34)$$

so that the ansatz becomes

$$H_{\mathbf{k}_0 \mathbf{q}}(\mathbf{r}, \mathbf{R}) \approx e^{i\mathbf{k}_0 \cdot \mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{R}} \psi_{\mathbf{q}}(\mathbf{r}, \mathbf{R}). \quad (35)$$

The approximation sign here is the same one already discussed in Equation 28: it comes from the reduced multiband ansatz, not from the algebraic manipulations that follow. Because $\mathbf{r}$ and $\mathbf{R}$ are independent lifted variables, the fast gradient acts only on the $\mathbf{k}_0$ phase and the slow gradient acts only on the $\mathbf{q}$ phase. This suggests the lean notation

$$D_{\mathbf{r}} := \nabla_{\mathbf{r}} + i\mathbf{k}_0, \quad D_{\mathbf{R}} := \nabla_{\mathbf{R}} + i\mathbf{q} \quad (36)$$

for the fast and slow covariant derivatives. With these definitions,

$$(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}}) H_{\mathbf{k}_0 \mathbf{q}} = e^{i\mathbf{k}_0 \cdot \mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{R}} (D_{\mathbf{r}} + \eta D_{\mathbf{R}}) \psi_{\mathbf{q}}, \quad (37)$$

and pushing the outer divergence through the same phase factors gives

$$-(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}}) \cdot [\varepsilon^{-1}(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}}) H_{\mathbf{k}_0 \mathbf{q}}] = e^{i\mathbf{k}_0 \cdot \mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{R}} \mathcal{L}_{\text{TE,eff}} \psi_{\mathbf{q}}, \quad (38)$$

with the symmetric effective operator

$$\mathcal{L}_{\text{TE,eff}} := -(D_{\mathbf{r}} + \eta D_{\mathbf{R}}) \cdot [\varepsilon^{-1}(\mathbf{r}, \mathbf{R})(D_{\mathbf{r}} + \eta D_{\mathbf{R}})] \quad (39)$$

acting on the periodic core $\psi_{\mathbf{q}}$. The factorization of the moire Bloch phase has therefore turned the slow momentum $\mathbf{q}$ into an exact rigid shift $\nabla_{\mathbf{R}} \mapsto \nabla_{\mathbf{R}} + i\mathbf{q}$ throughout the TE operator.

We can now separate the operator into powers of the scale-separation parameter,

$$\mathcal{L}_{\text{TE,eff}} = \mathcal{L}_{\text{TE}}^{(0)} + \eta \mathcal{L}_{\text{TE}}^{(1)} + \eta^2 \mathcal{L}_{\text{TE}}^{(2)}, \quad (40)$$

where the three orders are:

TE Expanded Operators

$$\begin{aligned}
\mathcal{L}_{\text{TE}}^{(0)} &:= -D_{\mathbf{r}} \cdot (\varepsilon^{-1} D_{\mathbf{r}}) \\
\mathcal{L}_{\text{TE}}^{(1)} &:= -D_{\mathbf{r}} \cdot (\varepsilon^{-1} D_{\mathbf{R}}) - D_{\mathbf{R}} \cdot (\varepsilon^{-1} D_{\mathbf{r}}) \\
\mathcal{L}_{\text{TE}}^{(2)} &:= -D_{\mathbf{R}} \cdot (\varepsilon^{-1} D_{\mathbf{R}}).
\end{aligned} \tag{41}$$

The notation is intentionally compact. The slow covariant derivative $D_{\mathbf{R}}$ acts on everything to its right, including the explicit $\mathbf{R}$ -dependence of $\varepsilon^{-1}(\mathbf{r}, \mathbf{R})$ through the registry map Equation 11, so the slow-coefficient terms are already built into the operator decomposition above without any additional bookkeeping.

This completes **Stage 1**: the TE problem has been reorganized into a hierarchy of operators adapted to the microscopic and moire scales. We now proceed to **Stage 2** and evaluate this hierarchy order by order.

From this point onward, we use the following shorthand throughout the explicit derivation:

Shorthand Notation

$$\begin{aligned}
u_n &:= u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R}) & f_n &:= f_{n\mathbf{q}}(\mathbf{R}) \\
\lambda_n &:= \lambda_n(\mathbf{R}; \mathbf{k}_0) & \varepsilon &:= \varepsilon(\mathbf{r}, \mathbf{R}) \\
\varepsilon^{-1} &:= \varepsilon^{-1}(\mathbf{r}, \mathbf{R}).
\end{aligned} \tag{42}$$

Since $\mathbf{k}_0$, $\mathbf{q}$, and the coordinate pair $(\mathbf{r}, \mathbf{R})$ remain fixed throughout, this shorthand loses no information. The only dependencies that matter for tracking the algebra are those on $\mathbf{r}$ and $\mathbf{R}$.

3.5.1 Zeroth Order: Local Band Energies

Since the envelopes f_n depend only on $\mathbf{R}$, the fast covariant derivative $D_{\mathbf{r}}$ passes through them. The zeroth-order operator therefore acts on each u_n through the local eigenproblem Equation 23 at the carrier momentum, giving $\mathcal{L}_{\text{TE}}^{(0)}\psi_{\mathbf{q}} = \sum_{n=1}^N \lambda_n f_n u_n$. Projecting onto $\langle u_m, \cdot \rangle_{\Omega}$ and using orthonormality extracts the diagonal band-energy matrix

$$\Lambda_{mn}(\mathbf{R}; \mathbf{k}_0) := \lambda_n \delta_{mn}. \tag{43}$$

No slow derivatives, no moire momentum, and no interband coupling appear at this order.

3.5.2 First Order: Velocity Coupling and Slow Derivatives

The first-order operator $\mathcal{L}_{\text{TE}}^{(1)} = -D_{\mathbf{r}_i}(\varepsilon^{-1} D_{\mathbf{R}_i}) - D_{\mathbf{R}_i}(\varepsilon^{-1} D_{\mathbf{r}_i})$ couples fast and slow scales. Applying it to $\psi_{\mathbf{q}} = \sum_n f_n u_n$ and distributing $D_{\mathbf{R}_i}$ via the product rule generates two classes of terms: those where the slow derivative acts on the envelope (proportional to $D_{\mathbf{R}_i} f_n$), and those where it acts on the Bloch state or the dielectric (proportional to f_n).

The first class is organized by the local TE velocity operator, defined as the $\mathbf{k}$ -derivative of the Bloch operator at the carrier momentum,

$$\mathcal{V}_i := \left. \frac{\partial \mathcal{L}_0(\mathbf{R}, \mathbf{k})}{\partial k_i} \right|_{\mathbf{k}=\mathbf{k}_0}, \tag{44}$$

with $\mathcal{L}_0(\mathbf{R}, \mathbf{k}) := -D_{\mathbf{r}}(\mathbf{k}) \cdot (\varepsilon^{-1} D_{\mathbf{r}}(\mathbf{k}))$. Differentiating gives

$$\mathcal{V}_i \varphi = -i [D_{\mathbf{r}_i}(\varepsilon^{-1} \varphi) + \varepsilon^{-1} D_{\mathbf{r}_i} \varphi], \tag{45}$$

and the velocity matrix elements are

$$v_{mn}^{(i)} := \langle u_m, \mathcal{V}_i u_n \rangle_{\Omega}. \tag{46}$$

The second class, where $D_{\mathbf{R}_i}$ acts on u_n or on ε^{-1} , is collected into the exact first-order remainder

$$\Gamma_{mn}^{(1)} := - \sum_{i=x,y} [i \langle u_m, \mathcal{V}_i (\partial_{\mathbf{R}_i} u_n) \rangle_{\Omega} + \langle u_m, (\partial_{\mathbf{R}_i} \varepsilon^{-1}) D_{\mathbf{r}_i} u_n \rangle_{\Omega}]. \tag{47}$$

Projecting the full first-order action onto the retained basis then gives

TE First-Order Projection

$$\left(\mathcal{H}_{\text{TE}}^{(1)}\mathbf{f}_q\right)_m = -iv_{mn}^{(i)}D_{R_i}f_n + \Gamma_{mn}^{(1)}f_n. \quad (48)$$

The moire Bloch momentum enters only through $D_{R_i} = \partial_{R_i} + iq_i$.

3.5.3 Second Order: Direct Slow-Kinetic Projection

The second-order operator $\mathcal{L}_{\text{TE}}^{(2)} = -D_{R_i}(\varepsilon^{-1}D_{R_i})$ contains only slow derivatives. Distributing D_{R_i} twice through ε^{-1} and u_n , and projecting onto $\langle u_m, \cdot \rangle_\Omega$, yields

TE Direct Second-Order Projection

$$\left(\mathcal{H}_{\text{TE,dir}}^{(2)}\mathbf{f}_q\right)_m = -G_{mn}D_{R_i}^2f_n - B_{mn}^{(i)}D_{R_i}f_n + \Gamma_{mn}^{(2)}f_n, \quad (49)$$

with the direct second-order coefficient matrices

$$\begin{aligned} G_{mn} &:= \langle u_m, \varepsilon^{-1}u_n \rangle_\Omega \\ B_{mn}^{(i)} &:= \langle u_m, \partial_{R_i}(\varepsilon^{-1}u_n) + \varepsilon^{-1}\partial_{R_i}u_n \rangle_\Omega \\ \Gamma_{mn}^{(2)} &:= - \sum_{i=x,y} \langle u_m, \partial_{R_i}(\varepsilon^{-1}\partial_{R_i}u_n) \rangle_\Omega. \end{aligned} \quad (50)$$

The metric G encodes the ε^{-1} -weighted overlap of retained Bloch states, B and $\Gamma^{(2)}$ capture the slow variation of both the basis and the dielectric. Note that these direct projected coefficients are gauge-dependent: an $\mathbf{R}$ -dependent unitary rotation $U(\mathbf{R}) \rightarrow U(\mathbf{R})W(\mathbf{R})$ of the retained frame changes each of them individually. They are intermediate quantities; the covariant operator assembled below is the gauge-meaningful object, with one restriction that the assembly makes explicit. Because the band-energy matrix Λ is kept diagonal and the Löwdin denominators carry band labels, the admissible frame changes $W(\mathbf{R})$ are phase rotations of the individual retained states, permutations, and unitary rotations inside degenerate blocks. A general $\mathbf{R}$ -dependent mixing of non-degenerate retained states would require Λ to be rotated to $W^\dagger \Lambda W$ and the downfolding below to be carried out with matrix-valued denominators. These are only the direct retained-space contributions; the virtual corrections from remote bands enter through the Löwdin step below.

3.5.4 The Retained Subspace and Geometric Leakage

Building the effective Hamiltonian requires more than the direct retained-space projections above. We must also account for virtual transitions into the remote complement. The first step is choosing which N local bands at the carrier momentum $\mathbf{k}_0$ serve as active degrees of freedom.

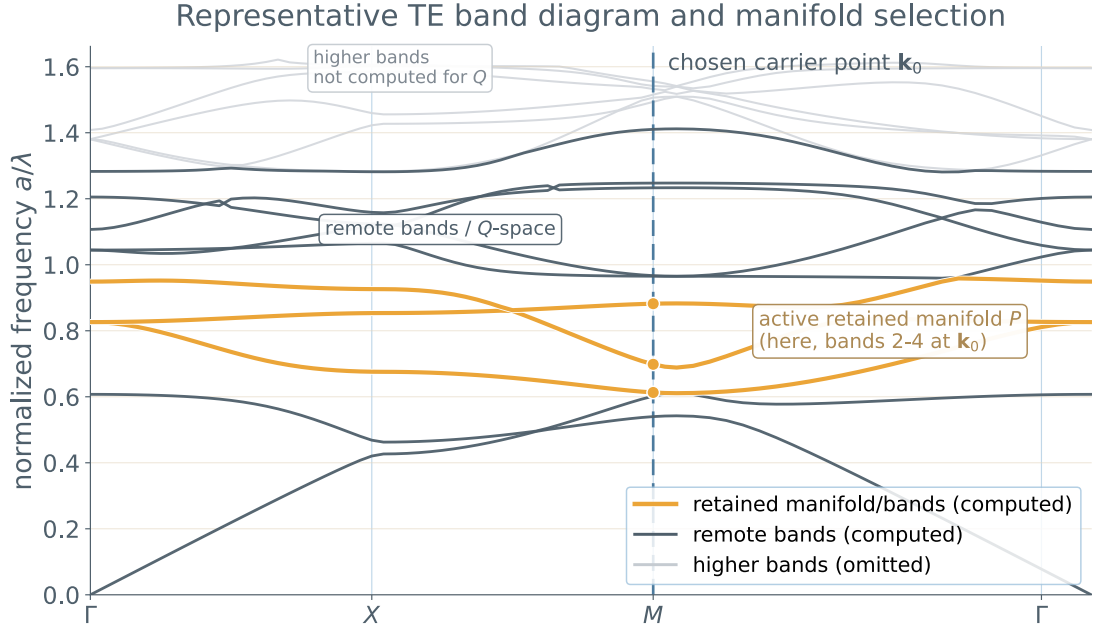


Figure 22: Representative TE band diagram of a square-lattice photonic crystal along $\Gamma - X - M - \Gamma$, computed here with 16 bands for illustration. The dashed line marks a chosen carrier point $\mathbf{k}_0$, taken here at M . The highlighted bands 2–4 define the retained manifold, or P -space. The darker bands indicate the computed remote bands used to approximate the complementary space Q , whereas the light-grey bands represent the remainder of the exact infinite complement. Because highly distant bands have minimal impact on the effective Hamiltonian, they can deliberately be omitted from the numerical Q -space approximation to save computational effort.

Figure 22 illustrates the two essential spaces: the *retained manifold* (P -space) and the *remote complement* (Q -space). We write P for the projector onto the retained subspace and $Q = 1 - P$ for the complement. The figure is a visual aid for what these spaces mean; it should *not* be read as a selection recipe. A spectral gap separating the retained bands from the rest in the band diagram is a *necessary* condition for a well-defined envelope expansion, but it is not *sufficient*: the subspace must also remain spectrally isolated across the full registry domain $\delta(\mathbf{R})$, not just at a single crystal configuration. If the retained manifold is chosen poorly, strong mixing with remote bands persists and the envelope approximation breaks down. In practice the exact infinite complement is truncated to a finite window of nearby remote bands, because the Löwdin denominators suppress distant contributions. The direct terms G , B , and $\Gamma^{(2)}$ found above are what P -space produces alone; the remaining correction comes from projecting through Q and back.

As $\mathbf{R}$ varies, the local Bloch states $u_n(\mathbf{r}; \mathbf{R})$ change. This slow variation has two geometric consequences: the retained states can rotate into one another within P -space, producing the *non-Abelian Berry connection*, and the slow derivative can twist states out of P into Q , producing a kinetic energy penalty known as the *Born-Huang potential*.

3.5.5 Assembly of the Effective Hamiltonian

The assembly now proceeds in two steps. First, we project onto the retained sector itself and rewrite the resulting terms in a geometrically transparent form. Second, we project through the remote sector and back, thereby collecting the virtual corrections that the retained manifold feels from states it does not explicitly keep. To do this cleanly without writing out band indices for every derivative, we package the retained Bloch functions columnwise into the operator $U(\mathbf{R})$ defined by $U(\mathbf{R})e_n := u_n(\mathbf{r}; \mathbf{R})$, assuming that a globally smooth retained frame exists over the moire cell (i.e., that the retained bundle is trivializable; for a topologically nontrivial bundle the construction would need to be carried out patchwise). This lets us define the projection operators on the fast-cell Hilbert space as

$$U^\dagger U = \mathbb{1}_N, \quad P := UU^\dagger, \quad Q := 1 - P. \quad (51)$$

Taking the slow derivative of the retained frame reveals exactly how the basis changes. Because U is orthonormal, its derivative splits into an in-subspace rotation and an out-of-subspace leakage term:

$$A_i := iU^\dagger \partial_{R_i} U, \quad \partial_{R_i} U = -iU A_i + \Xi_i, \quad \Xi_i := Q \partial_{R_i} U. \quad (52)$$

Here, A_i is the non-Abelian Berry connection. The factor of i is introduced by convention so that A_i is Hermitian, which is the natural form for an effective gauge potential. The remainder Ξ_i is the exact geometric leakage into the remote Q -space. This decomposition induces the covariant slow derivative and its corresponding gauge-covariant momentum,

$$\mathcal{D}_i := D_{R_i} - iA_i, \quad \Pi_i := -i\mathcal{D}_i, \quad (53)$$

so that the retained-field ansatz satisfies the exact product rule

$$D_{R_i}(U \mathbf{f}_q) = U \mathcal{D}_i \mathbf{f}_q + \Xi_i \mathbf{f}_q. \quad (54)$$

The exact remainder decompositions and Löwdin split behind this reorganization are recorded in Appendix B.

From this point onward, repeated Cartesian indices $i, j \in \{x, y\}$ are summed unless an explicit sum is written.

The first projection, namely the retained-space part $P\mathcal{L}P$, is what produces the direct coefficients already found: the metric-like term G , the first-derivative term B , and the local scalar remainder $\Gamma^{(2)}$. The second projection, namely the excursion $P\mathcal{L}Q$ followed by propagation in Q and return through $Q\mathcal{L}P$, accounts for the remote-band dressing of the active manifold. To include this second piece rigorously, we assume that the retained manifold is separated from the remote complement by a nonzero local spectral gap $\Delta(\mathbf{R}) > 0$ uniformly over the full registry domain, and write the exact lifted periodic core as

$$\Psi = U \mathbf{f}_q + \eta \chi + O(\eta^2), \quad Q\chi = \chi, \quad R_Q := \left[Q \left(\mathcal{L}_{\text{TE}}^{(0)} - \lambda_{\text{ref}} \right) Q \right]^{-1}, \quad (55)$$

where χ is the small virtual response leaking into the remote sector, $Q\chi = \chi$ enforces that it lives entirely in the complement, and R_Q is the reduced resolvent at a reference energy inside the retained manifold. Standard Löwdin partitioning then resolves χ and gives the closed effective operator through order η^2 as

$$\mathcal{H}_{\text{eff}} = \Lambda + \eta U^\dagger \mathcal{L}_{\text{TE}}^{(1)} U + \eta^2 \left[U^\dagger \mathcal{L}_{\text{TE}}^{(2)} U - U^\dagger \mathcal{L}_{\text{TE}}^{(1)} Q R_Q Q \mathcal{L}_{\text{TE}}^{(1)} U \right]. \quad (56)$$

Evaluating this operator order by order reveals the physical meaning of each term. The zeroth-order contribution is exactly the diagonal band-energy matrix Λ . At first order, the direct projection from Equation 48 can be reorganized into the Berry-covariant form

$$\mathcal{H}_{\text{TE,exact}}^{(1)} = \frac{1}{2} (v^{(i)} \Pi_i + \Pi_i v^{(i)}) + U_{\text{rem}}^{(1)}, \quad (57)$$

where $U_{\text{rem}}^{(1)}$ collects the exact first-order terms that are not absorbed into the symmetrized drift. Its explicit form, given in Equation 88, is built from the out-of-subspace leakage Ξ_i , slow dielectric gradients, the slow derivative of the velocity field, and the commutator $\frac{1}{2} [A_i, v^{(i)}]$ that converts the exact covariant form $-iv^{(i)} \mathcal{D}_i$ into its symmetrized version. The Berry connection enters rigorously through Π_i , and only once: the symmetrization must not count it a second time. The remainder $U_{\text{rem}}^{(1)}$ is a separate, nonvanishing matrix operator.

At second order, the direct bare metric G supplies only part of the slow kinetic term. The Löwdin correction generated by $\mathcal{L}_{\text{TE}}^{(1)}$ adds the remote-band curvature. Inserting the spectral decomposition $R_Q = \sum_{\ell \in Q} |u_\ell\rangle \langle u_\ell| / (\lambda_\ell - \lambda_{\text{ref}})$ into Equation 56 and then applying the standard Hermitian Löwdin symmetrization of quasi-degenerate perturbation theory [34], namely replacing λ_{ref} by λ_n or λ_m according to whether the retained-band label sits on the ket or bra, yields the full Hermitian inverse mass tensor

$$(M_{ij}^{-1})_{mn} := 2\delta_{ij} G_{mn} + \sum_{\ell \notin P} \left[\frac{v_{m\ell}^{(i)} v_{\ell n}^{(j)}}{\lambda_n - \lambda_\ell} + \frac{v_{m\ell}^{(j)} v_{\ell n}^{(i)}}{\lambda_m - \lambda_\ell} \right]. \quad (58)$$

The remaining second-order terms are scalar or one-derivative remainders. The cleanest way to state the direct part is the flux form. The second-order operator $\mathcal{L}_{\text{TE}}^{(2)} = -D_{R_i} \varepsilon^{-1} D_{R_i}$ is the ε^{-1} -weighted square of the slow flux, and by Equation 54 the slow flux of the ansatz is $U \mathcal{D}_i \mathbf{f}_q + \Xi_i \mathbf{f}_q$. Projecting the square onto the retained frame gives

$$\mathcal{H}_{\text{TE,dir}}^{(2)} = -\mathcal{D}_i(G\mathcal{D}_i + K_i) + K_i^\dagger \mathcal{D}_i + \Xi_i^\dagger \varepsilon^{-1} \Xi_i, \quad K_i := U^\dagger \varepsilon^{-1} \Xi_i, \quad (59)$$

with the slow derivatives acting on everything to their right. This expression is exact and equivalent to Equation 49: the two are alternative bookkeepings of the same operator, and the scalar $\Gamma^{(2)}$ of the raw form is already contained in the leakage and K terms of the flux form. Either form is complete on its own; adding $\Gamma^{(2)}$ to the flux form would count the leakage twice. The last term is the exact TE leakage penalty, and it is weighted,

$$U_{\text{BH,exact}} = \Xi_i^\dagger \varepsilon^{-1} \Xi_i. \quad (60)$$

The commonly used unweighted form $U_{\text{BH}} \approx \Xi_i^\dagger \Xi_i$ is a modeling simplification, not an identity. Together with the one-derivative K terms above, the one-derivative Löwdin cross-terms, and the scalar Löwdin term of the remote-band excursion, these terms form the second-order remainder $U_{\text{rem}}^{(2)}$. The full decomposition, with the remote-band term in its manifestly Hermitian form $-S^\dagger R_Q S$, is recorded in Appendix B.

Collecting all contributions, the TE effective operator obtained by collecting all terms retained through $O(\eta^2)$ is

TE Effective Hamiltonian $\mathcal{H}_{\text{eff}} = \Lambda + \eta \left[\frac{1}{2} (v^{(i)} \Pi_i + \Pi_i v^{(i)}) + U_{\text{rem}}^{(1)} \right] + \eta^2 \left[\frac{1}{2} \Pi_i M_{ij}^{-1} \Pi_j + U_{\text{rem}}^{(2)} \right] + O(\eta^3). \quad (61)$

The mass tensor M^{-1} and the Berry connection entering through Π_i are therefore exact through the retained order of the two-scale/Löwdin expansion under the assumptions stated above. The remainder operators $U_{\text{rem}}^{(1)}$ and $U_{\text{rem}}^{(2)}$ are explicit, nonvanishing matrix fields: Equation 88 gives the exact first-order remainder, whereas Equation 59 and Equation 91 give the direct and the remote-band parts of $U_{\text{rem}}^{(2)}$. The complete expanded operator, every term written out with every symbol defined, is displayed for both polarizations in Appendix A. The dominant contributions within $U_{\text{rem}}^{(2)}$ are the Born-Huang leakage potential from geometric frame rotation out of the active space and the slow-coefficient potentials from registry variation of ε^{-1} .

A brief note on terminology: $\mathcal{H}_{\text{eff}}$ is not a Hamiltonian in the quantum-mechanical sense, since the underlying Maxwell equation is not a Schrödinger equation. The name *effective Hamiltonian* is nevertheless standard in the $\mathbf{k} \cdot \mathbf{p}$ and envelope-function literature [21,35,36], and we adopt it here for consistency with the condensed-matter conventions that inspired the photonic moire framework.

3.6 The TM Case: Generalized and Hermitized Expansions

The exact logic and moire-Bloch factorization established for the TE polarization apply equally to the TM case. However, the vector geometry of the Maxwell equations leads to a fundamentally different operational structure. Rather than executing a fully detailed, step-by-step derivation as done for TE, this section highlights only the most crucial mathematical differences. These structural distinctions are too profound to skip over: simply stating the final result would obscure the physical origin of the TM operator's unique local terms and fail to do justice to the rigorous theoretical work required.

For TE, the starting point was a standard scalar eigenproblem. For TM, where the out-of-plane electric field E_z is the active component, the corresponding master equation is instead a generalized scalar eigenproblem,

$$-\Delta_{\mathbf{x}} E^\eta(\mathbf{x}) = \lambda \varepsilon^\eta(\mathbf{x}) E^\eta(\mathbf{x}). \quad (62)$$

Here, the non-uniform permittivity $\varepsilon^\eta(\mathbf{x})$ appears strictly as a material weight on the right-hand side. Multiplying by a^2 and reusing λ for the resulting dimensionless eigenvalue, the identical two-scale lift $\nabla_{\mathbf{x}} = \frac{1}{a}(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}})$ with independent fast and slow coordinates transforms this into

$$-(\nabla_{\mathbf{r}} + \eta \nabla_{\mathbf{R}})^2 E(\mathbf{r}, \mathbf{R}) = \lambda \varepsilon(\mathbf{r}, \mathbf{R}) E(\mathbf{r}, \mathbf{R}). \quad (63)$$

Following the established blueprint, we apply the two-scale moire-Bloch ansatz, factoring the field into a fast carrier phase and a slow moire phase:

$$E_{\mathbf{k}_0, \mathbf{q}}(\mathbf{r}, \mathbf{R}) \approx e^{i\mathbf{k}_0 \cdot \mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{R}} \psi_{\mathbf{q}}(\mathbf{r}, \mathbf{R}). \quad (64)$$

Pushing the gradients through these phase factors introduces the covariant equivalents $D_{\mathbf{r}} = \nabla_{\mathbf{r}} + i\mathbf{k}_0$ and $D_{\mathbf{R}} = \nabla_{\mathbf{R}} + i\mathbf{q}$. This isolates the generalized envelope problem entirely on the periodic core $\psi_{\mathbf{q}}$,

$$\mathcal{A}_{\text{TM}}^{\eta} \psi_{\mathbf{q}} = \lambda \mathcal{B}_{\text{TM}} \psi_{\mathbf{q}}, \quad (65)$$

with the unexpanded operators

TM Unexpanded Operators

$$\mathcal{A}_{\text{TM}}^{\eta} := -(D_{\mathbf{r}} + \eta D_{\mathbf{R}})^2, \quad \mathcal{B}_{\text{TM}} := \varepsilon(\mathbf{r}, \mathbf{R}). \quad (66)$$

Because $\mathcal{B}_{\text{TM}}$ is purely multiplicative and requires no expansion, expanding $\mathcal{A}_{\text{TM}}^{\eta}$ in powers of the scale separation parameter η provides a mathematically straightforward exact generalized hierarchy:

$$\begin{aligned} \mathcal{A}_{\text{TM}}^{(0)} &= -D_{\mathbf{r}} \cdot D_{\mathbf{r}} \\ \mathcal{A}_{\text{TM}}^{(1)} &= -(D_{\mathbf{r}} \cdot D_{\mathbf{R}} + D_{\mathbf{R}} \cdot D_{\mathbf{r}}) \\ \mathcal{A}_{\text{TM}}^{(2)} &= -D_{\mathbf{R}} \cdot D_{\mathbf{R}}. \end{aligned} \quad (67)$$

While rigorously exact, this generalized form does not yet match the structure we want. $\mathcal{A}_{\text{TM}}^{\eta}$ acts as a generalized operator, not a genuine Hamiltonian defined on a standard, unweighted Hilbert space. To achieve an effective band formalism matching the TE case, complete with standard orthogonality and projection rules, we must transform it into a standard eigenvalue problem.

3.6.1 Exact Hermitization and Explicit Gradients

We reduce the generalized TM eigenproblem to standard Hermitian form by absorbing the dielectric weight into the field. Defining the transformed field $\tilde{E} := \varepsilon^{\frac{1}{2}} E$ and multiplying the entire lifted equation from the left by $\varepsilon^{-\frac{1}{2}}$, and performing the same transformation on the periodic envelope, $\tilde{\psi}_{\mathbf{q}} := \varepsilon^{\frac{1}{2}} \psi_{\mathbf{q}}$, yields the exact standard eigenproblem

$$\tilde{\mathcal{H}}_{\text{TM,eff}}^{\eta} \tilde{\psi}_{\mathbf{q}} = \lambda \tilde{\psi}_{\mathbf{q}}, \quad (68)$$

housing the complete, exact TM effective Hamiltonian

TM Hermitized Operator

$$\tilde{\mathcal{H}}_{\text{TM,eff}}^{\eta} = -\varepsilon^{-\frac{1}{2}} (D_{\mathbf{r}} + \eta D_{\mathbf{R}})^2 \varepsilon^{-\frac{1}{2}}. \quad (69)$$

This is the exact, structural TM counterpart to the TE operator. However, its expansion is dramatically more intricate. The expansion parameter η is now wedged between the spatially varying roots of the dielectric function. Organizing this exact hermitized operator sequentially rigorously generates explicit spatial derivatives of ε that function as gauge-like drifts and scalar quasi-potentials.

For the explicit product-rule formulas below we continue to assume that $\varepsilon(\mathbf{r}, \mathbf{R})$ is strictly positive and sufficiently smooth in both variables. For sharp-interface media the same expressions should be read formally, or replaced by the corresponding weak-form identities with interface contributions.

Setting $\rho := \varepsilon^{-\frac{1}{2}}$ and evaluating the action on an arbitrary smooth test function φ , we unpack the explicit orders $\tilde{\mathcal{H}}_{\text{TM,eff}}^{\eta} = \tilde{\mathcal{H}}_{\text{TM}}^{(0)} + \eta \tilde{\mathcal{H}}_{\text{TM}}^{(1)} + \eta^2 \tilde{\mathcal{H}}_{\text{TM}}^{(2)}$.

Zeroth Order: The local microscopic operation begins as

$$\tilde{\mathcal{H}}_{\text{TM}}^{(0)} \varphi = -\rho D_{\mathbf{r}} \cdot D_{\mathbf{r}} (\rho \varphi). \quad (70)$$

Applying the exact product rule and restoring all instances of ε , we obtain

TM Zeroth Order

$$\begin{aligned}\tilde{\mathcal{H}}_{\text{TM}}^{(0)}\varphi = & -\varepsilon^{-1}D_{\mathbf{r}} \cdot D_{\mathbf{r}}\varphi + \varepsilon^{-2}(\nabla_{\mathbf{r}}\varepsilon) \cdot D_{\mathbf{r}}\varphi \\ & + \left[\frac{1}{2}\varepsilon^{-2}\Delta_{\mathbf{r}}\varepsilon - \frac{3}{4}\varepsilon^{-3}|\nabla_{\mathbf{r}}\varepsilon|^2 \right]\varphi.\end{aligned}\quad (71)$$

This term immediately sets TM apart from TE. Hermitized TM is not trivially $-\varepsilon^{-1}D_{\mathbf{r}}^2$. Already at leading order, it binds an explicit fast drift to the microscopic momentum $D_{\mathbf{r}}$ alongside a strict, purely local scalar potential shaped solely by the fast spatial gradients of the cell material.

First Order: The first-order cross terms define the critical interaction between microscopic cells and their slow moire environment:

$$\tilde{\mathcal{H}}_{\text{TM}}^{(1)}\varphi = -\rho(D_{\mathbf{r}} \cdot D_{\mathbf{R}} + D_{\mathbf{R}} \cdot D_{\mathbf{r}})(\rho\varphi). \quad (72)$$

Exhaustively distributing the exact derivatives produces

TM First Order

$$\begin{aligned}\tilde{\mathcal{H}}_{\text{TM}}^{(1)}\varphi = & -\varepsilon^{-1}(D_{\mathbf{r}} \cdot D_{\mathbf{R}} + D_{\mathbf{R}} \cdot D_{\mathbf{r}})\varphi \\ & + \varepsilon^{-2}(\nabla_{\mathbf{R}}\varepsilon) \cdot D_{\mathbf{r}}\varphi + \varepsilon^{-2}(\nabla_{\mathbf{r}}\varepsilon) \cdot D_{\mathbf{R}}\varphi \\ & + \left[\varepsilon^{-2} \sum_{i=x,y} \partial_{r_i} \partial_{R_i} \varepsilon - \frac{3}{2}\varepsilon^{-3} \sum_{i=x,y} (\partial_{r_i} \varepsilon)(\partial_{R_i} \varepsilon) \right] \varphi.\end{aligned}\quad (73)$$

Deviating decisively from the simple kinetic coupling seen in TE, the fully expanded TM operator demonstrates three distinct new cross-scale interactions:

1. A microscopic covariant derivative $D_{\mathbf{r}}$ actively drifting with the **slow** gradient of the moire registry.
2. A slow covariant derivative $D_{\mathbf{R}}$ actively drifting with the **fast** microscopic material landscape.
3. A purely mixed scalar pseudo-potential constructed symmetrically from cross-scale variations.

Second Order: The mechanism governing the slow quadratic scale is given by,

$$\begin{aligned}\tilde{\mathcal{H}}_{\text{TM}}^{(2)}\varphi = & -\rho D_{\mathbf{R}} \cdot D_{\mathbf{R}}(\rho\varphi) \\ = & -\varepsilon^{-1}D_{\mathbf{R}} \cdot D_{\mathbf{R}}\varphi + \varepsilon^{-2}(\nabla_{\mathbf{R}}\varepsilon) \cdot D_{\mathbf{R}}\varphi \\ & + \left[\frac{1}{2}\varepsilon^{-2}\Delta_{\mathbf{R}}\varepsilon - \frac{3}{4}\varepsilon^{-3}|\nabla_{\mathbf{R}}\varepsilon|^2 \right]\varphi.\end{aligned}\quad (74)$$

The underlying slow kinetic operator is therefore accompanied by a persistent moire drift generated from the local environment map and a slow scalar confining potential.

3.6.2 Projection and the Final TM Operator

The expanded operators act on the full fast Hilbert space. To obtain the $N \times N$ envelope operator, we project onto the hermitized local Bloch states $\tilde{u}_n(\mathbf{r}; \mathbf{R})$ that diagonalize $\tilde{\mathcal{H}}_{\text{TM}}^{(0)}$ with standard orthonormality $\langle \tilde{u}_m, \tilde{u}_n \rangle_{\Omega} = \delta_{mn}$, then apply the same Löwdin partitioning used for TE.

Every coefficient matrix that results differs from its TE counterpart in a systematic way: the hermitizing sandwich $\rho(\dots)\rho$ entangles each matrix element with the spatially varying dielectric. The TM velocity operator inherits the compact form

$$\tilde{\mathcal{V}}_i\varphi := -2i\rho D_{r_i}(\rho\varphi). \quad (75)$$

Compare the TE form $\mathcal{V}_i\varphi = -i[D_{r_i}(\varepsilon^{-1}\varphi) + \varepsilon^{-1}D_{r_i}\varphi]$ from Equation 45, where ε^{-1} sits between the derivatives rather than flanking them through $\rho = \varepsilon^{-1/2}$. The direct second-order metric becomes the weighted overlap

$$\tilde{G}_{mn} = \langle \tilde{u}_m, \varepsilon^{-1}\tilde{u}_n \rangle_{\Omega}, \quad (76)$$

which has the same ε^{-1} -weighted structure as the TE metric $G_{mn} = \langle u_m, \varepsilon^{-1} u_n \rangle_\Omega$, but with the hermitized states $\tilde{u}_n = \varepsilon^{1/2} u_n^{\text{TM}}$ in place of the bare TE Bloch states. The first-order remainder $\tilde{\Gamma}^{(1)}$ acquires an additional term proportional to $\partial_{R_i} \rho$ from the slow variation of the hermitizing factor. This term has no TE analogue; its explicit form and the remaining TM coefficient definitions are recorded in Appendix B.

In the flux form Equation 59 the hermitizing factor travels with the leakage. The slow flux of the hermitized ansatz is $D_{R_i}(\rho \tilde{U} \mathbf{f}_q) = \rho \tilde{U} \mathcal{D}_i \mathbf{f}_q + Y_i \mathbf{f}_q$ with the TM leakage flux

$$Y_i := \rho \tilde{\Xi}_i + (\partial_{R_i} \rho) \tilde{U}, \quad \tilde{\Xi}_i := Q \partial_{R_i} \tilde{U}, \quad (77)$$

so the direct TM second-order operator is $-\mathcal{D}_i(\tilde{G} \mathcal{D}_i + \tilde{K}_i) + \tilde{K}_i^\dagger \mathcal{D}_i + Y_i^\dagger Y_i$ with $\tilde{K}_i = \tilde{U}^\dagger \rho Y_i$. The TM Born-Huang penalty $Y_i^\dagger Y_i$ contains, besides the ε^{-1} -weighted frame leakage, the slow variation of the hermitizing factor itself.

With these definitions in place, the Löwdin mass tensor takes the same structural formula as Equation 58 but with tilded velocities and the TM metric replacing its TE counterpart. Collecting all contributions, the TM effective operator obtained by the same bookkeeping through $O(\eta^2)$ is

TM Effective Hamiltonian

$$\mathcal{H}_{\text{TM,eff}} = \Lambda + \eta \left[\frac{1}{2} (\tilde{v}^{(i)} \Pi_i + \Pi_i \tilde{v}^{(i)}) + \tilde{U}_{\text{rem}}^{(1)} \right] + \eta^2 \left[\frac{1}{2} \Pi_i \tilde{M}_{ij}^{-1} \Pi_j + \tilde{U}_{\text{rem}}^{(2)} \right] + O(\eta^3). \quad (78)$$

This is structurally identical to the TE result Equation 61. The Berry connection, covariant momentum, and Löwdin mass tensor enter in the same way. Every coefficient, however, carries the hermitizing factor ρ : tilded velocities include a dielectric drift, the metric is weighted, and the remainders contain mixed slow-fast derivatives of $\varepsilon^{1/2}$ with no TE counterpart. The structural sameness is the payoff of the hermitization strategy: by absorbing the dielectric weight into the states at the start, we ensure the downstream Löwdin algebra is identical in form.

One practical warning deserves emphasis. Computing $\varepsilon^{\pm 1/2}$ accurately as operators on the Bloch basis is the genuine numerical bottleneck of the TM polarization. Errors in the hermitizing transformation contaminate every downstream coefficient. This makes TM not only algebraically harder than TE but numerically more demanding at the solver level.

3.7 The Resummed Limit

The expansion above is organized in powers of η , and it is worth asking what the series converges to. Every term generated by the slow derivatives acting on a frame frozen at the carrier momentum $\mathbf{k}_0$ has one origin. An envelope with moire momentum $\mathbf{q}$ represents a physical Bloch state at the monolayer momentum $\mathbf{k}_0 + \eta \mathbf{q}$, and the local Bloch data at that momentum, $u_n(\mathbf{r}; \mathbf{R}, \mathbf{k})$ and $\lambda_n(\mathbf{R}, \mathbf{k})$, are analytic in $\mathbf{k}$. The velocity term is the first Taylor coefficient of λ_n in $\mathbf{k}$; the direct metric together with the Löwdin sum is its second coefficient, which is the mass sum rule of $\mathbf{k} \cdot \mathbf{p}$ theory; the Born-Huang and remainder terms are the corresponding coefficients of the frame itself. The η -expansion is the Taylor expansion of the local band data in the small momentum $\eta \mathbf{q}$ around the carrier.

This observation has a practical consequence: nothing forces the frame to stay frozen at $\mathbf{k}_0$. For an envelope that is periodic on the moire lattice, the admissible momenta form the discrete set $\mathbf{k}_p = \mathbf{k}_0 + \eta \mathbf{G}_p$, with $\mathbf{G}_p$ running over the moire reciprocal lattice, and one may use for each harmonic p the exact local Bloch state at exactly that momentum. All orders of the expansion in $\eta \mathbf{q}$ are then summed at once. For the TM pencil the resulting model is particularly transparent. Let the registry-averaged local crystal (the average of ε_{loc} over the registry torus, which for a weak second layer is the first layer alone) provide the frames $u_1(\mathbf{r}; \mathbf{k}_p)$ of one retained band. In the Galerkin projection of the exact supercell problem onto these trial states, distinct harmonics are distinct momentum cosets, so the kinetic block is diagonal with entries $\lambda_1(\mathbf{k}_p)$, and only the registry-dependent part of the dielectric, the Fourier harmonics c_h of the second layer, couples different harmonics. The envelope eigenproblem becomes

$$\text{diag}(\lambda_1(\mathbf{k}_p)) \mathbf{c} = \lambda (\mathbb{1} + V) \mathbf{c}, \quad V_{pp'} = c_h \langle u_1(\mathbf{k}_p), e^{i\mathbf{h} \cdot \mathbf{r}} u_1(\mathbf{k}_{p'}) \rangle_\Omega \quad \text{for} \quad \mathbf{G}_p - \mathbf{G}_{p'} = \mathbf{W}^T \mathbf{h}, \quad (79)$$

and $V_{pp'} = 0$ otherwise. Here W is the integer matrix through which the registry map turns a monolayer harmonic $\mathbf{h}$ of the second layer into a moire harmonic; it is the reciprocal-space image of $\delta(\mathbf{R}) = -J\mathbf{R}$ restricted to a commensurate cell. Exact local band data enter on the left, and the interlayer coupling enters as a nearest-neighbor hopping in the space of moire harmonics on the right. No supercell object appears anywhere, and the cost is one monolayer solve per harmonic. We call this the *resummed-frame model*. Its remaining error is the next effect that the two-scale picture neglects: the registry dressing of the frames themselves, which enters at second order in the interlayer coupling. Section 5 measures both the order-by-order convergence of the truncated expansion toward this limit and the residual error of the limit itself.

3.8 From Effective Hamiltonian to Computable Data

The derivation is now complete. After two full expansions, Bloch-cell projections, and Löwdin downfolding, we arrive at the envelope effective Hamiltonian. The moire-periodic envelope $\mathbf{f}_q$ satisfies

$$\mathcal{H}_{\text{eff}}\mathbf{f}_q = \lambda\mathbf{f}_q, \quad (80)$$

with the $N \times N$ matrix operator $\mathcal{H}_{\text{eff}}$ from Equation 61. Once discretized on a moire-reciprocal grid, this becomes a standard Hermitian eigenproblem whose solution is computationally routine (e.g., using SciPy’s `eigsh` [37]). The actual challenge lies in assembling the structural coefficients that enter $\mathcal{H}_{\text{eff}}$: the band energies $\Lambda(\mathbf{R})$, the velocity couplings $v^{(i)}(\mathbf{R})$, the inverse mass tensor $M^{-1}(\mathbf{R})$, the Berry connection $A_i(\mathbf{R})$, and the remainder operators $U_{\text{rem}}^{(1)}(\mathbf{R})$ and $U_{\text{rem}}^{(2)}(\mathbf{R})$.

Each of these terms is a matrix field varying over the moire cell, extracted by solving a local Bloch problem at the corresponding moire position $\mathbf{R}$. The moire cell is therefore discretized into a grid of registry points δ_j , and at each point, the local two-atomic crystal defined by $\varepsilon_{\text{loc}}(\mathbf{r}; \delta_j)$ must be fully diagonalized.

This procedure, the *registry sweep*, is conceptually simple. We fix a carrier momentum $\mathbf{k}_0$ (typically a high-symmetry point) and iterate over the sample grid δ_j . For each shift, the Bloch eigenproblem is solved to compile eigenvalues and eigenvectors for both the retained and remote bands, allowing us to extract all necessary operator matrix elements. The result is a complete tabulation of effective Hamiltonian coefficients over one period of the registry. Because this tabulation is independent of the twist angle, it forms a *universal master map*: once computed, it can be reused for any moire geometry by simply evaluating along the appropriate registry path.

While conceptually simple, the data demands of this sweep are severe. The solver must deliver far more than basic eigenfrequencies; it must supply the full eigenvectors, explicit operator matrices, and their variations. This includes $\mathbf{k}$ -derivatives for velocities and mass tensors, as well as registry derivatives for Berry connections and Born-Huang terms. Because these quantities involve matrix elements coupling the retained P -space to the remote Q -space, the solver must compute many more bands than are ultimately retained. In practice, retaining $N = 4$ bands often requires solving for 16 or more total bands at each of the thousands of registry points. Generating this massive dataset of eigenfrequencies, eigenvectors, derivatives, and cross-subspace couplings on a dense grid is a formidable numerical task that heavily dictates the choice of the underlying wave solver.

3.8.1 The Solver Landscape and Next Steps

The registry sweep demands two things simultaneously: *data transparency* (access to eigenvectors, the explicit operator matrix, and derived matrix elements) and *throughput* (thousands of solves in reasonable time). These requirements interact badly with existing tools.

MPB [25] is the standard open-source plane-wave solver for photonic crystals. It is fast, well-tested, and freely available. However, MPB uses iterative, matrix-free techniques tied to its internal data structures. It does not build or expose the explicit operator matrix. Extracting off-diagonal velocity matrix elements or cross-subspace couplings would require workarounds that are either numerically fragile or architecturally impractical. Each solve also carries MPB’s well-known geometry-setup overhead that penalizes the rapid-fire regime of thousands of registry samples.

Legume [38] takes the opposite approach: it builds the photonic operator explicitly in a plane-wave basis and exposes it as a dense array. In principle, we could extract every required matrix element from Legume. The difficulty is throughput. Legume is written in Python with NumPy backends, and dense diagonalization scales as $O(N_{\text{pw}}^3)$. At the resolutions needed for remote bands ($N_{\text{pw}} \approx 1000\text{--}4000$), each solve is slow, and doing thousands in an interpreted language becomes prohibitive.

Real-space methods (FDFD, FEM) discretize on spatial grids. They are flexible for complex geometries but suffer from numerical dispersion at high frequencies and lack native analytic k -derivatives.

In short: MPB gives fast solves but the wrong data; Legume gives the right data but too slowly. No existing open-source tool combines explicit matrix access with the throughput needed for dense registry sweeps. A sufficiently patient researcher *could* build the pipeline on top of Legume, or even modify MPB's C/Fortran codebase to expose its internal operators. The envelope theory does not logically require a new solver. But the practical distance between *possible in principle* and *feasible in practice* turned out to be wide enough to justify a purpose-built tool: a plane-wave eigensolver designed from the start around the specific extraction problem posed by the envelope pipeline. The next section describes this tool.

4 Blaze2D: A Custom Plane-Wave Solver

The previous section ended at a practical bottleneck: the envelope approximation requires not just eigenvalues, but solved local Bloch problems together with eigenvectors, operator matrix elements, and derived couplings, repeated over a dense grid of moire registries. This is not a one-off band-structure calculation but a high-throughput extraction problem. The solver feeding the pipeline must therefore be accurate, expose Bloch-level data explicitly, and sustain thousands of solves across slightly varying crystal configurations. Existing tools satisfy these requirements only partially. A dedicated solver was therefore built to close this gap.



Figure 23:
Blaze2D logo.

Blaze2D is a two-dimensional plane-wave expansion (PWE) eigensolver written in Rust, designed specifically to produce the local Bloch data processed by the envelope framework. It was developed as part of this thesis and forms a central technical component of the presented workflow. Blaze2D is open-source ( GitHub [39]) and published as a Python package ( PyPI [40]). The individual components, plane-wave discretization of Maxwell's equations, iterative eigensolvers, and subpixel smoothing are well established [25,41]. The novelty lies in their assembly: a solver optimized end-to-end for sweeping over many crystal configurations at moderate resolution, with mixed-precision arithmetic and native multithreading, while exposing exactly the Bloch-level data that the envelope theory needs.

4.1 Design Choices

Three foundational choices were made from the start, each driven by a concrete requirement of the envelope pipeline.

Method: plane-wave expansion. The PWE method discretizes the Bloch eigenproblem in reciprocal space by expanding both the dielectric function and the field in Fourier modes on the reciprocal lattice. For a given $\mathbf{k}$ -point and resolution (number of retained plane waves N_{pw}), the problem becomes a dense $N_{\text{pw}} \times N_{\text{pw}}$ matrix eigenproblem. The reason for choosing PWE over real-space methods is direct: the envelope framework requires not just eigenvalues but Bloch functions and their Fourier coefficients, and the PWE basis delivers these natively. Additionally, PWE eigenvalues converge spectrally with resolution, providing high accuracy at moderate grid sizes [25].

Algorithm: LOBPCG. The locally optimal block preconditioned conjugate gradient (LOBPCG) method [41] solves for the lowest eigenpairs of a Hermitian operator without forming or factorizing the full matrix. It is iterative, works in blocks (solving for several eigenpairs simultaneously), and accepts a preconditioner. These properties make it the natural choice for the photonic PWE problem, where only the lowest bands are needed and a good preconditioner is available. MPB uses the same algorithmic family [25].

Language: Rust. The solver must run millions of operator applications across thousands of crystal configurations. Rust provides predictable memory layout, no garbage-collection pauses, and safe concurrency. These properties matter once the solver runs inside a tight parameter-sweep loop. The compiled performance is comparable to C/Fortran, while the type system eliminates entire classes of memory bugs that would otherwise surface only under heavy workloads.

4.2 Geometry and the Permittivity Matrix

The first module to build is the *geometry*: translating a crystal specification (lattice vectors, shapes, dielectric constants) into the Fourier-space permittivity matrix $\varepsilon_{\mathbf{G},\mathbf{G}'}$ processed by the PWE operators.

Blaze2D uses the same analytical subpixel smoothing as MPB. Rather than sampling $\varepsilon(\mathbf{x})$ on a pixel grid, each geometric primitive (cylinder, ellipse, block) is treated as an exact shape whose overlap with every grid cell is computed analytically. The smoothed ε^{-1} is then obtained via the anisotropic averaging procedure of Farjadpour *et al.* [42], which avoids the staircasing artifacts that naive pixelization introduces at dielectric interfaces.

Validating this module is straightforward: the permittivity matrix can be compared element-by-element against MPB for any crystal geometry. Figure 24 shows such a comparison for a square lattice of dielectric rods ($\varepsilon = 8.9$, $r = 0.45a$) at resolutions $N = 8$ to 128. Only the coarsest grid ($N = 8$) exhibits appreciable error (mean

$|\Delta\varepsilon| \approx 3 \times 10^{-2}$, peak ≈ 0.68); for $N \geq 16$ the mean error drops below 8×10^{-3} and reaches $\approx 5 \times 10^{-4}$ at $N = 128$. The remaining residual peaks of order 0.1–0.2 are localized at the rod–air interface, where the two solvers discretize the material boundary slightly differently. Agreement to this level at every resolution confirms that the geometry pipeline is correct before any eigensolve is attempted.

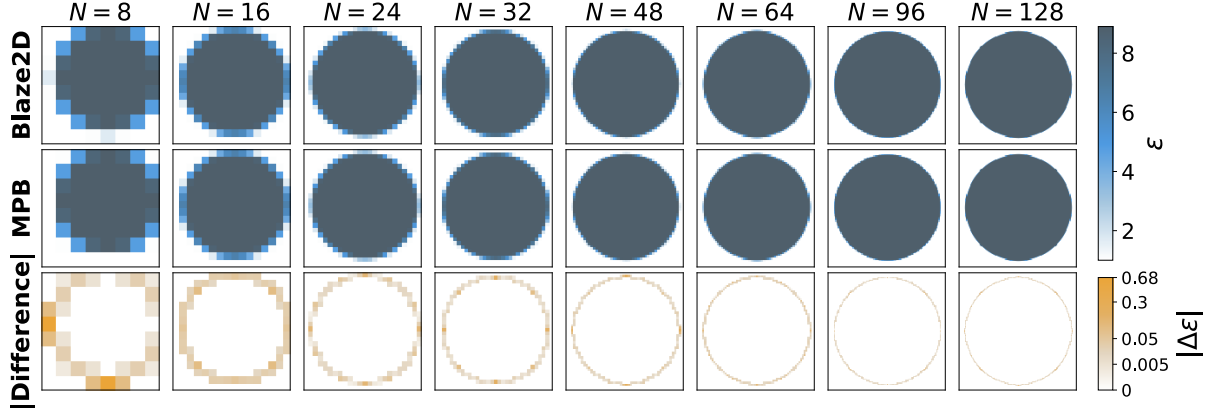


Figure 24: Smoothed permittivity maps from Blaze2D and MPB at resolutions $N = 8$ to 128, with the bottom row showing the absolute difference $|\Delta\varepsilon|$ on a power-law color scale ($\gamma = 0.3$) to magnify small discrepancies.

With the geometry validated, the remaining task is a spectral analysis: construct the TE and TM operators on a Fourier basis and solve them efficiently.

4.3 Eigenvalue Operators and Their Application

With the permittivity matrix in hand, the next step is to discretize the eigenvalue operators from Equation 3 and Equation 4 explicitly. In contrast to MPB, which works from the full curl–curl operator and projects onto the relevant polarization, Blaze2D implements the TE and TM operators directly:

$$\begin{aligned} \text{TE : } A_{\text{TE}} &= -(\mathbf{k} + \mathbf{G}) \cdot [\varepsilon^{-1}]_{\mathbf{G}, \mathbf{G}'} (\mathbf{k} + \mathbf{G}'), & B_{\text{TE}} &= \mathbb{1} \\ \text{TM : } A_{\text{TM}} &= |\mathbf{k} + \mathbf{G}|^2 \delta_{\mathbf{G}, \mathbf{G}'}, & B_{\text{TM}} &= \varepsilon_{\mathbf{G}, \mathbf{G}'} \end{aligned} \quad (81)$$

The operator classes are implemented generically: the LOBPCG solver receives an abstract operator interface, making the TE and TM cases interchangeable at the API level.

Operator application proceeds in the standard PWE fashion. Multiplication by ε^{-1} in reciprocal space is a dense matrix–vector product, while the gradient terms $(\mathbf{k} + \mathbf{G})$ act as diagonal multiplications. In practice, these operations dominate the runtime and their memory-access pattern determines performance.

At high dielectric contrast, the Fourier coefficients of ε^{-1} decay slowly, and individual reciprocal-space components can develop large magnitudes that amplify numerical noise. Blaze2D applies the same clamping and regularization strategy as MPB to suppress these artifacts without distorting the physically relevant low-frequency content. This direct TE/TM implementation is also what makes the data extraction convenient: the same operator objects used in the eigensolve can later be reused to expose explicit matrix elements to the envelope pipeline.

4.4 Preconditioning

The convergence rate of LOBPCG depends critically on the preconditioner. Each polarization admits a different strategy.

For TE, the preconditioner is the one described in Ref. [25]: an approximation to A_{TE}^{-1} built from the diagonal kinetic term $(|\mathbf{k} + \mathbf{G}|^2)$ and a scalar estimate of ε^{-1} . This is the same advanced preconditioner used by MPB and is the more complex of the two.

For TM, the structure is simpler. Because A_{TM} is already diagonal in the plane-wave basis, its inverse is trivially available and serves as an effective preconditioner. The result is that TM consistently achieves lower condition numbers and converges in fewer iterations than TE, a systematic advantage rooted in operator structure.

Tuning the preconditioner accounted for roughly a quarter of the total development time. The MPB developers describe the same challenge: finding a good preconditioner “is something of a *black art* with lots of trial and error”¹ [25]. Because Blaze2D’s internal operator layout differs from MPB’s, the preconditioner could not be ported directly; it had to be re-derived and re-tuned against condition-number measurements at each stage.

4.5 The LOBPCG Solver

At the heart of Blaze2D lies the LOBPCG algorithm [41]. At each step, the solver maintains three subspaces: the current eigenvector candidates X (N_{band} vectors), the search directions P from the previous step, and the preconditioned residuals W . These are assembled into a trial basis $[X, P, W]$, and a small dense eigenproblem (the Rayleigh–Ritz projection) of dimension $\dim(X) + \dim(P) + \dim(W)$ is solved exactly. The new X is read off from the lowest eigenpairs of this projected problem. The structure of this search subspace is sketched in Figure 25.

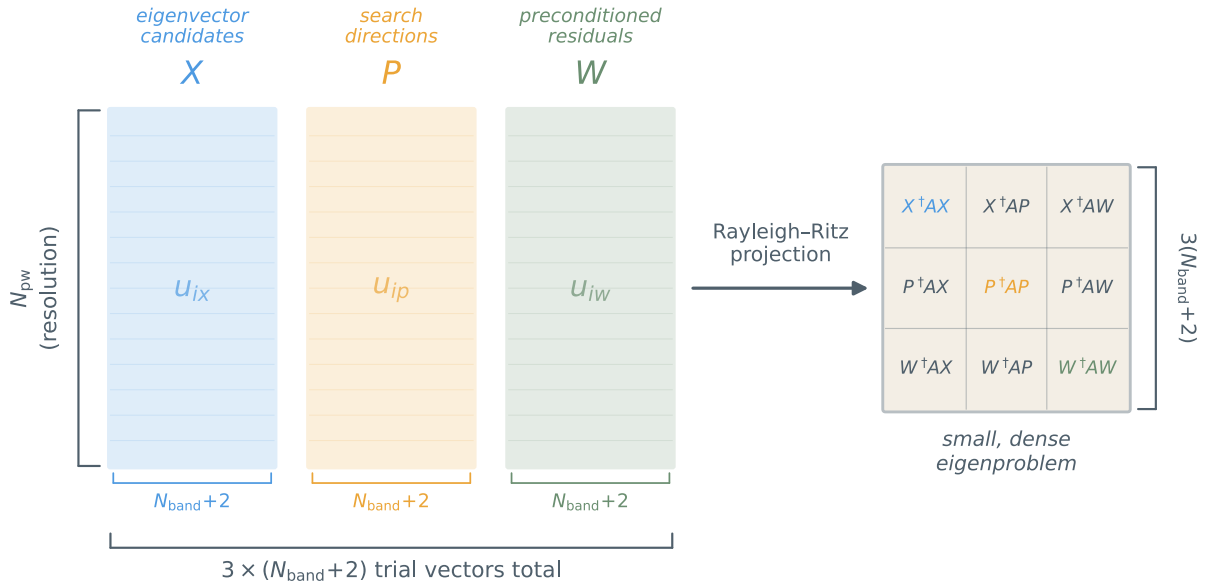


Figure 25: Structure of the LOBPCG search subspace. The trial basis $[X, P, W]$ defines a small, dense projected eigenproblem whose exact solution yields the updated eigenvector approximations. Rather than operating in the full N_{pw} -dimensional Hilbert space, each iteration works in a subspace of dimension $\dim(X) + \dim(P) + \dim(W)$.

Several implementation details proved decisive for performance and stability:

Subspace dimensions. Expanding the candidate space beyond the number of requested bands accelerates convergence significantly: adding one or two extra trial vectors to X provides the optimizer with additional variational freedom at modest cost. Conversely, shrinking or omitting either P or W degrades convergence severely. The best results were achieved when all three subspaces had roughly comparable dimensions.

Orthogonalization. Near-degenerate eigenvectors cause classical Gram–Schmidt orthogonalization to lose numerical rank, producing a singular Rayleigh–Ritz problem. Blaze2D uses the SVQB procedure [43], which orthogonalizes via a singular-value decomposition of the Gram matrix and is numerically stable even for tightly clustered eigenvalues.

Convergence criterion. MPB monitors the residual norm $\|Ax - \lambda Bx\|$ and declares convergence when it falls below a threshold (default 10^{-7}). Blaze2D instead monitors the relative change in eigenvalues between iterations. In practice, eigenvalues stabilize well before the residual reaches a tight tolerance, so eigenvalue-based convergence requires substantially fewer iterations per solve. While residual convergence carries a proven convergence-rate guarantee [41], eigenvalue convergence proved completely stable across all tested configurations, including difficult cases with accidental degeneracies at high-symmetry k -points.

¹From the MPB developer documentation, Developer Information: The Mathematics of MPB.

Warm-starting. The single largest lever for performance is also the simplest: initializing each $\mathbf{k}$ -point solve with the converged eigenvectors of the previous $\mathbf{k}$ -point. This adds no algorithmic complexity, yet it typically reduces the iteration count by an order of magnitude compared to a random initialization. MPB uses the same strategy.

Deflation strategy. Once a band converges, the solver must avoid rediscovering it. Because distinct Bloch modes are mathematically orthogonal, we can explicitly project all new search directions away from the already-converged states, a technique known as deflation. While solvers can *hard-lock* these converged bands by removing them from the active problem entirely, Blaze2D relies on *soft-locking*. Converged bands remain part of the small Rayleigh-Ritz projection, but the solver stops calculating new, computationally expensive search directions for them. This halts their active optimization, yet allows the converged states to mix with the active subspace to maintain strict orthogonality as the remaining bands settle. In practice, soft-locking proved far more numerically stable than hard-locking, especially near accidental degeneracies where bands must be handled carefully as a collective cluster rather than frozen one by one.

4.6 Mixed Precision

Modern eigensolvers are not compute-bound but memory-bandwidth-bound. Profiling both MPB and Blaze2D shows that actual floating-point arithmetic accounts for as little as 10% of CPU time; the remainder is spent moving data between memory and cache. This observation motivates a mixed-precision strategy: store all large arrays (eigenvectors, operator matrices, intermediate products) in single precision (f32) to halve the memory traffic, but promote to double precision (f64) on the fly for numerically sensitive operations (inner products, Rayleigh-Ritz projections, and orthogonalization steps) before rounding the result back to f32 for storage.

The natural objection is: if the result is rounded back to f32, what is gained by computing in f64? The answer is that certain intermediate accumulations require f64 for numerical stability (a dot product of 10^4 terms, for instance, can lose several significant digits in f32), while the *result* of that dot product (a single scalar or a small matrix) is representable in f32 without meaningful loss. The precision is needed transiently, not persistently.

This mixed-precision approach yields a nearly clean $2 \times$ speedup with no significant loss in eigenvalue accuracy. The same conclusion was reached independently in a 2023 study of mixed-precision LOBPCG for electronic-structure calculations [44], a paper discovered only after the approach had already been implemented in Blaze2D. The strategy itself is standard in modern data science and high-performance computing.

4.7 Validation

Blaze2D was validated against MPB across a representative set of two-dimensional photonic crystals by comparing full band diagrams, $|\mathbf{u}|^2$ mode profiles, and convergence behavior. The validation process was the most time-consuming part of the project. MPB uses several nonstandard coordinate conventions, most notably a half-pixel-shifted grid center, which produced false discrepancies that had to be identified and accounted for one by one.

The validation narrative follows the same logic as the solver itself. First, the global spectral output must agree. Second, the eigenvectors must represent the same physical modes. Third, both solvers must converge in the same way as the discretization is refined. The following subsections address these three checks in turn.

4.7.1 Band-Diagram Agreement

The primary metric is the relative eigenvalue error across all $\mathbf{k}$ -points and bands. Bloch-function phases were not compared directly, because MPB's phase conventions differ from Blaze2D's in ways that scramble the complex phases without affecting physically observable quantities. However, the squared modulus $|u_{n\mathbf{k}}(\mathbf{r})|^2$ was compared and found to agree, and improvements in mode-profile agreement tracked improvements in eigenvalue accuracy, confirming that the band diagram is a sufficient validation metric.

One systematic difference remains: when tracking bands across avoided crossings, MPB tends to follow a given band adiabatically to higher eigenvalues, while Blaze2D reports the true N lowest eigenvalues at each $\mathbf{k}$ -point and does not track crossings. For isolated bands away from topmost-band crossings, both solvers agree to high precision. This behavior is visible in Figure 26.

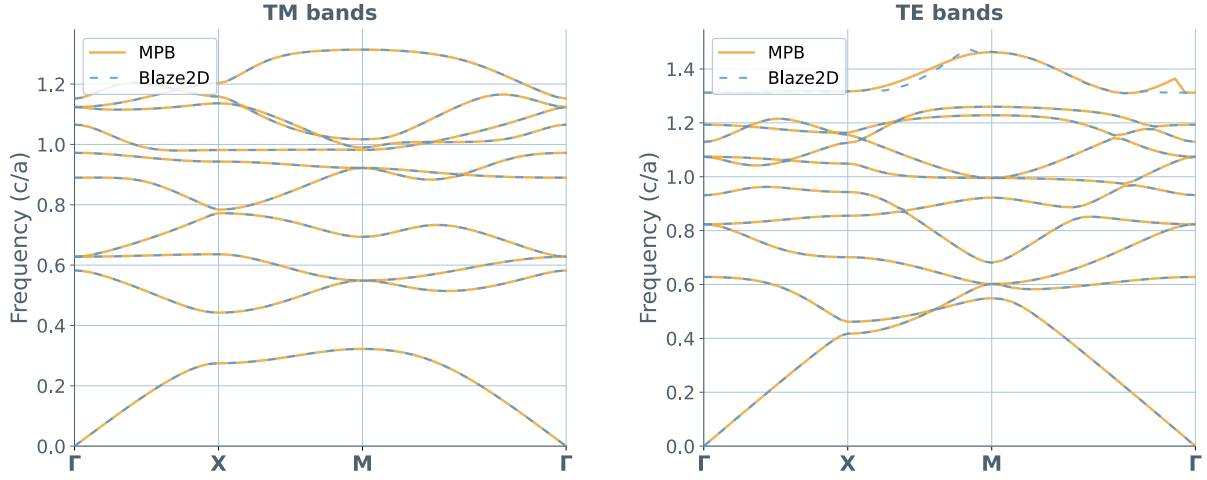


Figure 26: Band-diagram comparison for a square lattice ($\epsilon = 8.9$ rods, $r = 0.2a$), showing the 10 lowest bands. **Left:** TM polarization; **right:** TE polarization. Both solvers show near-perfect agreement, with small deviations visible only in the topmost TE band due to differing band-tracking behavior across avoided crossings.

To quantify the agreement beyond the visual overlap of Figure 26, Figure 27 shows the RMS relative eigenvalue difference between the two solvers for the lowest eight bands, evaluated over 61 k -points along $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$, as a function of resolution. At $N = 128$, relative differences reach $\approx 2 \times 10^{-5}$ on average, with per-band maxima below 10^{-4} . This is consistent with Blaze2D’s internal eigenvalue convergence tolerance of 10^{-5} in mixed-precision mode; the residual plateau beyond $N \approx 48$ reflects that tolerance floor rather than a systematic discrepancy between the two solvers.

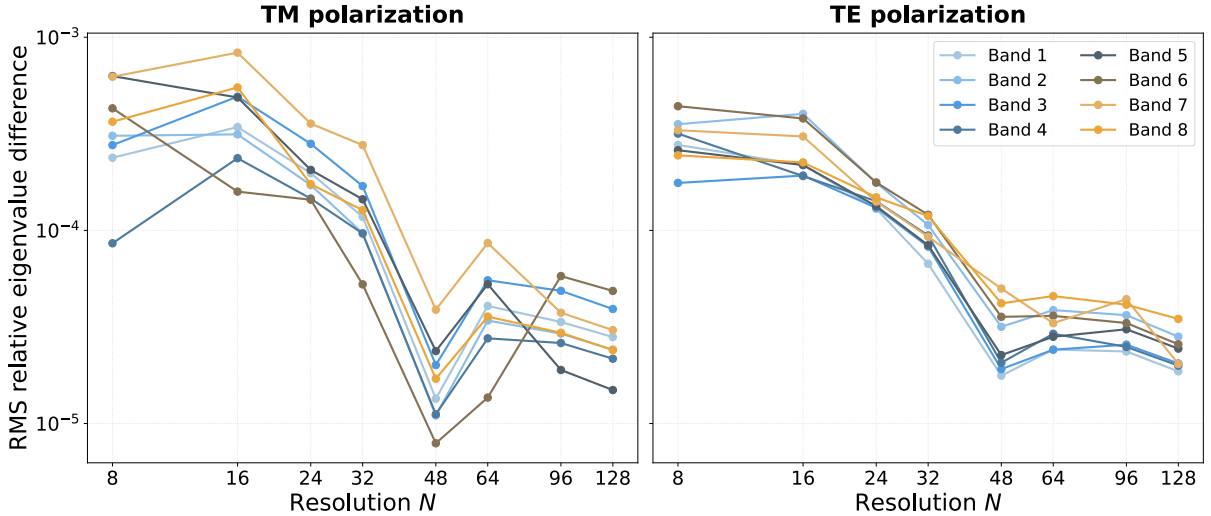


Figure 27: RMS relative eigenvalue difference between Blaze2D and MPB for the eight lowest bands of a square lattice ($\epsilon = 8.9$ rods, $r = 0.2a$). TM (left) and TE (right) polarizations.

Taken together, Figure 26 and Figure 27 establish a precise agreement: at the resolutions relevant for the registry sweep, Blaze2D reproduces MPB’s eigenvalues to within the mixed-precision solver tolerance.

4.7.2 Mode Profiles

Eigenvalue agreement alone is not sufficient: the envelope pipeline ultimately processes eigenvectors and matrix elements built from them. For that reason, representative real-space mode profiles were compared as well. Figure 28 shows the squared Bloch amplitude $|\mathbf{u}|^2$ for several bands and k -points.

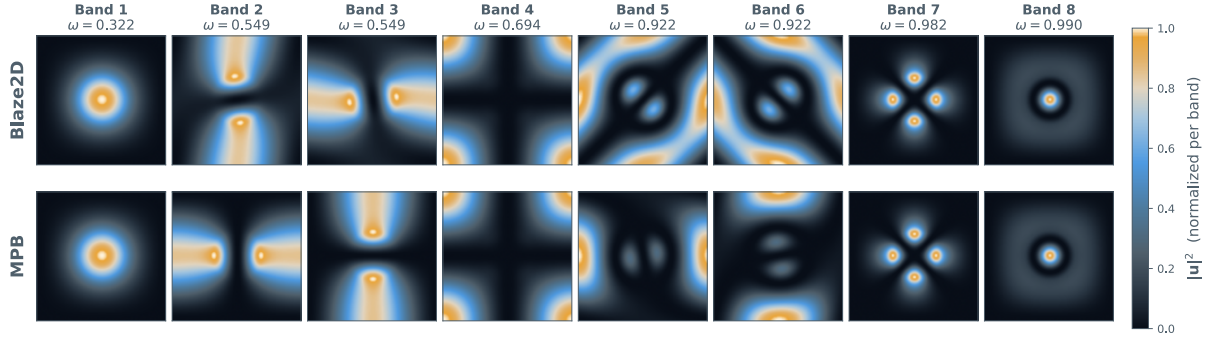


Figure 28: Comparison of $|u|^2$ mode profiles from Blaze2D and MPB for a representative set of bands, k -points and a resolution of 64 px/ a . The spatial intensity distributions agree well for non-degenerate frequencies; at degenerate frequencies, the modes may be superposed or swapped, leading to expected visual discrepancies.

The agreement is strong wherever the eigenvalue is non-degenerate: nodal structure, localization, and symmetry match visually across the unit cell. The only clearly visible mismatches occur at or near degeneracies, where any orthonormal basis of the degenerate subspace is equally valid. In those cases MPB and Blaze2D may return rotated or swapped representatives of the same physical subspace, which changes the plotted pattern without indicating a physical disagreement. This is precisely why the comparison is carried out on $|u|^2$ rather than on the complex Bloch phase itself.

Despite the strong agreement, small yet visual mismatches for bands 2 and 3 can be seen in Figure 28. The spatial modes do not appear perfectly symmetric; these are deviations from MPB that have not been investigated or quantified in this thesis. Because the envelope pipeline is built from Bloch-function data, these deviations should be kept in mind when judging how reliable the final envelope results are.

4.7.3 Convergence with Resolution

Agreement at a single resolution could still be accidental. A stronger test is whether both solvers approach the continuum limit at the same rate as the plane-wave cutoff is increased. That comparison is shown in Figure 29.

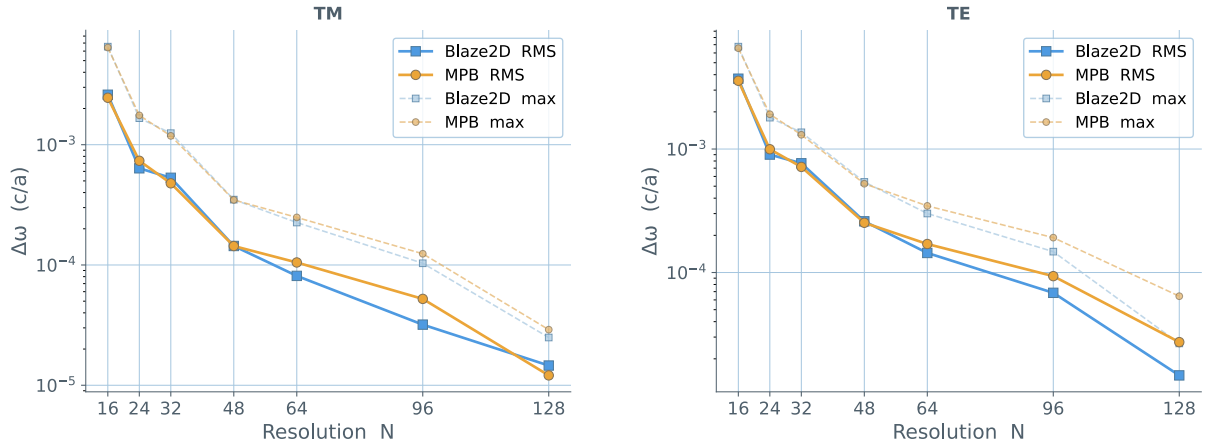


Figure 29: Eigenvalue convergence for a square lattice ($\varepsilon = 8.9$ rods, $r = 0.2a$). Solid lines: RMS deviation $\Delta\omega_{\text{RMS}}$ of the four lowest bands along $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$; dashed lines: worst-case deviation $\max|\Delta\omega|$. All deviations are measured against a higher resolution $N = 192$ reference. Both solvers converge at comparable rates.

The two curves track each other closely in both polarizations, for both RMS and worst-case errors. This matters because it rules out a hidden cancellation in the direct MPB comparison: Blaze2D does not merely match one reference calculation, but exhibits the same resolution dependence as an established solver. For the purposes of the envelope pipeline, this is the relevant notion of correctness, since all extracted matrix elements are ultimately built on these converged Bloch states.

4.8 Benchmarks

Accuracy alone would not justify a new solver. The point of Blaze2D is that it must also execute the dense registry sweep from Section 3.8 in reasonable time. The runtime comparison is shown in Figure 30, while the iteration counts, per-iteration costs, and memory footprint are broken down in Figure 31.

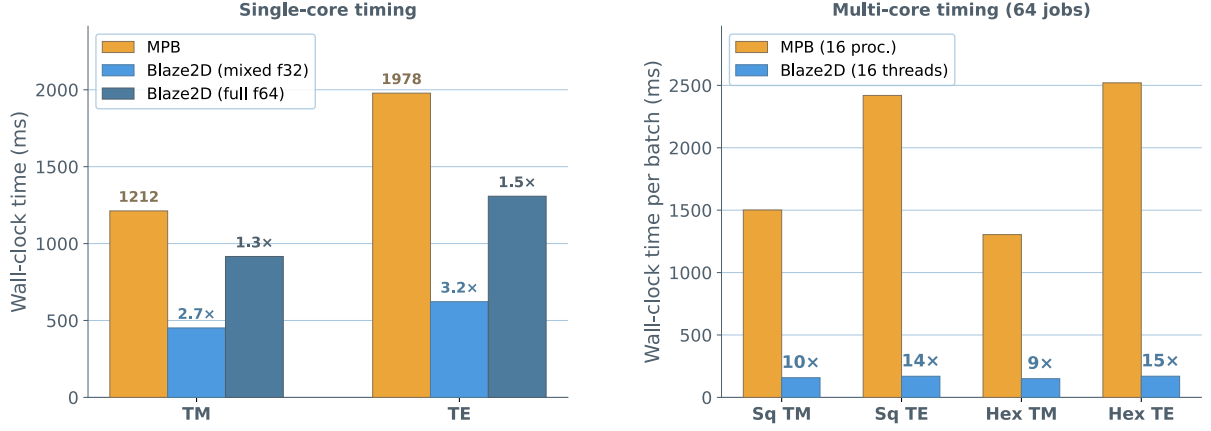


Figure 30: Single-core and multi-core wall-clock comparison of MPB and Blaze2D in mixed and full precision.

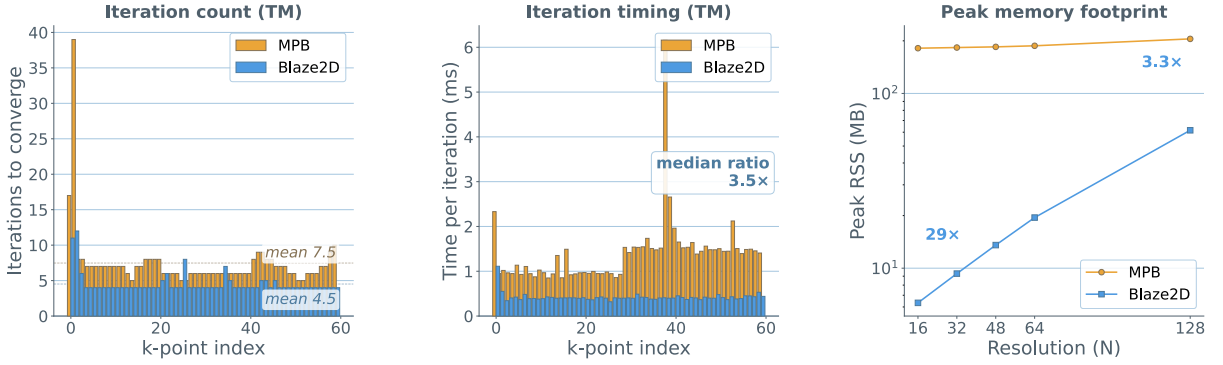


Figure 31: Iteration count per k -point, time per iteration, and peak memory footprint for MPB vs. Blaze2D.

A few observations from these benchmarks deserve comment. The TM polarization converges in fewer iterations than TE for both solvers, consistent with the simpler preconditioner structure discussed above. Mixed precision does not increase the iteration count; the eigenvalue trajectory is indistinguishable from the full-precision run. The speedup seen in Figure 30 therefore comes almost entirely from reduced memory traffic rather than from altered convergence behavior.

The decomposition in Figure 31 makes this interpretation more concrete. Time per iteration falls under mixed precision, while memory consumption scales predictably with N_{pw}^2 for the stored matrices and $N_{pw} \times N_{band}$ for the eigenvector block, with f32 storage halving both contributions relative to f64. For the registry sweep, this reduction matters twice: it shortens each individual solve and increases the number of configurations that can be processed concurrently.

4.9 From Solver to Pipeline

With the eigensolver validated, the remaining task is to extract the matrix elements required by the envelope effective Hamiltonian and export them to the Python layer where the moire-scale problem is assembled and solved.

The extraction module computes, for each crystal configuration δ on the moire grid, the local eigenvalues $\lambda_{n(\delta, \mathbf{k}_0)}$, the Bloch functions $u_{n\mathbf{k}_0}(\mathbf{r}; \delta)$, and the derived operator matrix elements (Berry connections, effective-mass tensors, and the coupling terms entering the effective Hamiltonian of Section 3). These are written as structured arrays and exposed through Python bindings generated via Rust's foreign-function interface.

Basic sanity checks on the extracted data (Hermiticity of the effective Hamiltonian blocks, expected magnitudes of the Berry-connection components, correct symmetry under lattice operations) confirm that the plumbing

between solver and pipeline introduces no artifacts. At this point the narrative closes back onto the envelope construction: the effective theory derived in the previous section has been reduced to computable local data, and Blaze2D is the tool that provides it. The moire-grid solver that processes this data is the subject of the next section.

5 The Envelope Framework in Practice

The preceding chapters developed two components in parallel: a multiband envelope approximation that reduces the photonic moire eigenproblem to a set of moire-scale envelope equations (Section 3), and a purpose-built plane-wave eigensolver, Blaze2D, designed to extract the local Bloch data that this approximation requires (Section 4). With both tools in hand, we can now assemble and solve concrete moire systems. But running the pipeline is only the beginning: we must also ask whether its results are trustworthy, how they compare against independent references, and what physical content they carry. This section addresses all three questions in a single narrative. We begin by walking through the EA pipeline itself, then establish independent reference solvers, compare their outputs, probe internal consistency, and finally turn to the physics that the framework is explicitly built to reveal.

5.1 The Envelope Approximation Pipeline

The envelope approximation translates the continuous two-scale theory of Section 3 into a concrete computational pipeline. The key structural insight is that this pipeline splits cleanly into two phases with very different roles and computational profiles.

5.1.1 Phase 1: Building the Effective Hamiltonian

Phase 1 performs the *registry sweep* introduced in Section 3.8. Blaze2D solves the local Bloch eigenproblem (Equation 23) at the chosen carrier momentum $\mathbf{k}_0$ for every registry point δ on a discrete grid covering one period of the registry torus. At each point, the solver extracts the full set of ingredients that enter the effective Hamiltonian Equation 61: the local band energies $\Lambda_{mn} = \lambda_n \delta_{mn}$ (Equation 43), the interband velocity matrices $v_{mn}^{(i)}$ (Equation 46), the Löwdin-corrected inverse mass tensor M_{ij}^{-1} (Equation 58), the non-Abelian Berry connection A_i (Equation 52), the Born-Huang leakage potential U_{BH} (Equation 60), and the slow-coefficient corrections arising from $\partial_{R_j} \varepsilon^{-1}$ (Equation 22). These form the layers of a multiband data structure defined on the registry grid.

All ingredients share the same spatial domain: they are scalar or matrix fields over the registry torus $\delta \in \mathbb{R}^2/\Lambda$. Because the registry map $\delta(\mathbf{R})$ (Equation 11) is fully determined by the lattice geometry and does not involve the twist angle, the entire Phase 1 output is *twist-angle invariant*. The registry sweep depends only on the crystal configuration (lattice type, ε , r/a , polarisation) and the expansion momentum $\mathbf{k}_0$. Once computed, this *universal master map* can be reused for any twist angle: only Phase 2, which introduces the moire momentum scaling $\eta = a/L$, needs to know θ . This separation is a major computational advantage, because the registry sweep, which requires solving thousands of local Bloch problems with full eigenvector extraction, is by far the more expensive phase.

The Hamiltonian ingredients can be visualised as a stack of scalar and tensor fields defined over the registry grid of the moire unit cell. Figure 32 shows this stack for a 7×7 registry sweep.

To verify that the extraction pipeline produces mathematically sound ingredients, we examine four configurations: the lowest TE and TM bands for a square lattice of rods at the M point, and for a hexagonal lattice of holes at the K corner of the zone. For each case, we sweep over a 7×7 grid of local registries δ , directly assembling the ingredients via Blaze2D at a resolution of $48 \text{ px}/a$.

Across all 7×7 registry sweeps and the four test configurations, the core iterative solver achieves a perfect 100% convergence rate. The resulting matrix fields, principally the local connection W and the inverse mass tensor M , satisfy hermiticity to the iterative machine-precision limit: the maximum non-Hermitian residuals are bounded below 10^{-9} for TE fields and are exact floating-point zeros for the diagonal TM blocks.

The moire envelope Hamiltonian combines field contributions of varying derivative order: the local potential (λ), the group velocity ($\mathbf{v} \cdot \mathbf{D}$), the kinetic energy ($\mathbf{D}^\dagger M \mathbf{D}$), and the Born-Huang potential. To verify that all scales interact appropriately, Figure 33 compares their relative geometric strengths at a representative moire envelope wavevector $q_{\text{ref}} = 0.1 \times 2\pi/a$.

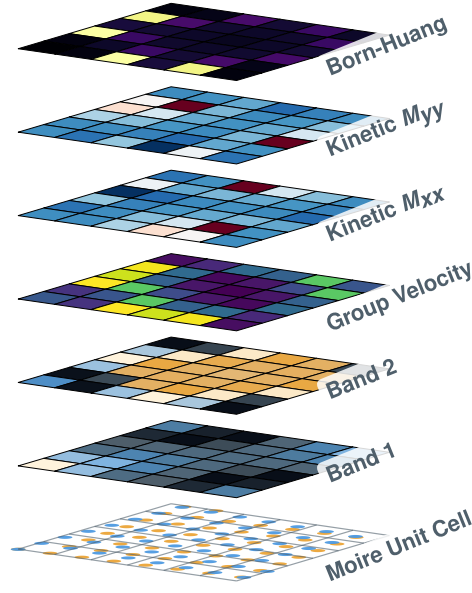


Figure 32: Conceptual layout of the 7×7 mathematical ingredients mapped across the local moire unit cell sub-registries.

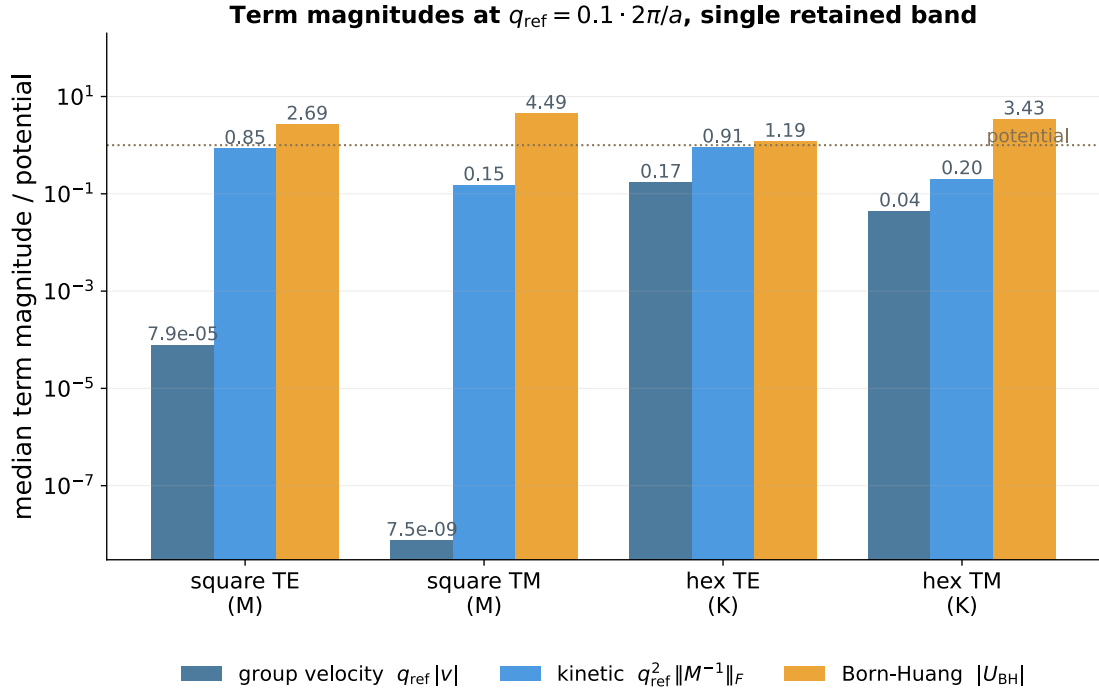


Figure 33: Median magnitudes over the registry grid of the effective-Hamiltonian terms evaluated at a characteristic moire momentum $q_{\text{ref}} = 0.1 \times 2\pi/a$, normalized to the local potential λ , for a single retained band. Square rods at M (TE, TM) and hexagonal holes at K (TE, TM); the K carrier is the zone corner $(2/3, 1/3)$.

The observed magnitudes align with the underlying symmetries. At the M point of the square lattice a single band sits at a time-reversal-symmetric extremum for every registry, so the local group velocity vanishes; the extracted data show the velocity term suppressed by four to seven orders of magnitude. At the K corner of the hexagonal lattice the picture depends on the registry. In the aligned configuration the lowest TE band is non-degenerate and its velocity vanishes by the three-fold symmetry, while the lowest TM band is degenerate with the next one, so a single-band description there is marginal; at generic registries the shift breaks the three-fold

symmetry and a single band acquires a first-order slope, which is what the medians report (17 % of the potential for TE, 4 % for TM). The Born-Huang term outweighs the kinetic term in every configuration and exceeds the potential itself in three of four; the geometric terms of the effective Hamiltonian are not corrections but leading contributions.

5.1.2 Phase 2: Solving the Envelope Eigenproblem

With the effective Hamiltonian ingredients tabulated, Phase 2 assembles and solves the moire-scale eigenproblem. This is where the twist angle finally enters: the scale-separation parameter $\eta = \frac{a}{L}$ sets the physical moire period L and thereby fixes the momentum scaling of the derivative operators $\Pi_i = -i\mathcal{D}_i$ (Equation 53) that appear in the first- and second-order terms of the effective Hamiltonian Equation 61.

Concretely, Phase 2 begins by mapping the Phase 1 registry data onto a moire-scale grid in fractional coordinates $\mathbf{s} \in [0, 1)^2$. The covariant slow derivatives are discretized using finite differences with Bloch-periodic boundary conditions, and the Cartesian velocity and mass-tensor data from Phase 1 are transformed into the moire fractional-coordinate basis through the moire lattice matrix $B = [\mathbf{L}_1 \mid \mathbf{L}_2]$. The resulting sparse $N_s N_b \times N_s N_b$ Hermitian matrix (where N_s is the number of moire grid points and N_b the number of retained bands) is solved by shift-invert Lanczos iteration (SciPy's eigsh) centred on a target eigenvalue σ .

The choice of σ deserves emphasis. The envelope approximation is a local expansion around the carrier momentum $\mathbf{k}_0$, and its effective Hamiltonian is most reliable for eigenvalues near the local band energies $\lambda_n(\mathbf{R}; \mathbf{k}_0)$. Like a Taylor polynomial that diverges far from its expansion point, the EA loses fidelity for eigenfrequencies that lie far from the target manifold. The natural choice is therefore to centre σ within the spectral range of the diagonal potential Λ , typically at the mean or median of the local band energies across the moire cell. Modes found near this target are the most trustworthy; modes at the spectral periphery should be treated with increasing caution.

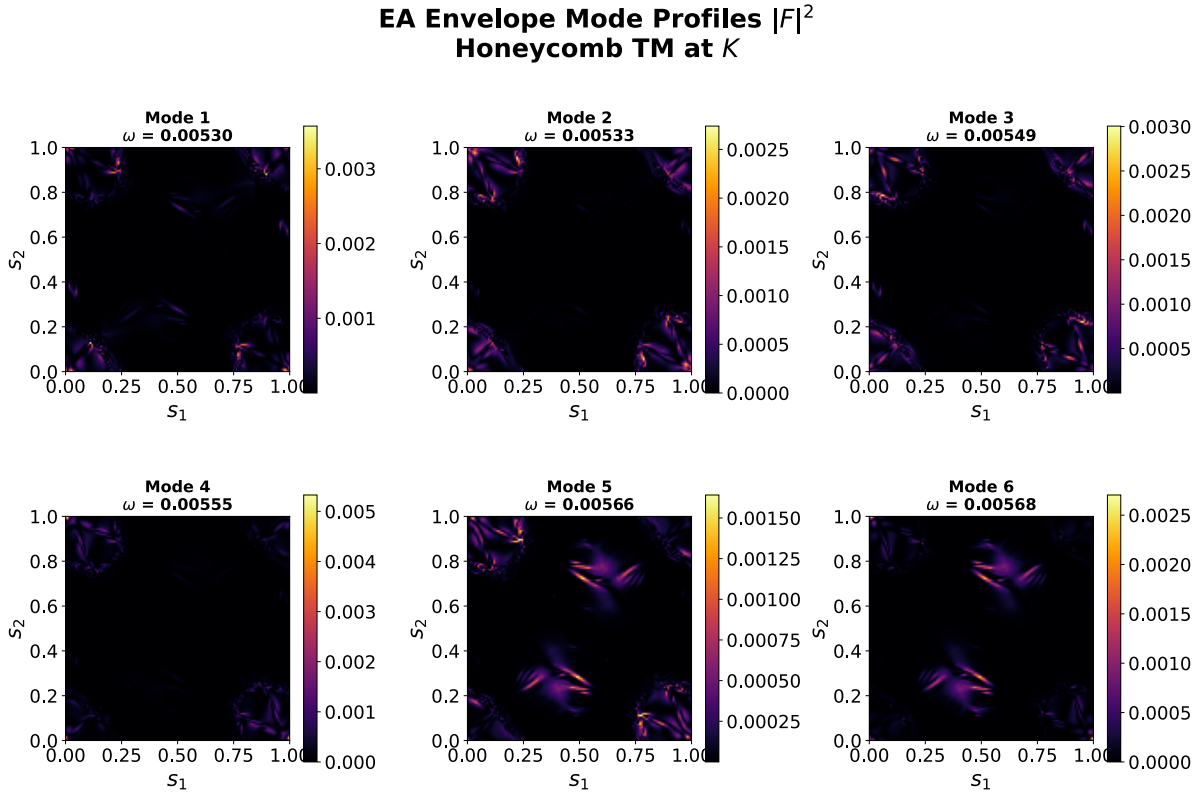


Figure 34: EA envelope mode profiles for a representative moire configuration, demonstrating that the pipeline produces physically plausible moire-scale eigenstates with well-defined nodal structure.

5.2 The Need for Independent Validation

The pipeline produces eigenfrequencies, envelope mode profiles, and moire-scale band structures. But a natural question arises: how do we know any of this is correct? We can inspect the internal data for plausibility, as done

above, but internal checks alone cannot tell us whether the results are generally well-behaved or whether the framework produces physically meaningful eigenvalues.

The existing photonic moire crystal literature is almost entirely concerned with *slab* geometries [10–19] (see [20] for a broader overview). In slabs, the two layers couple through evanescent fields across a finite gap, and it is this interlayer coupling that gives rise to flat bands and magic-angle phenomenology [11,13,15]. In a pure 2D photonic crystal the bilayer permittivity is simply the pointwise sum of the two layers (Equation 10), with no adjustable gap or evanescent decay. The physics is qualitatively different, and results from one setting do not transfer to the other. Some two-dimensional studies do exist [45–47], but these either use moire-inspired geometries as a single-layer unit-cell design technique or remain in the slab regime, so none of them provides a supercell eigenvalue spectrum against which the envelope approximation could be compared.

This absence of external comparison data makes it necessary to construct our own reference. The strategy is to select crystal configurations and twist angles for which independent brute-force solvers can produce reliable eigenvalues, and then to compare these eigenvalues against the envelope predictions. The two solvers available for this purpose are MPB [25], a well-established plane-wave expansion (PWE) solver, and our own finite-difference frequency-domain (FDFD) eigensolver.

5.3 Reference Solvers: MPB and FDFD

The ideal scenario would be to choose a crystal configuration and twist angle small enough for the envelope approximation to be accurate, build the corresponding commensurate moire supercell, solve it exactly with a conventional eigensolver, and compare. In practice, this is constrained from both ends.

On the *solver side*, MPB requires a resolution of at least 32–64 px/ a for reliable results. Because the number of unknowns scales as $R^2 N_{\text{cells}}$, where R is the resolution and N_{cells} the number of unit cells in the supercell, this limits MPB to commensurate angles no smaller than about 4° . That, in turn, is a regime where the two-atomic crystal approximation underlying the envelope theory begins to degrade for many crystal configurations (see Figure 18). FDFD, whose real-space discretization does not suffer from the same Fourier truncation problems as PWE, offers a complementary path: it is roughly three times more memory efficient at the same resolution and, as we will show, remains accurate even at resolutions far below what MPB requires.

On the *theory side*, the envelope approximation improves as the twist angle decreases, because the scale-separation parameter $\eta = a/L$ shrinks and longer-range moire modulations become smoother. The best regime for the approximation is therefore the worst regime for brute-force solvers, and vice versa.

To understand why this is the case, and why FDFD is a better complement to the envelope approximation than MPB, we now compare how the two solvers discretize the same eigenproblem.

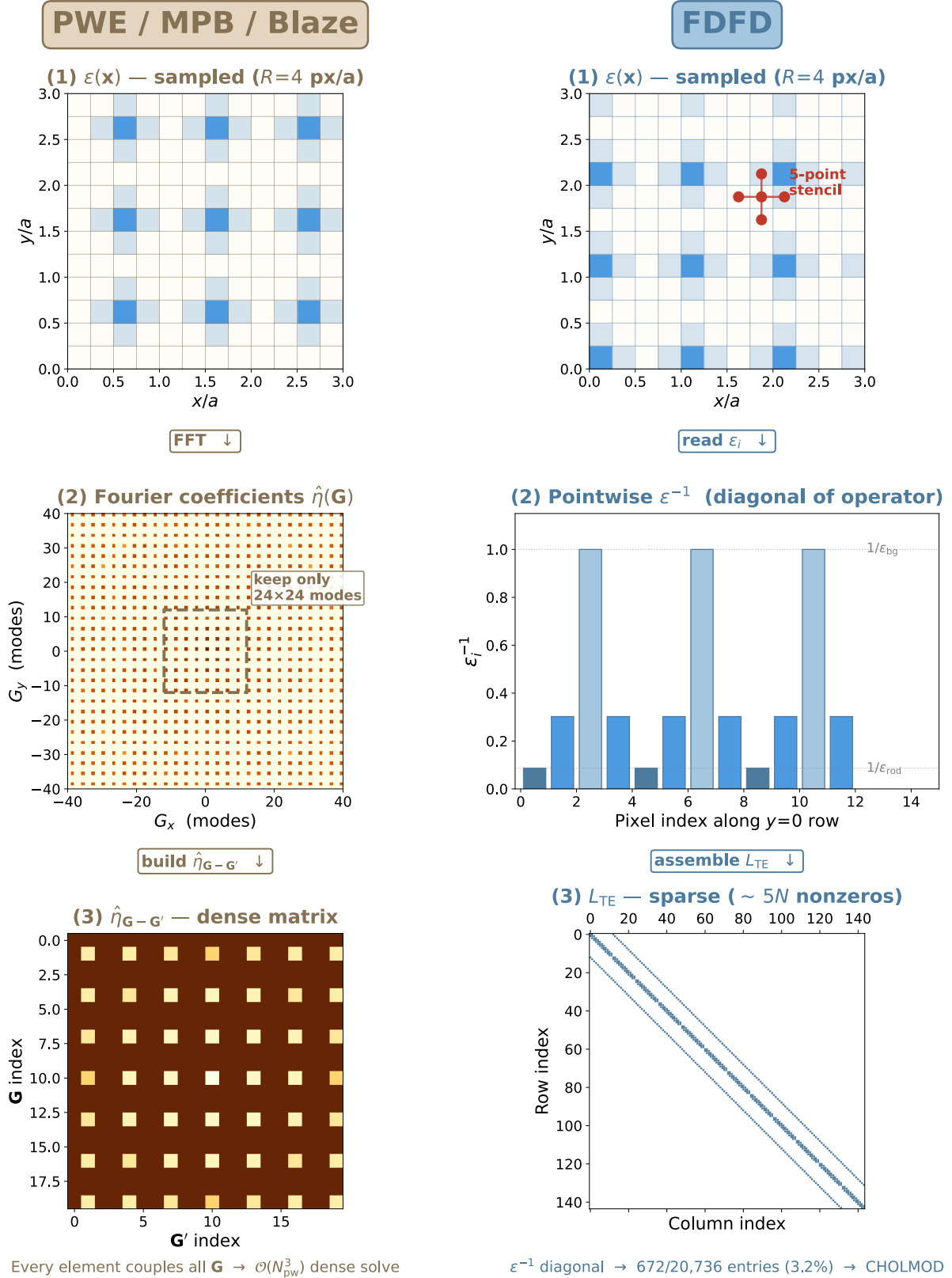


Figure 35: Side-by-side overview of the PWE (left) and FDFD (right) discretization pipelines for a 3×3 monolayer tile at $R = 4$ px/a. **Row (1):** Both methods discretize $\epsilon(x)$ on a finite grid with their own sub-pixel smoothing; the left panel shows MPB's internal ϵ grid, the right panel shows the FDFD grid. **Row (2):** PWE enters the eigenproblem through truncated Fourier coefficients $\hat{\eta}(\mathbf{G})$: only $R \cdot L/a = 4 \times 3 = 12$ modes per direction are retained ($= 24 \times 24$ two-sided), discarding everything outside the dashed box; FDFD reads ϵ^{-1} at each grid point directly (the bar chart shows the $y = 0$ row cutting through rod centres, with sub-pixel-smoothed boundary pixels at intermediate values). **Row (3):** The resulting matrix is dense ($\mathcal{O}(N_{pw}^3)$ eigensolver) for PWE vs. sparse ($\sim 5N$ nonzeros, CHOLMOD factorisation) for FDFD.

Plane-Wave Expansion (PWE / MPB). The PWE method expands the Bloch-periodic field and the inverse dielectric function in Fourier series. Writing $H_z(\mathbf{x}) = \sum_{\mathbf{G}} c_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}}$ and $\varepsilon^{-1}(\mathbf{x}) = \sum_{\mathbf{G}} \hat{\eta}_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{x}}$, the master equation becomes a matrix eigenproblem in reciprocal space:

PWE eigenproblem (TE)

$$\sum_{\mathbf{G}'} (\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}') \hat{\eta}_{\mathbf{G}-\mathbf{G}'} c_{\mathbf{G}'} = \frac{\omega^2}{c^2} c_{\mathbf{G}} \quad (82)$$

The material enters exclusively through the Fourier convolution $\hat{\eta}_{\mathbf{G}-\mathbf{G}'}$. Because the product $\varepsilon^{-1}(\mathbf{x})\nabla H_z$ is a pointwise multiplication in real space, it becomes a *convolution* in reciprocal space: every plane-wave coefficient $c_{\mathbf{G}'}$ couples to every other $c_{\mathbf{G}}$ through $\hat{\eta}_{\mathbf{G}-\mathbf{G}'}$. The matrix in Equation 82 is therefore fully dense, *regardless* of how simple or complex the material is (see Row (3) left of Figure 35).

At finite resolution R (pixels per lattice constant), the solver retains at most $\sim R^2$ plane waves per unit cell. For a supercell containing N_{cells} unit cells with side length $L = \sqrt{N_{\text{cells}}} \cdot a$, this gives $(R \cdot L/a)^2 = R^2 N_{\text{cells}}$ plane waves total; equivalently, RL/a modes per supercell side. Sharp material boundaries (e.g. rod edges) have slowly decaying Fourier coefficients, so truncation smears boundaries, distorts rod shapes, and introduces systematic errors into *every* matrix element (see Row (2) left of Figure 35). Crucially, the reconstruction is a finite sum of plane waves and therefore *smooth and continuous* in real space: the “discretization” occurs in reciprocal space (a finite set of $\mathbf{G}$ vectors), not on a real-space grid. What the eigensolver sees is a blurred, continuous approximation of ε with softened boundaries and reduced dielectric contrast, not a pixelated map.

Finite-Difference Frequency-Domain (FDFD). FDFD discretizes the *same* continuous equation on a real-space grid. Using fractional supercell coordinates $(s_1, s_2) \in [0, 1)^2$ with $\mathbf{x} = s_1 \mathbf{L}_1 + s_2 \mathbf{L}_2$, the Cartesian derivatives become $\frac{\partial}{\partial} x_i = \sum_{\alpha} (B^{-1})_{\alpha i} \frac{\partial}{\partial} s_{\alpha}$ where $B = [\mathbf{L}_1 \mid \mathbf{L}_2]$. The Laplacian is assembled from forward-difference operators D_{α}^{+} with Bloch-periodic boundaries, weighted by the contravariant metric $g^{\alpha\beta} = (B^{-1} B^{-T})_{\alpha\beta}$:

FDFD eigenproblem (TE)

$$L_{\text{TE}} = \sum_{\alpha\beta} g^{\alpha\beta} (D_{\alpha}^{+})^{\dagger} \varepsilon^{-1} D_{\beta}^{+}, \quad L_{\text{TE}} \mathbf{u} = \frac{\omega^2}{c^2} \mathbf{u} \quad (83)$$

Here ε^{-1} is a *diagonal matrix* of pointwise $1/\varepsilon$ values on the grid (see Row (2) right of Figure 35). No Fourier transform of the material is needed. Because each D_{α}^{+} is a nearest-neighbour finite-difference operator (the five-point stencil shown in Row (1) right), the product $D^{\dagger} \varepsilon^{-1} D$ couples each grid point only to itself and its immediate neighbours. The material merely *reweights* these local couplings without introducing new ones. The resulting operator L_{TE} is therefore sparse, with at most $\sim 5N$ nonzero entries for $N = R^2 \times N_{\text{cells}}$ grid points, *independent* of the material complexity (see Row (3) right of Figure 35).

Why the discretization matters. The structural difference in how ε enters each eigenproblem has direct consequences for accuracy and scalability:

- **PWE:** material enters through Fourier coefficients $\hat{\eta}_{\mathbf{G}-\mathbf{G}'}$. Sharp boundaries require many harmonics; truncation corrupts the matrix globally. Solving the dense $N_{\text{pw}} \times N_{\text{pw}}$ eigenproblem costs $\mathcal{O}(N_{\text{pw}}^3)$ in time and $\mathcal{O}(N_{\text{pw}}^2)$ in memory.
- **FDFD:** material enters as pointwise grid values ε_i^{-1} , which are spatially local and well-defined even on coarse grids via sub-pixel averaging. The sparse operator has only $\sim 5N$ nonzero entries, so storing it costs $\mathcal{O}(N)$ rather than $\mathcal{O}(N^2)$.

Because L_{TE} is sparse, symmetric, and positive-definite (after a spectral shift), it can be factored with a sparse Cholesky decomposition. We use CHOLMOD [48] for this step, which factors the shifted operator $L_{\text{TE}} - \sigma I$ once; each subsequent shift-invert iteration then reduces to a sparse triangular solve. For a 2D grid the fill-in of the Cholesky factor scales as $\mathcal{O}(N \log N)$, and the factorisation cost is $\mathcal{O}(N^{3/2})$, compared to $\mathcal{O}(N^3)$ for a dense eigensolver. At the same resolution R , both methods have $N = R^2 N_{\text{cells}}$ unknowns, but PWE must store and diagonalise a dense $N \times N$ matrix while FDFD only stores and factors a sparse one. This makes FDFD roughly

three times more memory-efficient in practice, allowing it to reach lower twist angles than MPB for the same hardware budget.

At low resolution, the PWE Fourier coefficients are badly truncated, introducing systematic errors into *every* matrix element. FDFD’s diagonal ε values, by contrast, are simply spatial averages over each pixel: physically meaningful effective-medium values at any resolution. Figure 36 and Figure 37 illustrate this difference directly.

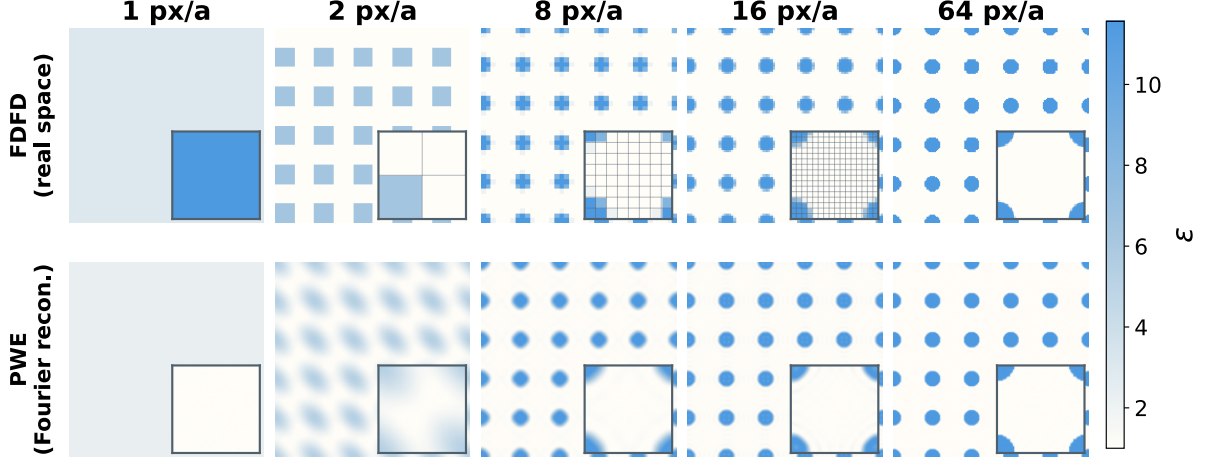


Figure 36: Material representation at seven resolutions for a square-lattice monolayer ($\varepsilon_{\text{rod}} = 11.56$, $r/a = 0.20$). **Top row:** Real-space ε grid as used by FDFD (nearest-neighbour rendering). **Bottom row:** The same data represented via truncated Fourier reconstruction (what the PWE eigenproblem “sees”). At low resolution, FDFD’s pixel averages remain physically meaningful, while the PWE Fourier reconstruction, which is inherently a smooth sum of plane waves (no real-space grid), smears rod boundaries and distorts their shapes: the sharp circular profiles are replaced by diffuse blobs with reduced dielectric contrast.

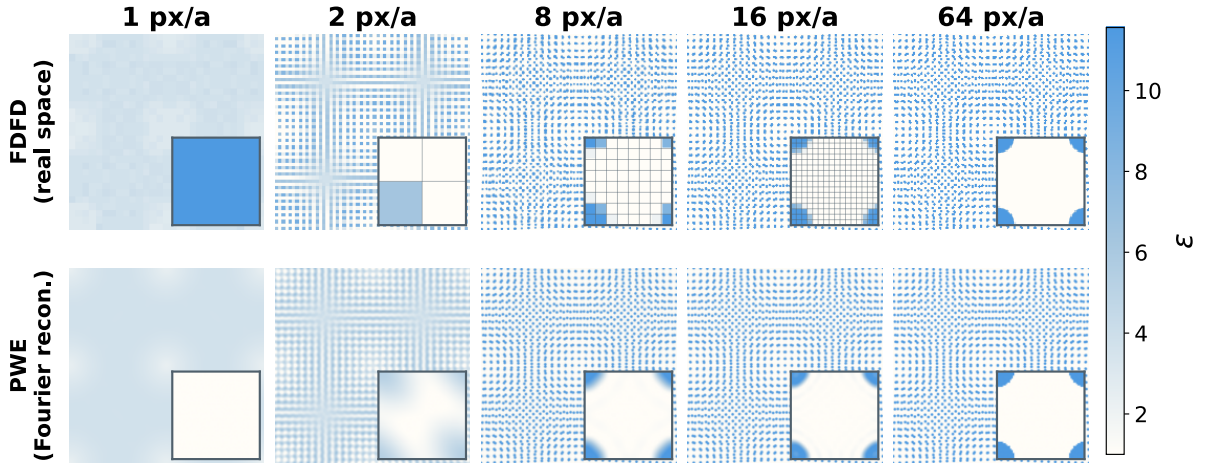


Figure 37: Same comparison as Figure 36, but for a commensurate moire supercell (square bilayer, $\theta \approx 4^\circ$, $m = 29$, $n = 1$, $N_{\text{cells}} = 842$). At 1–2 px/a the sub-cell rod structure has vanished; what survives in both representations is the slowly varying *moire-scale modulation* of ε , precisely the information that the envelope approximation models. The PWE Fourier reconstruction smears out the fine rod structure and introduces diffuse boundary artifacts, while FDFD’s pixel averages remain clean.

5.3.1 Monolayer Band Structure: MPB vs FDFD

Before turning to moire supercells, it is useful to compare the two solvers on the simplest possible test case: a single unit cell. Figure 38 shows the band structure for a square monolayer ($r/a = 0.2$, $\varepsilon_{\text{rod}} = 8.9$) along $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$, computed with both MPB and FDFD at resolution 128, for TM and TE polarization (five bands each). The two solvers agree to better than 10^{-3} in relative error across almost the entire path, with TE errors slightly higher than TM. The isolated spikes near symmetry points are band-crossing artifacts where eigenvalue sorting becomes ambiguous. This level of agreement confirms that the two discretization schemes

produce consistent results on a standard geometry, and sets a baseline for interpreting any larger discrepancies that appear in supercell calculations below.

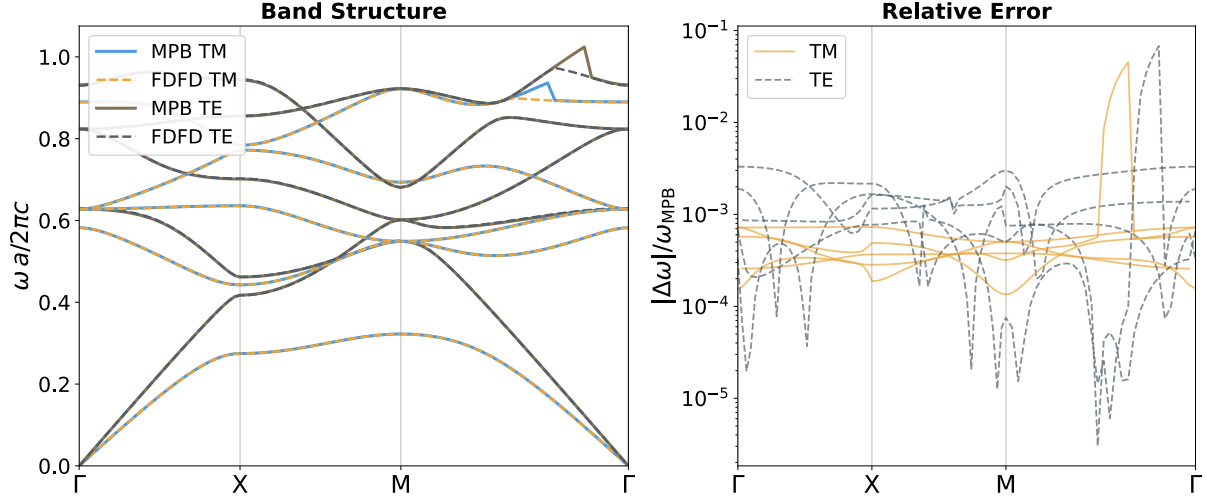


Figure 38: Monolayer band structure comparison for a square lattice ($r/a = 0.2$, $\varepsilon_{\text{rod}} = 8.9$, resolution 128). **Left:** TM and TE bands from MPB (solid) and FDFD (dashed) along $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$. **Right:** Relative frequency error $|\Delta\omega|/\omega_{\text{MPB}}$ on a logarithmic scale. Typical agreement is 10^{-4} for TM and 10^{-3} for TE; isolated spikes near Γ are eigenvalue-sorting artifacts at band crossings.

5.3.2 The Lower Limit of FDFD Resolutions

Since memory and compute time scale quadratically with the resolution per a , every factor saved in resolution translates directly into the ability to reach lower twist angles, which is precisely the regime where the envelope approximation operates and where validation data is most scarce.

Figure 39 shows the result for a $(m, n) = (38, 1)$ square-lattice CML supercell ($\theta \approx 3^\circ$, $N_{\text{cells}} = 1445$, 50 lowest TM modes at Γ). The left panel overlays eigenfrequency ladders for FDFD at 1, 2, 4, 16, and 64 px/ a against an MPB-128 reference. For roughly the lower half of the spectrum, every resolution, including 1 px/ a , traces the reference curve almost exactly. Only near the upper end of the spectrum do the lowest resolutions begin to deviate. The right panel quantifies the convergence: measuring intra-method error against FDFD-64 isolates the pure discretisation convergence from any systematic cross-method offset. Mean and maximum relative errors drop by roughly four orders of magnitude between 1 and 16 px/ a . A small but constant $\approx 0.9\%$ offset persists between any FDFD resolution and MPB-128, reflecting the systematic difference between the two numerical methods rather than a discretisation error.

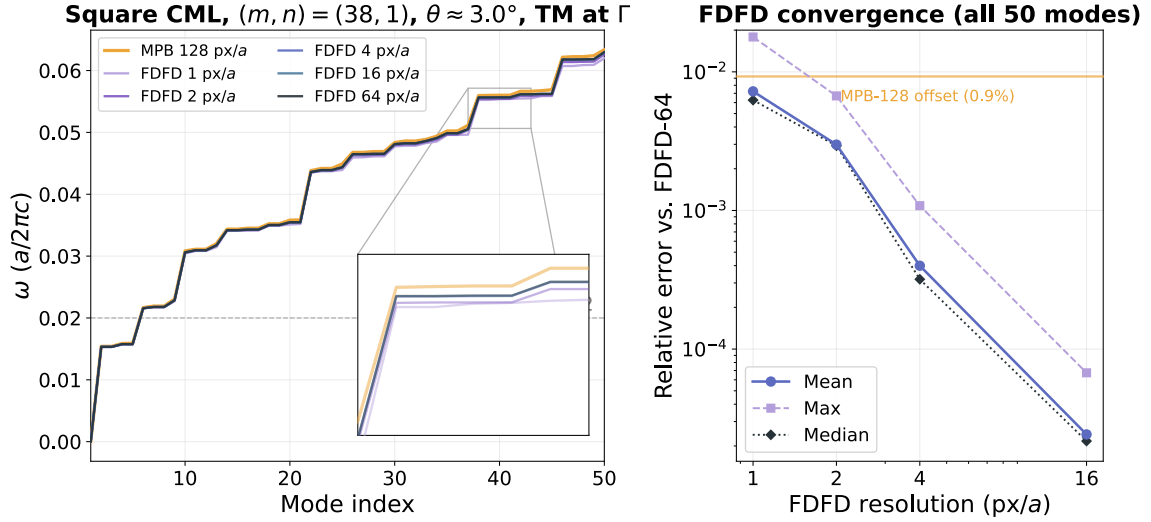


Figure 39: FDFD resolution convergence for a square-lattice CML supercell ($(m, n) = (38, 1)$, $\theta \approx 3.0^\circ$, $N_{\text{cells}} = 1445$, TM at Γ , 50 lowest modes). **Left:** Sorted eigenfrequencies vs. mode index; MPB-128 reference (golden) overlaid with FDFD at 1–64 px/a. The inset zooms into modes 37–43 to reveal the tiny inter-resolution spread. **Right:** Mean, median, and maximum relative error vs. FDFD-64 (same method) on a log-log scale, isolating the pure discretisation convergence. The horizontal line marks the systematic $\approx 0.9\%$ cross-method offset against MPB-128, which is resolution-independent.

Figure 40 presents the same data as an eigenvalue-stripe overview, where each horizontal lane shows the 50 lowest eigenfrequencies as vertical lines. The visual impression is striking: for the lower part of the spectrum, the stripes from 1 px/a are indistinguishable from those at 64 px/a or the MPB-128 reference. A visible spread develops only near the upper end, predominantly at 1–2 px/a.

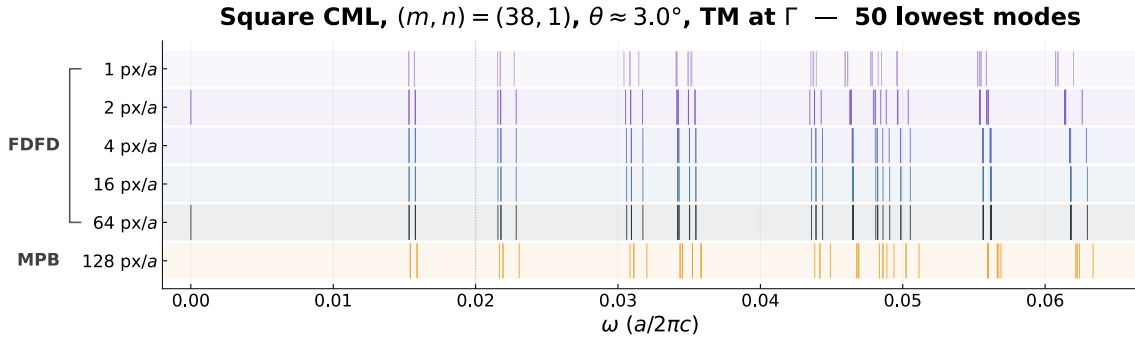


Figure 40: Eigenvalue stripe overview for the same supercell as Figure 39. Each lane shows the 50 lowest TM eigenfrequencies at Γ as vertical lines. The five FDFD lanes span 1–64 px/a (top to bottom by ascending resolution); the bottom lane is the MPB-128 reference. At low frequencies the eigenvalues are virtually indistinguishable across all resolutions, while a visible spread develops only near the upper end of the spectrum.

The observation that FDFD at 1 px/a recovers the low-frequency spectrum at all was one of the most surprising findings of this thesis. One pixel per lattice constant means a single grid value represents an entire unit cell. Returning to the material maps in Figure 37, the 1 px/a supercell has no discernible rod structure: the circular rods, the air gaps, the sharp dielectric boundaries have all been *completely* averaged into a single number per cell. The resulting grid looks almost like noise, yet it produces the correct eigenvalues.

This result is surprising enough to ask for a closer look at what is actually happening, and how it relates to the envelope approximation developed in Section 3.

In the FDFD pipeline, each pixel stores the spatial average of ϵ^{-1} over one unit cell. Because the moire pattern modulates the local registry $\delta(\mathbf{R})$ on a scale $L \gg a$ (Equation 11), the cell-averaged dielectric varies slowly across the supercell. It is this slowly varying field, the moire-scale modulation of the material, that the 1 px/a grid captures faithfully. Everything that varies on the sub-cell scale is averaged away; everything that varies on the moire scale is preserved.

This is precisely the separation exploited by the envelope approximation. In Section 3, the two-scale lift promotes the physical coordinate into an independent fast variable $\mathbf{r}$ (monolayer scale) and a slow variable $\mathbf{R}$ (moiré scale). The lifted permittivity $\varepsilon(\mathbf{r}, \mathbf{R}) = \varepsilon_{\text{loc}}(\mathbf{r}; \delta(\mathbf{R}))$ (Equation 18) encodes the fast structure through the local two-atomic crystal and the slow structure through the registry map. The envelope eigenproblem then projects out the fast degrees of freedom entirely: its zeroth-order term is the diagonal matrix of local band energies $\Lambda_{mn}(\mathbf{R}) = \lambda_n(\mathbf{R})\delta_{mn}$ (Equation 43), and its higher-order corrections involve only moiré-scale derivatives and coupling coefficients. The fast Bloch functions $u_{n\mathbf{k}_0}(\mathbf{r}; \mathbf{R})$ serve as a basis that is *integrated over* in the Bloch-cell projection and never appear as independent degrees of freedom in the final eigenproblem.

FDFD at 1 px/a performs an analogous operation by brute force: it replaces each unit cell by a single effective dielectric value, thereby collapsing the fast variable and retaining only the moiré-scale variation. The resulting sparse eigenproblem has one degree of freedom per moiré unit cell, the same count as the discretised envelope equation. The two approaches are not formally identical: the envelope approximation projects onto a specific band subspace and includes velocity and mass-tensor corrections through the first- and second-order terms in η , while FDFD at 1 px/a simply solves the full operator on a maximally coarse grid. But they share the same structural premise: for low-lying modes, the eigenvalue spectrum is determined by the slow spatial variation of the material, not by the sub-cell geometry.

This interpretation is confirmed directly by the eigenvectors. Figure 41 compares the lowest six nontrivial TM mode profiles at Γ for the same $\theta \approx 3^\circ$ square supercell, computed with FDFD at 1 px/a and MPB at 32 px/a. The coarse 1 px/a solutions already reproduce the same moiré-scale envelopes as the high-resolution MPB solver. The MPB row resolves the intra-cell structure, but the large-scale pattern is already fixed by the slowly varying moiré modulation.

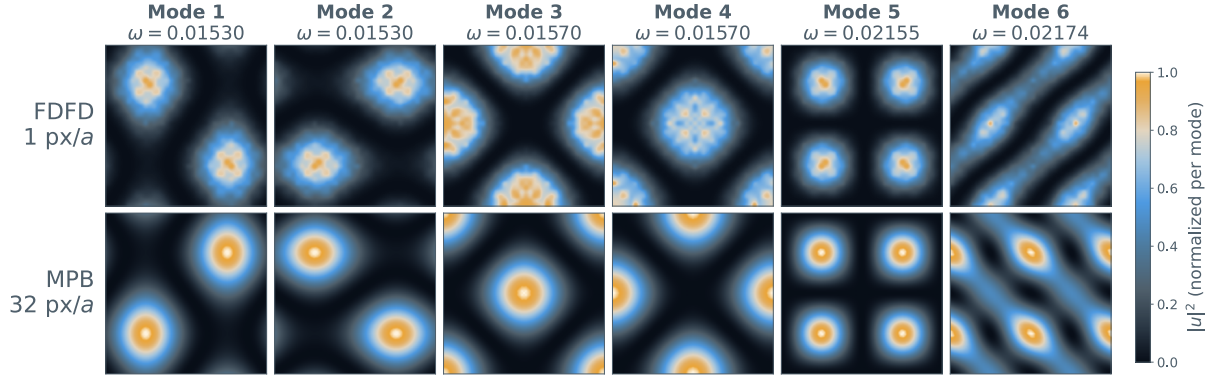


Figure 41: Mode-profile comparison for the same square-lattice CML supercell as Figure 39 ($(m, n) = (38, 1)$, $\theta \approx 3.0^\circ$, TM at Γ). Rows: FDFD at 1 px/a and MPB at 32 px/a. Columns: the six lowest nontrivial modes, shown as normalized $|u|^2$. The moiré-scale envelopes agree across both rows; the MPB row restores the intra-cell structure while the large-scale pattern is already captured at 1 px/a. Degenerate pairs may appear rotated relative to each other because the basis inside a degenerate subspace is not unique.

This finding has also a direct practical consequence. Because FDFD memory scales as $R^2 N_{\text{cells}}$, dropping from 16 px/a to 1 px/a reduces the matrix dimension by a factor of 256. For the supercells needed at $\theta \lesssim 2^\circ$, this is the difference between a feasible computation and one that exceeds available memory. The low-resolution FDFD solutions therefore provide a cheap and independent reference for validating the envelope framework at small twist angles, which is precisely the regime where the two-scale expansion is most accurate and where no other brute-force solver can reach.

5.4 What a Faithful Comparison Requires

With both the envelope pipeline and the brute-force reference solvers characterised, we arrive at the central question: do the two produce the same eigenvalues? Before comparing a single number we state what such a comparison must satisfy. The requirements below were established one by one, each after a comparison had failed for the lack of it, and the square-lattice comparisons that opened this campaign could not have succeeded for reasons that are now precisely known.

Spectral isolation, everywhere. The retained manifold must be separated from every other band at every registry, and the separation must hold across the whole monolayer Brillouin zone, not only at the carrier. The operational criterion is a *registry-common gap*: the maximum of band n over all registries and all $\mathbf{k}$ must lie below the minimum of band $n + 1$ over the same set. Without such a gap the target states sit inside the folded continuum of a neighbouring band at some registry, hybridise with it, and dissolve into resonances; no method, exact or approximate, can then match them one by one. Inspecting the eigenvalue landscape at the carrier momentum alone, as a first manifold selection naturally does, is necessary but not sufficient.

Certified counts. Both sides must enumerate every state in the comparison window, and the two counts must agree before any residual is read. Count mismatches are the first symptom of a broken comparison and the easiest to hide. For a plane-wave reference the number of eigenvalues below any λ follows exactly from the inertia of the factorised pencil $K - \lambda S$ (Sylvester’s law); the same factorisation certifies the FDFD count; the envelope model’s count is fixed by construction once its trial space is built on a declared set of moire harmonics.

Sorted, index-aligned matching. No assignment algorithm. Any two ladders of comparable density can be matched to within a level spacing, and an optimal assignment reports agreement that a rigid shift of the same pool reproduces equally well. Once the counts agree, sorted ladders are compared index by index and nothing else.

Extrapolated references. An FDFD ladder at one resolution is not a reference at the 10^{-6} level. Each state is extrapolated in the grid spacing from three resolutions with a fitted convergence order and an uncertainty; the plane-wave reference is converged in its cutoff and certified by residuals. Two independent references that agree with each other define the floor below which no claim is made.

Symmetry bookkeeping. The commensurate $(m, 1)$ cell used throughout this chapter is a centred cell: $(L_1 + L_2)/2$ is a lattice vector of both layers, so the cell is twice the true primitive cell and every level at the folded X momentum is an exact doublet of that hidden translation. The two monolayer valleys X and X' fold onto the same supercell momentum and are related by the four-fold rotation of the twisted bilayer. A comparison that does not resolve these sectors compares mixtures.

A sound operator. An earlier implementation of the envelope operator carried four defects that were invisible in aggregate comparisons and fatal in exact ones: the diagonal kinetic term was assembled as the square of a first-derivative stencil, whose discrete symbol vanishes at the Nyquist momentum as well as at zero, so the operator supported four interleaved copies of the envelope spectrum; the remote-band term was assembled as $LR_Q R'$ with $R' \neq L^\dagger$ and injected a spurious attractive potential; the registry derivatives of the discretised rod boundaries entered as grid-divergent fields; and the eigenproblem was solved in single precision. All four were repaired before any number reported below was produced, and every claim below was made with the repaired operator or with the resummed-frame model of Section 3.7, which contains none of these terms.

Figure 42 applies the first requirement to the thesis crystal. For equal rods the X -point manifold of band 1 lies inside the continuum of band 0 at other registries: the local crystal morphs from an aligned to a checkerboard configuration as the registry sweeps the torus, and no frequency window is gap for all of them. A supercell eigenvector classified by its Fourier weight near the X star confirms the consequence: at 2° every FDFD state in the comparison window carries an X -star weight below two percent. The states the envelope model was asked to reproduce did not exist as isolated states. Making the second layer a weak perturber (rods of half the radius) keeps the gap of the first layer open at every registry, and band 1 at X becomes an isolated manifold with a registry-common gap and a headroom of 0.12 to band 2. This asymmetric bilayer is the thesis crystal from here on.

5.5 The Thesis Crystal Revisited

5.5.1 The Strong-Coupling Wall

Even with an isolated manifold, the square bilayer is a hard case, and the reason can be read off monolayer data before any supercell is solved. Solving the local two-atomic crystal at X on a 6×6 registry grid gives the registry-resolved band positions, in units of the dimensionless eigenvalue λ : band 0 spans $[2.445, 3.004]$, band 1 spans $[5.316, 7.612]$, band 2 spans $[11.80, 16.28]$. The registry potential seen by band 1, the range of $\Lambda_{11}(\mathbf{R})$, is therefore $V = 2.30$, while the gap to band 0 is 2.31 and the gap to band 2 is 4.19. The moire potential is as deep as the band gap that isolates it: $V/\Delta \approx 1$. At 2° the kinetic quantum of the envelope, $\frac{1}{2} M^{-1} (2\pi\eta)^2$, is about

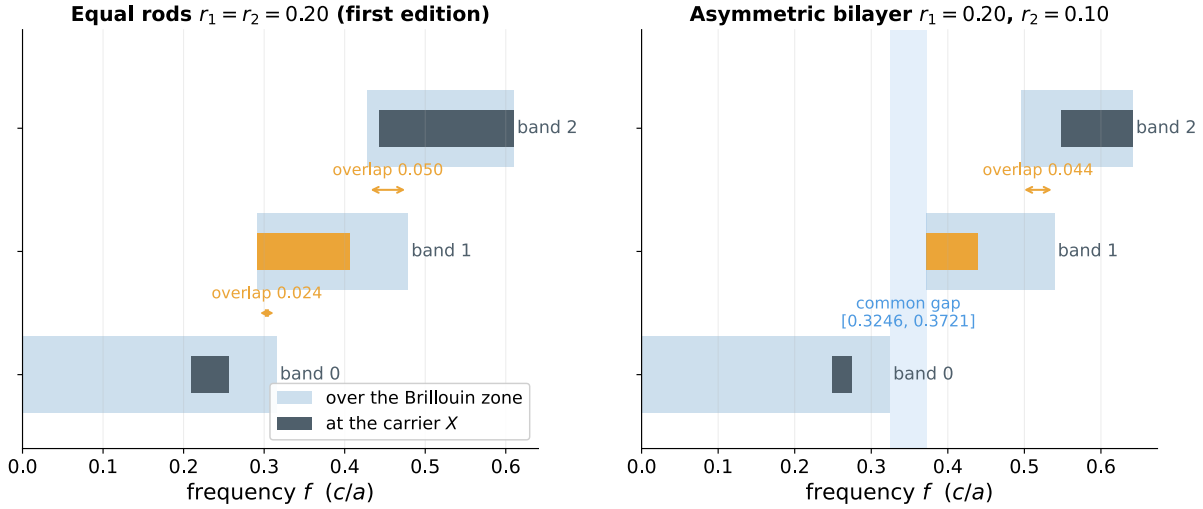


Figure 42: Registry-resolved band windows of the square TM bilayer at the carrier X and over the Brillouin zone, for the equal-rod crystal ($r_1 = r_2 = 0.20$, left) and the asymmetric bilayer ($r_1 = 0.20, r_2 = 0.10$, right); $\varepsilon = 8.9$ in both. Bars span the range of each band over a 5×5 registry grid; the pale bars span the full zone. A registry-common gap exists only where the pale bar of band n ends below the pale bar of band $n + 1$ begins. For equal rods the band-0 continuum overlaps the band-1 window at X and the manifold dissolves; the weak second layer restores the gap by continuity.

0.024 in the same units, so the potential exceeds the kinetic energy by a factor near one hundred. The two-scale expansion assumes a slow modulation on top of a rigid local band; here the modulation rivals the band structure itself.

Two consequences follow. First, the manifold states are pocket-bound: the supercell ground state sits 0.42 above the registry minimum of Λ_{11} , deep inside the wells, so any model built on the registry-averaged crystal starts 0.79 too high before any envelope physics is added. Second, the per-cell kinetic budget is tiny compared with the well depth, so the tower of envelope states above the floor is dense and its structure is dictated by the symmetry of the wells, not by the dispersion of the band. This is the quantitative form of the wall that every comparison on this crystal kept hitting. It is not an implementation defect, and it is computable a priori.

5.5.2 The Angle Ladder

Figure 43 shows the manifold tower of the asymmetric bilayer at five commensurate angles, in every solver that reaches the angle. Every solver consumes the identical analytic dielectric (the exact disk Fourier coefficients of both rod layers through a Lanczos window, converged in the plane-wave cutoff to 2×10^{-7} in λ). FDFD references at 7.63° , 3.95° and 2.01° are inertia-certified per resolution and Richardson-extrapolated with a fitted order of 2.05 at every angle; MPB at resolution 24 differs from the extrapolated FDFD by 1.4×10^{-4} in frequency on the same states, which is MPB's own un-extrapolated discretisation error. The envelope model is the registry-adapted resummed-frame model of Section 3.7 with a 6×6 envelope box, exact per-momentum frames, and the interlayer hops over the full second-layer star.

The floor is reproduced. The envelope model places the manifold bottom at 3.0×10^{-4} , 6.7×10^{-5} and 1.0×10^{-4} in frequency from the extrapolated FDFD value at 7.63° , 3.95° and 2.01° , inside MPB's own discretisation error at every reference angle. The tower is not reproduced. At 2.01° the lowest fourteen envelope rungs span 0.0084 in frequency where the FDFD rungs span 0.0040; enlarging the envelope box from 6×6 to 8×8 harmonics moves the median rung error from 1.1×10^{-2} to 8.4×10^{-3} only, so trial truncation is not the cause. The cause is symmetry. The FDFD tower consists of four-fold degenerate quartets, the $X \oplus X'$ structure of the centred cell. A trial set closed under the four-fold rotation is necessary and was built (the rotation acts on envelope harmonics as an integer affine map $\mathbf{n} \rightarrow M\mathbf{n} + \mathbf{n}_0$), but it is not sufficient: the parallel-transport gauge used to smooth the registry-adapted frames picks a direction, so the trial span is not covariant under the rotation and the quartets still split. The gauge-free variant of the model, with registry-averaged frames and the registry entering only through the hops, has no such freedom and gives exactly degenerate quartets, but its floor lies 1.3×10^{-2} too high, because averaged frames cannot reach the pockets. On this crystal the accurate-floor

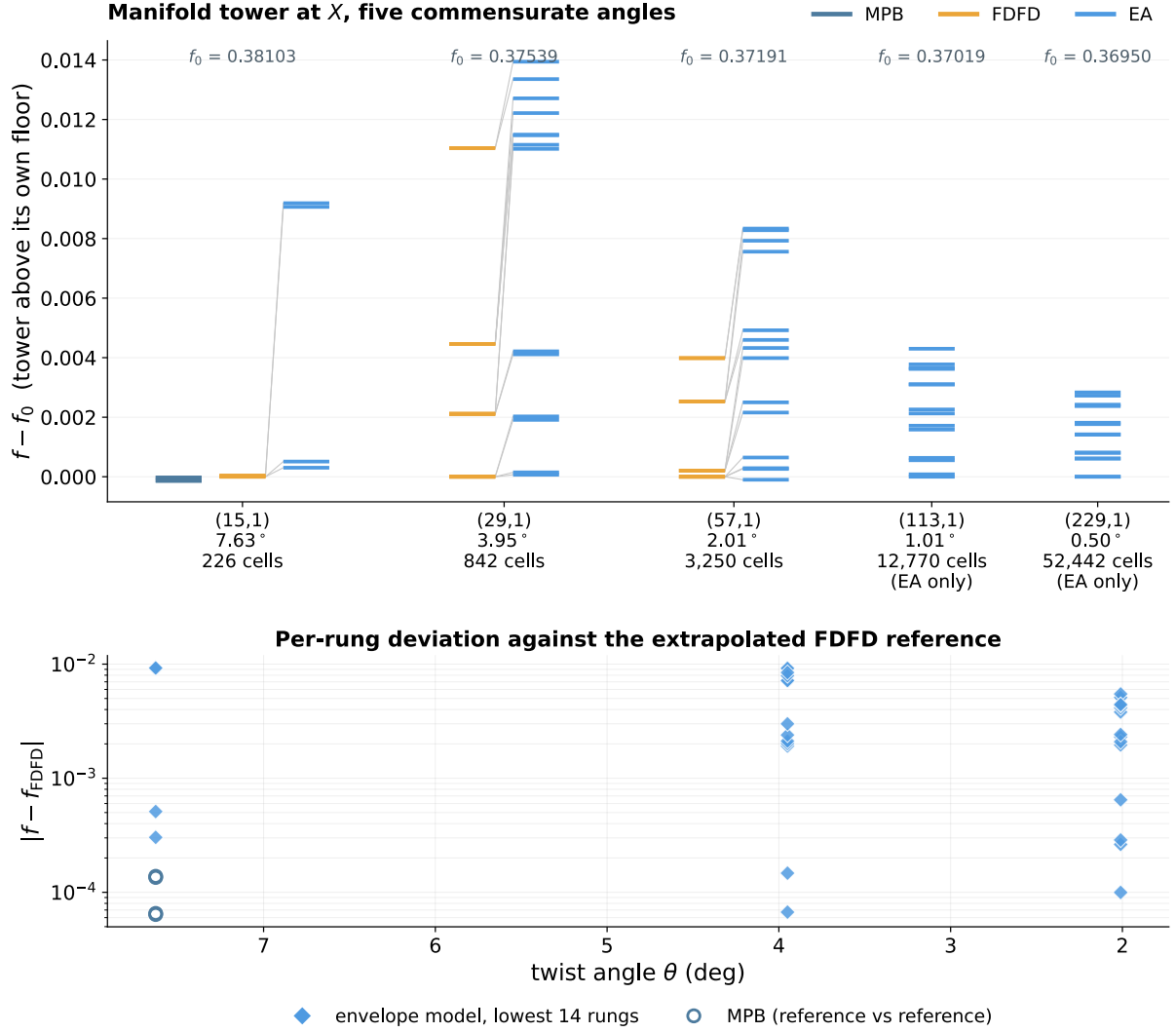


Figure 43: The thesis crystal angle by angle (square TM bilayer, $r_1 = 0.20$, $r_2 = 0.10$, $\varepsilon = 8.9$, carrier X , band 1). **Top:** the lowest fourteen rungs of the manifold tower in MPB (steel blue), extrapolated FDFD (orange) and the resummed-frame envelope model (sky blue), each group referred to its own floor f_0 ; grey lines join equal indices. At 1.01° and 0.50° only the envelope model exists. **Bottom:** per-rung deviation against the extrapolated FDFD reference where one exists; open circles are MPB against FDFD, the reference-versus-reference floor.

model and the exactly-symmetric model are still two different models. The missing piece, a gauge for the adapted frames that is covariant under the point group, is a bounded next step rather than an unknown.

5.5.3 The Cost Inversion

The ladder also shows where the envelope model stands as a solver. The FDFD reference took 13 s at 7.63°, 65 s at 3.95° and 3221 s at 2.01° (3.3 million unknowns at 32 px/a); the 1.01° cell would need 13 million unknowns and did not fit in memory. The envelope model went the other way. Its frame cache shrinks as the angle shrinks, from 226 to 81 to 25 to 9 k -cells for $m = 15, 29, 57$ and 113, because pocket-bound envelopes have a fixed width in moire harmonic units. The 0.50° case, 52,442 moire cells, took 533 s, and the remaining cost is the registry setup rather than the angle. Below about 2° the envelope model is the only solver in the room.

The angle ladder also settles the bandwidth question. For a kinetic-dominated tower the width of the lowest rungs scales as η^2 , and the FDFD data of the hexagonal test crystal in Appendix D follow that law. The thesis crystal does not: the certified FDFD towers span 0.0040 at 2.01° and 0.011 at 3.95°, a ratio of 2.7 where θ^2 predicts 3.9. A potential-dominated tower is set by the wells, and the quadratic law belongs to the regime the next section enters.

5.6 Where the Envelope Approximation Is Exact

5.6.1 A Candidate Built to the Requirements

If the square bilayer is the hard case, what does an easy one look like? The requirements of Section 5.4 translate into a design brief: an isolated manifold with a registry-common gap; a weak-to-moderate modulation, V small against the kinetic quantum; a twist angle inside the two-scale validity window at which a commensurate supercell is still brute-force solvable; a smooth, band-limited dielectric so that every solver consumes the identical analytic coefficients and the registry derivatives of the material are finite; and few enough unknowns that every solver can be over-converged. Nothing in the envelope derivation requires binary rods, and the fourth item removes at a stroke the sampling offsets, staircase errors and divergent boundary terms that had dominated the error budget of the hard case.

The candidate is a hexagonal lattice with $\varepsilon_0 = 9$, a host layer described by its three lowest Fourier stars with amplitudes 2.95, 2.25 and 2.60, detuned so that the three M points of the zone are no longer equivalent, and a weak second layer with a single star of amplitude $a_2 = 0.12$. Band 1 of the registry-averaged crystal has its minimum at one M point, M_2 , which is time-reversal invariant and therefore has no valley partner; the next M point lies 0.011 higher, the manifold window has depth $V = 0.023$, a registry-common gap extends 0.148 above the floor, and band 2 sits 0.611 higher still. The commensurate family $(m, m - 1)$ from $(4, 3)$ to $(9, 8)$ spans 37 to 217 primitive cells, so the full supercell is dense-solvable across the ladder, and V/E_{kin} runs from 0.1 to 0.8. The band-1 mass at M_2 is strongly anisotropic, roughly ten to one, which will matter below.

Two independent references were built on this material. The plane-wave reference uses the hermitized collocation operator, dense below 26,000 plane waves and otherwise a bottom-block Lanczos solve with certified residuals below 8×10^{-12} . The FDFD leg samples the analytic dielectric exactly, runs at 16, 24 and 32 px/ a , and extrapolates with a fitted order of 2.000 at every angle and an uncertainty near 4×10^{-7} in λ . The two agree to between 2.5×10^{-7} and 2.9×10^{-7} in λ , that is 1.7×10^{-8} in frequency, uniformly across the family. This is the floor of everything that follows.

5.6.2 The Triple Match

Figure 44 shows the deviation of the envelope model from the plane-wave reference for the manifold ground state across the family, for three model and scaling variants, and Figure 45 shows the same rung in all three solvers with the landing point resolved on a 10^{-6} axis. The three variants separate two things that the hard case had entangled: what the frame does, and what the family does.

Manifold ground state: envelope model against full-Maxwell references

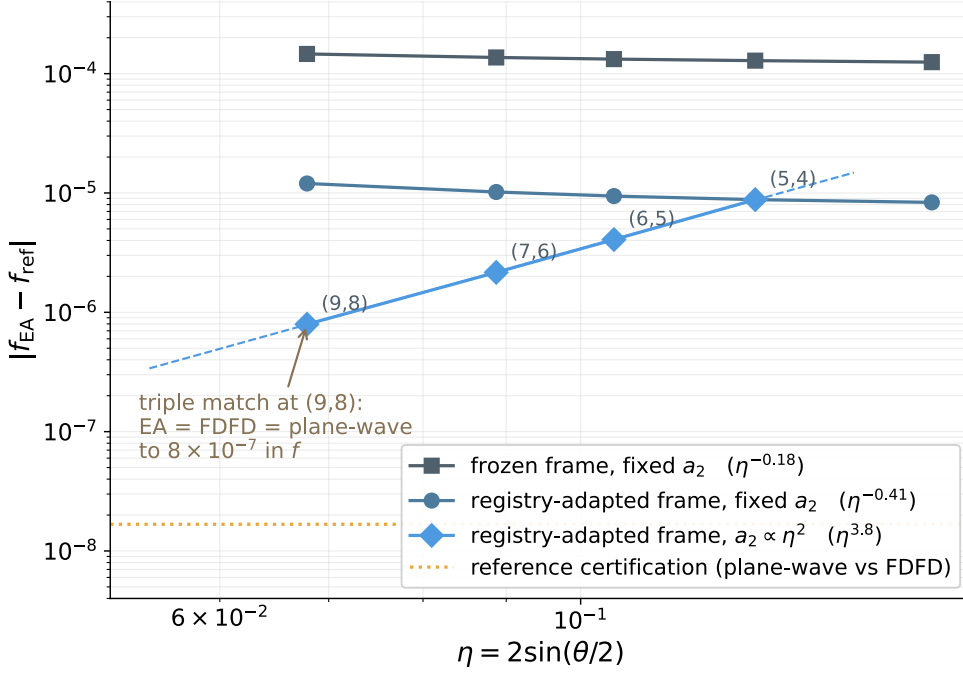


Figure 44: Deviation of the envelope model's manifold ground state from the certified plane-wave reference on the smooth single-valley candidate, against $\eta = 2\sin(\theta/2)$, for the frozen-frame single-band model at fixed material (grey), the registry-adapted single-band model at fixed material (steel blue), and the registry-adapted model on the uniform family $a_2 \propto \eta^2$ (sky blue, with the fitted power law). The dotted line is the agreement between the two references.

The frozen frame, a single Bloch function taken at the carrier and used at every registry, sits on a flat floor between 2.0×10^{-3} and 2.4×10^{-3} in λ with exponent $\eta^{-0.18}$. The floor is a material property: the frozen frame cannot follow the rotation of the Bloch state with the registry, and the resulting error is second order in the interlayer coupling and independent of the angle. The registry-adapted frame, in which the local Bloch function $u_1(\delta(\mathbf{R}))$ enters the product-space trial tensor at every slow point and the slow derivative differentiates through it (so that every frame-derivative, Berry and leakage contribution enters mechanically, with the trial space exactly orthonormal), is fifteen times better at fixed material, between 1.35×10^{-4} and 1.94×10^{-4} in λ , but still not asymptotic: the exponent is $\eta^{-0.41}$. It cannot be otherwise. At fixed material the family is not uniform, V/E_{kin} grows as η^{-2} , and the envelope sharpens into the wells faster than the expansion gains from the smaller η . The uniform family scales the second layer with the angle, $a_2 \propto \eta^2$, so that V/E_{kin} stays fixed. On that family the registry-adapted model converges as $\eta^{3.79}$, from 1.42×10^{-4} at (5, 4) to 1.28×10^{-5} in λ at (9, 8).

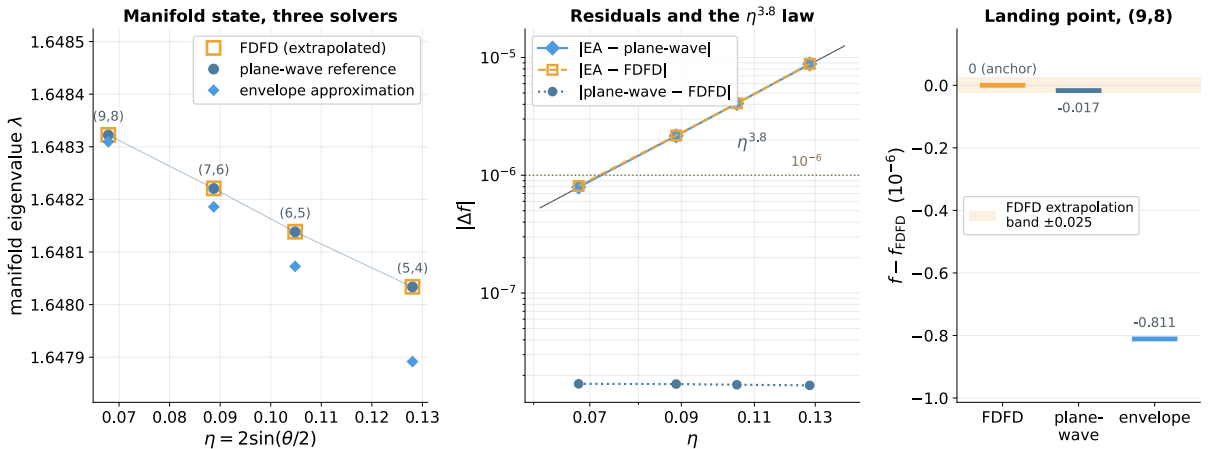


Figure 45: The manifold state across the scaled family. **Left:** its eigenvalue in FDFD (open squares), the plane-wave reference (dots) and the envelope model (diamonds). **Middle:** the residuals, with the fitted power law and the 10^{-6} line. **Right:** the landing point at (9, 8) on a 10^{-6} frequency axis, the FDFD extrapolation band shaded.

At the landing point the three solvers agree on the state:

$$|f_{\text{EA}} - f_{\text{PWE}}| = 7.9 \times 10^{-7}, \quad |f_{\text{EA}} - f_{\text{FDFD}}| = 8.1 \times 10^{-7}, \quad |f_{\text{PWE}} - f_{\text{FDFD}}| = 1.7 \times 10^{-8}. \quad (84)$$

Every knob of the envelope model was certified separately: the slow grid at 17 against 21 points moves the eigenvalue by 6×10^{-15} ; the monolayer cutoff at 4 against 5 and the fine grid at 192 against 256 by 10^{-6} in λ . One negative result belongs to the record. Multi-band frozen frames are poisoned at this carrier: the remote bands have nonzero slope at M_2 , their envelope parabolas extend far beyond their validity and dump spurious states into the window (a three-band frozen frame put seven of them there). Frames that are frozen and many is the worst combination; frames that are adapted and few is the right one.

5.6.3 Every State Accounted For

A single matched state is not a validation. The next question was how far up the tower the agreement extends, and answering it needed a reference that reaches forty to a hundred states and can prove it has not skipped one. The commensurate moire dielectric of finite-Fourier layers has an exact thirteen-term supercell Fourier series, so the plane-wave mass matrix is sparse and the TM pencil $Ku = \lambda Su$ with $K = \text{diag} |\mathbf{k}_s + \mathbf{G}|^2$ is a sparse symmetric pencil. Shift-invert reaches interior window states directly, 250 times faster than the Lanczos climb through the folded band-0 states underneath, and the LDL^T factorisation of $K - \lambda S$ gives the exact number of eigenvalues below λ by inertia. Every census below is certified. At (18, 17), 919 cells, the two references agree on all 47 states of the gap window to between 3×10^{-8} and 8×10^{-8} in frequency; at (32, 31), 2977 cells, on all 85.

Against such a tower the envelope model with the frozen frame does three things: it reproduces some rungs to 10^{-7} , it misses others, and it produces extra levels. A per-state diagnosis resolves all three. The valley weights of the reference eigenvectors are essentially binary, and every reference state the model misses belongs to another valley basin or lies above a ceiling; every extra envelope level carries a harmonic outside the model's domain. The ceiling is arithmetic: the three M points fold to pairwise distinct supercell sectors at every angle of the family, so a sector-resolved spectrum holds only the M_2 tower, but the sector's momenta $M_2 + \mathbf{G}_{\text{moire}}$ sample the whole monolayer zone, and above the floor of the M_3 basin, 0.0355 above M_2 , states of that basin legitimately enter the sector. No single-valley theory can claim anything above that line, and none is made.

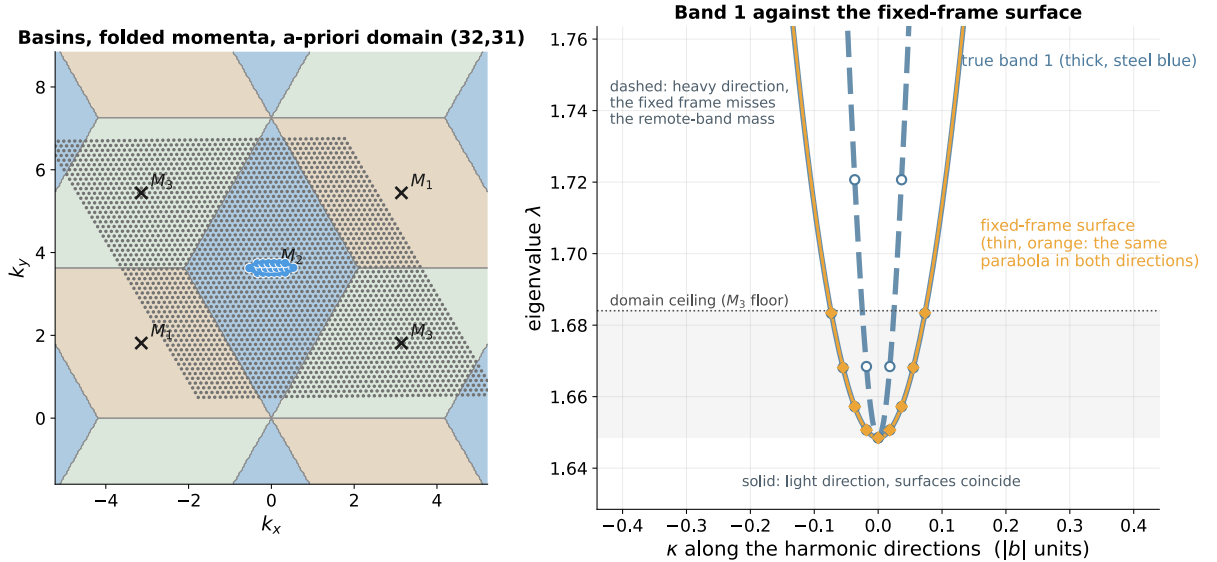


Figure 46: The momentum-space anatomy of the sector ladder at (32, 31). **Left:** the monolayer zone around M_2 partitioned into the basins of the three M points, the folded momentum lattice of the commensuration (dots), and the a-priori domain of the single-valley envelope theory (filled circles): harmonics in the M_2 basin at or below the M_3 floor (contour). **Right:** the registry-averaged band 1 along the two principal harmonic directions (thick) against the fixed-frame envelope surface (thin). Along the light direction the two coincide and the rungs match at 10^{-7} ; along the heavy direction the fixed frame misses the remote-band mass and assigns wrong energies inside the basin.

The sharper finding concerns direction rather than distance (Figure 46). The fixed-frame envelope surface $h_{11}(\kappa) = u_1(M_2)^\dagger C(M_2 + \kappa) u_1(M_2)$ is nearly isotropic, while the true band-1 surface is strongly anisotropic:

the first heavy-direction shell sits nine times above the first light one. At the same $|\kappa|$ the light-direction rungs match at 3.7×10^{-7} while the heavy-direction rungs err by 1.5×10^{-5} and more. The missing heavy mass lives in the remote-band coupling that a frame frozen at one momentum cannot carry. The dispersion gap $|h_{11} - \lambda_1|(\kappa)$ is computable from the monolayer alone, and it predicts the fixed-frame model's error rung by rung before any supercell is solved: predicted 3.8×10^{-7} , 1.6×10^{-6} , 3.7×10^{-6} and 7.2×10^{-6} on the light shells against measured values between 3.4×10^{-7} and 7.2×10^{-6} ; predicted about 10^{-3} on the heavy shells against measured 4×10^{-4} to 1.1×10^{-3} .

This suggests the protocol that makes the comparison reviewer-proof. Everything is declared from monolayer dispersion alone, before any comparison: the domain, namely the harmonics in the M_2 basin at or below the M_3 floor; for the fixed-frame model, additionally only rungs whose a-priori dispersion gap is below 10^{-5} in frequency; models built on the domain, so that counts are fixed by construction; reference censuses certified by inertia; matching sorted and one to one with no tolerance. Figure 47 shows the result at the largest supercell of the campaign, (55, 54), 8911 cells, $\theta = 0.607^\circ$, with FDFD as the only reference (2.28 and 3.56 million unknowns at 16 and 20 px/a, censuses certified by inertia on the FDFD matrix at both resolutions).

The a-priori census says 51 in-domain states; FDFD finds 51 below the ceiling, all of them M_2 -dominant by eigenvector classification. The exact-frame single-band model, one exact Bloch function of the registry-averaged

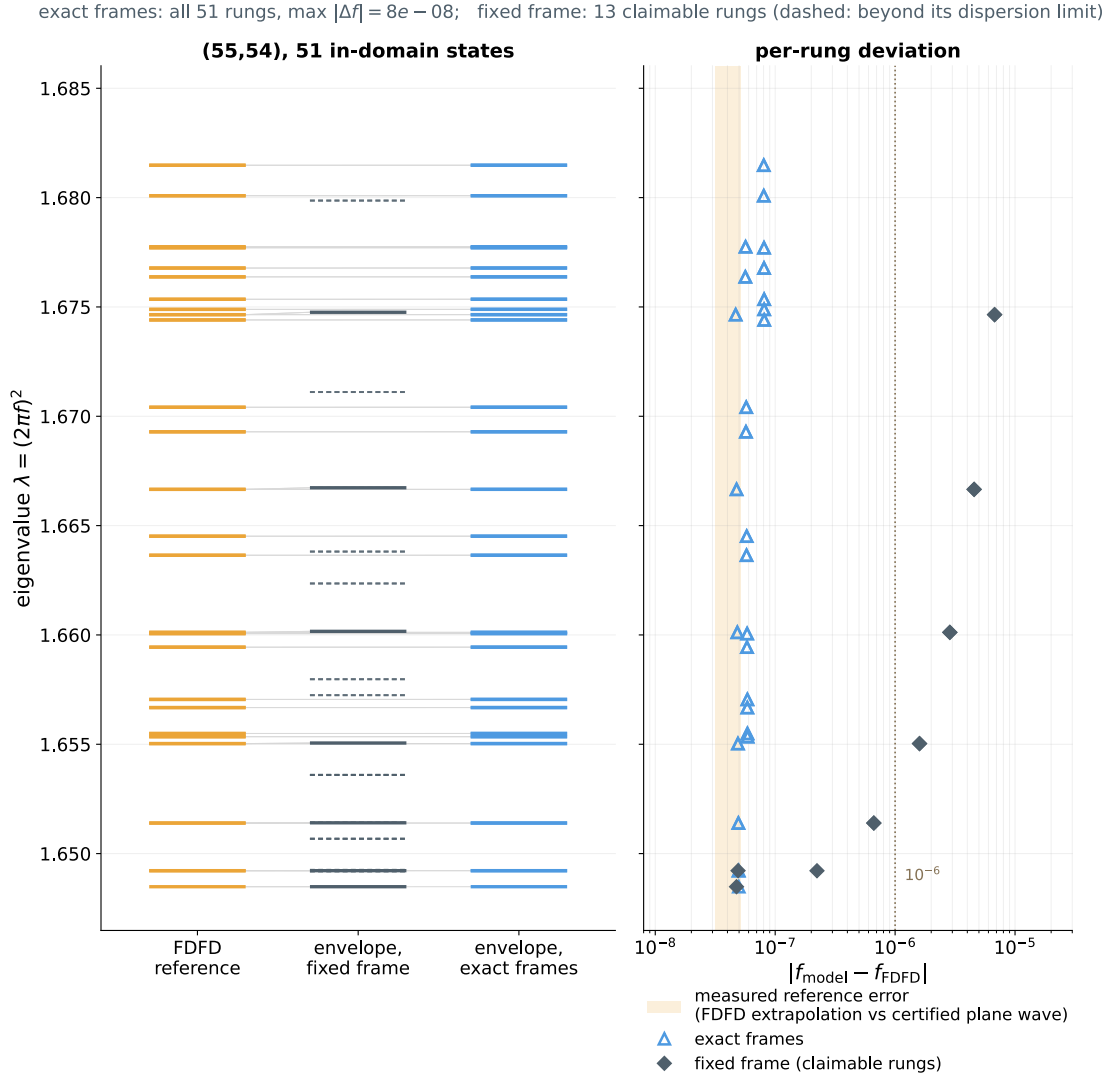


Figure 47: Every state of the declared single-valley domain at (55, 54), 8911 cells, 0.607° . **Left:** the FDFD reference, the fixed-frame envelope model (dashed where beyond its a-priori dispersion limit), and the exact-frame single-band model; matched rungs joined. **Right:** per-rung deviation of both models against the measured reference error, the difference between the FDFD extrapolation and the certified plane-wave pencil calibrated on the 21 in-domain states at (32, 31).

monolayer per in-domain folded momentum, matches all 51 rungs one to one with deviations between 4.7×10^{-8} and 8.1×10^{-8} in frequency, median 5.8×10^{-8} . The measured error of the reference itself is between 3.2×10^{-8} and 5.2×10^{-8} . The comparison is reference-limited: the envelope model matches the full-Maxwell solver to within the solver's own discretisation error, on every state it claims, with the counts fixed before the comparison. The fixed-frame model claims its 13 a-priori rungs and lands all 13 inside its declared 10^{-5} limit, but its trial count below the ceiling (59) does not close against the census (51). That count failure is part of the record, and only the exact-frame model achieves closure.

5.6.4 Order by Order

Is the exact frame an addition to the theory or already inside it? It is inside it. The η^2 Löwdin dressing by remote bands, the term derived in Section 3.5.3 and implemented in the pipeline, is the second-order piece of the resummed frame, and the remote-band content it carries is exactly the heavy mass that the fixed frame lacks. At the symbol level the sum rule closes: the raw fixed-frame surface is an exactly isotropic parabola with curvature 0.247, equal to the true light-direction curvature 0.2464; the true heavy curvature 2.350 is carried entirely by the second-order $\mathbf{k} \cdot \mathbf{p}$ sum, of which band 0 alone contributes 2.159, two bands close the sum to 0.08%, and the full sum closes to the finite-difference value at 10^{-5} relative.

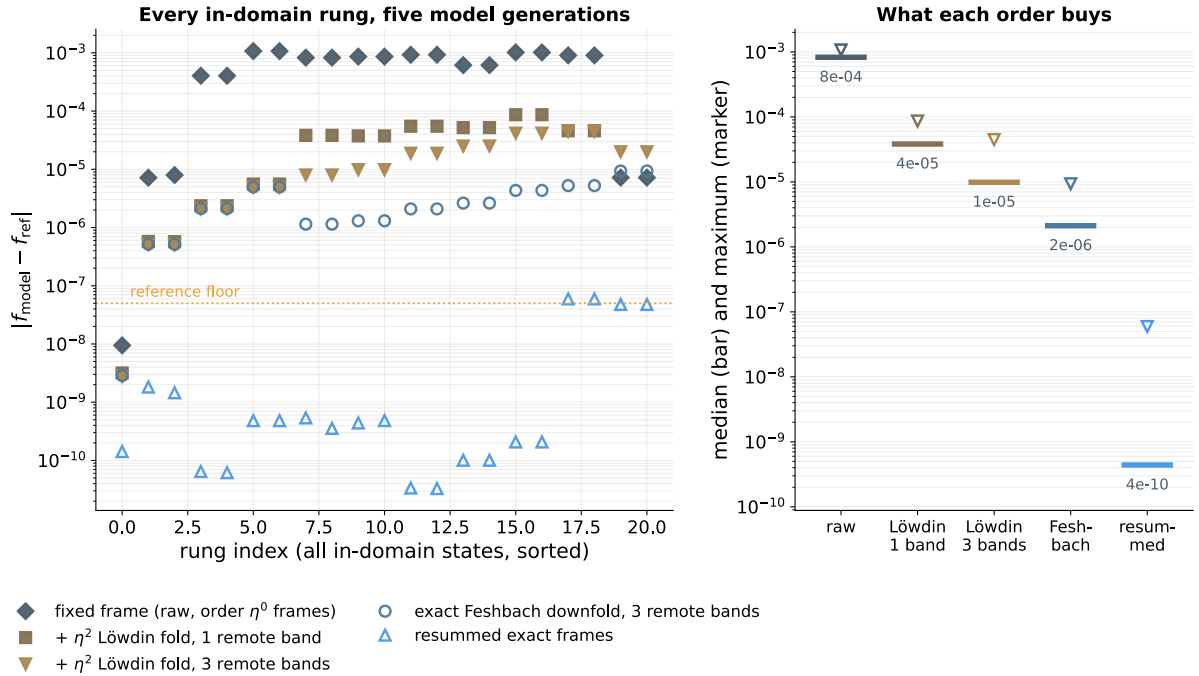


Figure 48: Completing the envelope approximation order by order at (32, 31), scaled family, all 21 in-domain rungs. **Left:** per-rung deviation from the certified reference for the raw fixed frame, the fixed frame with the η^2 Löwdin fold over one and over three remote bands, the exact Feshbach downfold of the same three-band content, and the resummed exact frames.

Right: medians (bars) and maxima (markers) of the same five models.

Figure 48 measures the ladder of orders on the same 21 rungs. The medians in frequency run from 8.3×10^{-4} for the raw fixed frame to 3.8×10^{-5} with the η^2 fold over one remote band, 9.9×10^{-6} with three, 2.1×10^{-6} with the exact Feshbach downfold of the same content, and 4.4×10^{-10} with resummed frames. The term the theory already contains recovers two to three decades, monotonically on every heavy rung. Two lessons come with it. The remote-band content must be folded into the retained block, as Löwdin or Feshbach do, and never jointly diagonalised: diagonalising the retained and remote blocks together lets the remote parabolas over-extend and dump spurious states into the window, which is why a three-band frozen frame was worse than a single band. And the fold carries its own fixed-frame dispersion error: it adds a wobble near 10^{-5} on the top light shells that the raw model already had at 7×10^{-6} , so the series is asymptotic rung by rung, not uniformly.

5.6.5 The Resummed Frame and Its Frontier

The resummed-frame model of Section 3.7, Equation 79, was implemented as a standalone monolayer computation: exact band-1 Bloch functions of the registry-averaged crystal at every in-domain folded momentum on

the left, the six-neighbour interlayer hop matrix on the right, no supercell anywhere. It reproduces the supercell-built exact-frame model to 10^{-14} in λ at (18, 17), (32, 31) and (55, 54), and it reproduces the 51-rung FDFD result of Figure 47 in under a second on a laptop core. One bug is worth recording because the first attempt did not show it: when the harmonic set spans several valleys, momentum cosets must be deduplicated (lattice copies of far valleys are the same Bloch state) and the hop lookup must then be coset-aware, re-indexing a representative column exactly, $u_1(g; k + G_0) = u_1(g + g_0; k)$. Without it the hops break at basin-copy seams and inter-copy doublets fail to split.

Validity frontier of the resummed-frame model, (18,17), 51 of 51 states

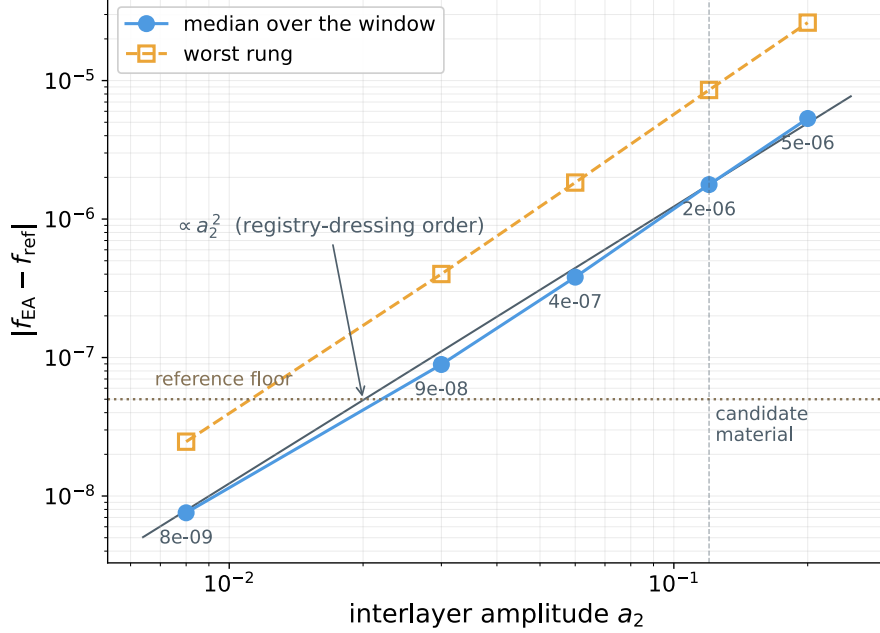


Figure 49: The validity frontier of the resummed-frame model at (18, 17): median and worst deviation from the certified reference over the full gap window, all valleys, 51 of 51 states at every point, against the interlayer amplitude a_2 . The grey line is the a_2^2 law of the registry-dressing order, pinned at the candidate material.

What remains is the next effect that the two-scale picture neglects, the dressing of the frames by the registry, and its size is measured in Figure 49. Over a sweep of the interlayer amplitude at fixed angle, full window, all valleys, the median deviation follows a clean a_2^2 law: 7.6×10^{-9} at $a_2 = 0.008$, 8.9×10^{-8} at 0.03, 3.8×10^{-7} at 0.06, 1.8×10^{-6} at 0.12 and 5.3×10^{-6} at 0.20. At the candidate material itself, $a_2 = 0.12$, the valley-agnostic model matches all 51 states of the gap window at or below 8.6×10^{-6} in frequency, the case in which the fixed frame had matched 13. A trial buffer of 0.024 above the claim edge removes the remaining top-shell tails (maximum in-domain deviation 1.8×10^{-9} at (32, 31), unchanged at twice the buffer), so the 5.8×10^{-8} median of Figure 47 is the reference's floor, not the model's. The next rung of the theory, registry-adapted momentum-dependent frames with an overlap metric, is defined and was not needed anywhere in this material family.

This settles the question that the square bilayer had left open. The envelope idea is not structurally single-valley or fixed-frame. With exact per-momentum frames it is valley-agnostic and reference-limited on an isolated weak-coupling manifold, its truncated orders converge toward that limit at measured rates, and its remaining error is the registry dressing at second order in the interlayer coupling, with a computable frontier. On the strongly coupled square bilayer it reproduces the floor within MPB's error and runs where brute force cannot, while the symmetry of its tower is the one open item.

5.7 Internal Consistency Tests

The comparisons of Section 5.5 and Section 5.6 used the resummed-frame model. The pipeline of Section 5.1, the truncated expansion on a registry grid and a moire grid, is what the geometric studies below and the magic-angle scan use, and its own convergence deserves the same scrutiny. All tests in this section use the honeycomb TM Dirac pair at the true K corner (Section 5.8) with the operator of Section 5.4, the parallel-transport gauge of Section 5.8 and a complex-double eigensolve, at $\theta = 1^\circ$ and the moire Γ point.

5.7.1 Sensitivity to the Registry and Moire Grids

Two grids enter Phase 1 and Phase 2. The registry grid discretises the Hamiltonian ingredients over the registry torus; the moire grid discretises the envelope. Figure 50 varies them separately. With the moire grid locked to the registry grid, the ten lowest eigenvalues move by 2.7×10^{-3} in frequency from a 16×16 to a 32×32 registry, by 3.5×10^{-4} to 48×48 and by 1.5×10^{-4} to 64×64 , a second-order approach that has not yet converged at the 48×48 production grid to better than about 10^{-4} . With the registry data fixed at 48×48 and the fields interpolated onto finer moire grids, the Phase 2 discretisation alone contributes 2.4×10^{-4} between 48 and 128 points per moire period and 10^{-5} between 96 and 128. At the level of the miniband widths of this crystal, between 5×10^{-5} and 10^{-3} , the production grids resolve the spectrum; at the 10^{-6} level of Section 5.6 they do not, which is one reason the exact comparisons used the resummed model on a spectral basis instead.

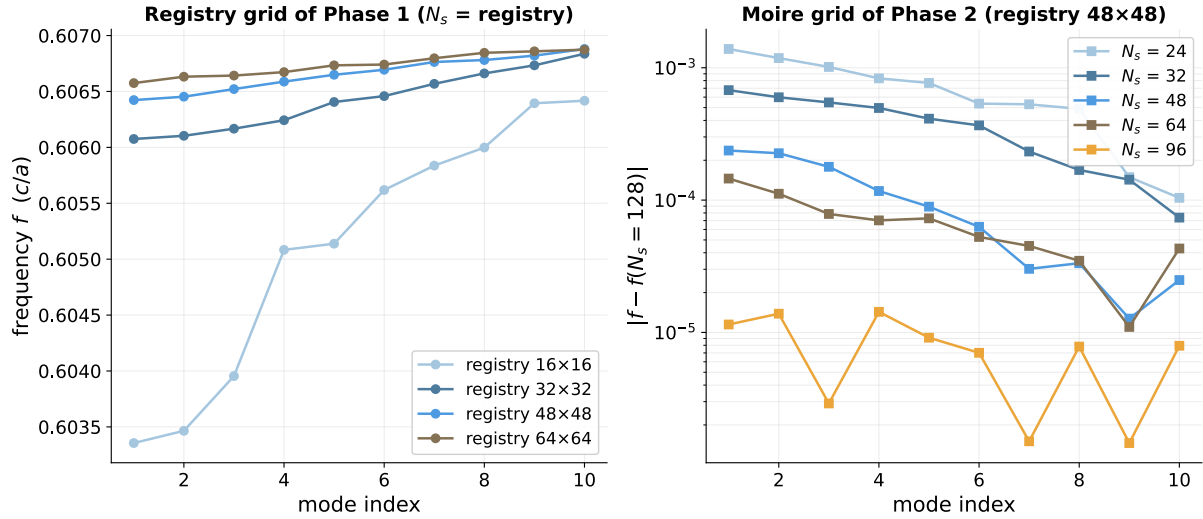


Figure 50: Convergence of the envelope eigenvalues of the honeycomb Dirac pair at $\theta = 1^\circ$, moire Γ point. **Left:** the ten lowest eigenvalues with the registry grid of Phase 1, the moire grid locked to it. **Right:** deviation from the 128×128 moire grid when only the Phase 2 grid is refined on fixed 48×48 registry data.

5.7.2 Sensitivity to the Retained and Remote Band Counts

The manifold-selection requirement of Section 5.4 says that a retained set which touches other bands at some registry degrades the approximation. The Dirac pair, bands 1 and 2, is isolated from band 0 by 0.17 and from bands 3 and 4 by 0.47 in frequency at the aligned registry, and bands 3 and 4 are themselves degenerate there. Figure 51 tests two things. First, the number of remote bands in the Löwdin mass tensor is varied from zero to eight with the pair fixed: the ten lowest eigenvalues move by at most 1.3×10^{-4} in frequency between no remote bands and eight, and by 7×10^{-5} between two and eight, while the trace of the dressed inverse mass changes by five percent. The Löwdin sum converges quickly here because the pair is far from every remote band over most of the registry torus. Second, the retained set is enlarged from the pair to bands 1–3 and 1–4. The spectrum barely moves, by 3×10^{-5} and 6×10^{-5} in the lowest eigenvalue, but the Born-Huang leakage quadruples as soon as band 3 is retained without its degenerate partner band 4, and stays there when band 4 is added, because the enlarged set now touches band 5 at other registries. The criterion behaves as it should: the geometric diagnostic reacts to a poorly isolated retained set long before the eigenvalues do.

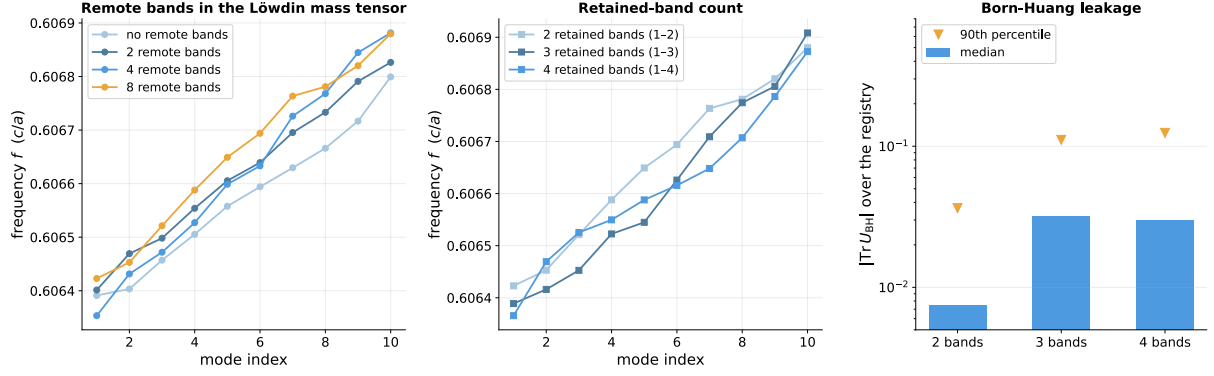


Figure 51: Sensitivity of the envelope spectrum of the honeycomb Dirac pair ($\theta = 1^\circ$, Γ) to the band counts. **Left:** the ten lowest eigenvalues with zero, two, four and eight remote bands in the Löwdin mass tensor. **Middle:** the same with two, three and four retained bands (bands 1–2, 1–3, 1–4). **Right:** median and 90th percentile of the Born-Huang trace over the registry for the three retained sets.

5.8 Dirac Physics of the Honeycomb Crystal

Throughout the preceding sections we have used the honeycomb TM crystal at K as a recurring test case. There is a deliberate reason: the K -point Dirac cone is the standard platform of photonic moire physics [11,13,15], and it is precisely the setting for which the multiband envelope approximation was built. Dirac physics in photonic moire systems could fill a thesis of its own; here we do what the envelope framework is designed for and inspect the effective Hamiltonian terms and the geometric data that the extraction produces.

Two choices precede the physics: the carrier and the gauge. The Dirac cone of this crystal (air rods of radius 0.408 in $\varepsilon = 3.78$) sits at the zone corner $K = (2/3, 1/3)$ in fractional reciprocal coordinates, in bands 1 and 2 (zero-based), at $f_D = 0.6394$. The point $(1/3, 1/3)$, which fractional coordinates invite as a guess for K , is an interior point on the Γ – K line at 58 % of the distance to the corner; bands 2 and 3 are accidentally near-degenerate there with a splitting of 10^{-4} , while at the corner they are split by 0.47, so a pair extracted at that point is not the Dirac pair. Every honeycomb figure of this chapter uses the corner as carrier with the Dirac pair as the retained manifold and all other computed bands as remote. The gauge matters because the Berry connection is the derivative of the retained frame with respect to the registry, and the frame returned by an eigensolver at neighbouring registry points carries an arbitrary phase per band and, inside a nearly degenerate pair, an arbitrary mixing. Finite differences of such frames produce noise. The pair frame is therefore transported along the registry grid: at every step the unitary polar factor of the overlap with the previous frame is removed, which makes neighbouring frames as parallel as the pair allows, and every retained block of the Hamiltonian is rotated into that gauge before it is assembled. The quantities that do not depend on the gauge at all, the inter-band gap, the velocity norm, the Born-Huang potential, the quantum-metric trace and the plaquette Berry curvature of the pair, are computed alongside and serve as the check.

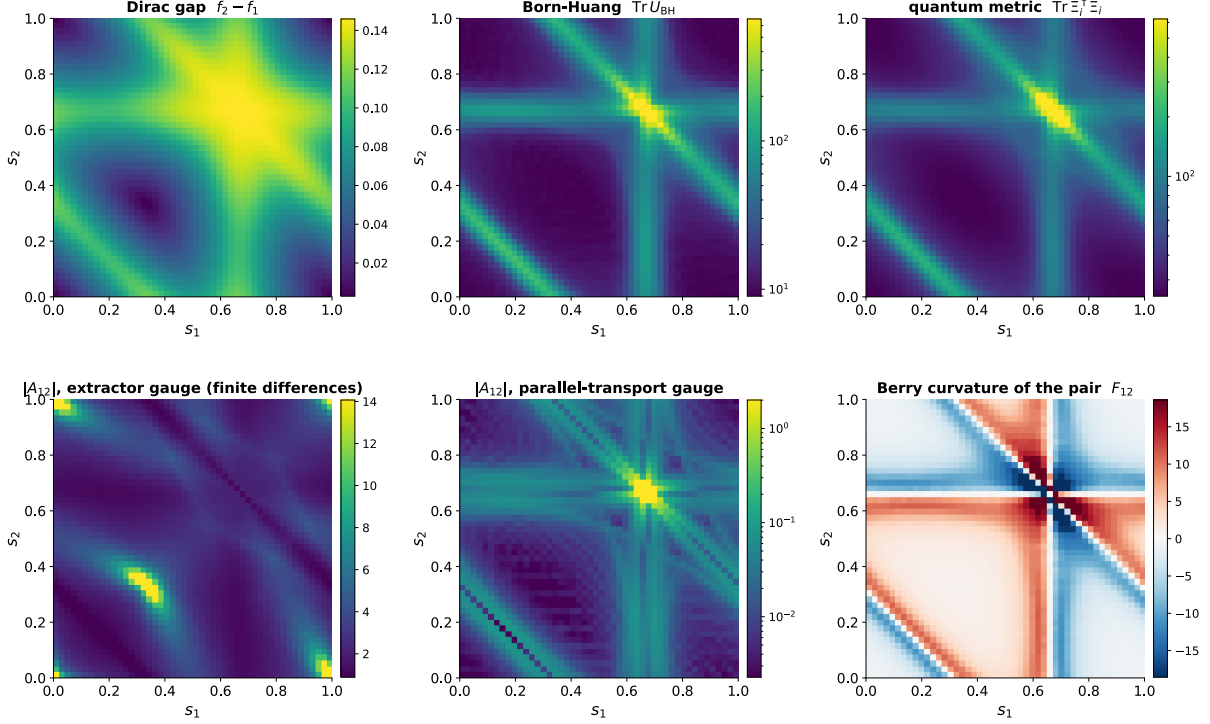


Figure 52: Registry-domain geometry of the Dirac pair of the honeycomb TM crystal at K (48×48 registry grid, resolution 64). **Top**: the gap between the two Dirac bands, the trace of the Born-Huang potential, and the trace of the quantum metric $\Xi_i^\dagger \Xi_i$ of the pair. **Bottom**: the Berry connection magnitude $|A_{12}|$ as returned by finite differences in the extractor’s own gauge, the same quantity in the parallel-transport gauge, and the gauge-invariant plaquette Berry curvature of the pair. The Dirac degeneracy sits at the aligned registry $(2/3, 2/3)$; the three lines of enhanced leakage through it are the registries where the two sublattices of the local crystal come closest.

Figure 52 shows the result. The Dirac gap closes at one registry, the aligned honeycomb, and opens to 0.14 in frequency where the two sublattices are maximally displaced. Everything geometric follows the gap. The Born-Huang potential and the quantum metric of the pair peak at the degeneracy and along the three lines through it where the sublattices approach each other; they are the same object seen twice, since the Born-Huang potential is the ε^{-1} -weighted quantum metric of Equation 60. The Berry connection in the extractor’s gauge is large everywhere and structured by the solver rather than by the crystal; in the transported gauge it is two orders of magnitude smaller away from the degeneracy and concentrates on the same lines. The plaquette curvature is gauge-invariant by construction and antisymmetric across the degeneracy, as a two-band Dirac touching demands; its integral over the registry torus is not a topological invariant of the pair, because the pair is degenerate at one point of the torus, and it is reported as a map, not as a number.

The full ingredient stack is shown in Appendix D, Figure 61. Reading it from bottom to top: the moire cell, the two Dirac bands over the registry torus, nearly degenerate around the aligned registry and split elsewhere; the inter-band gap; the velocity norm, which is the dominant first-order contribution as expected for a Dirac cone and largest where the pair is far from degenerate; the Berry connection and curvature; the two mass tensors, whose Löwdin dressing by the eight remote bands reflects the local curvature of the cone plus the virtual dressing; and the Born-Huang potential at the top. The twist-angle invariance of this data, Figure 62, is the Phase 1 invariance of Section 5.1.1 made visible: the same registry-domain landscapes are mapped onto moire cells of three different sizes, and only the cell changes.

This stack is the payoff of the pipeline. A supercell eigensolver produces eigenvalues and mode profiles; it cannot decompose them into velocity contributions, mass corrections, geometric phases and leakage penalties. The envelope extraction makes that decomposition explicit and spatially resolved, and the transported gauge makes it consistent.

5.9 Bandwidth Scaling and the Search for Magic Angles

The most celebrated prediction of moire physics in electronic systems is the existence of magic angles at which flat bands emerge and the group velocity vanishes [6]. It is natural to ask whether the photonic envelope framework predicts analogous angles for the honeycomb Dirac crystal.

We scan the miniband bandwidth against the twist angle on 237 angles between 0.2° and 10° , with the carrier and gauge of Section 5.8. At each angle the envelope eigenproblem of the Dirac pair is solved at nine $\mathbf{q}$ -points along $\Gamma-M-K-\Gamma$ of the moire zone for the twenty eigenvalues nearest the Dirac energy, on a 48×48 moire grid matched one to one to the registry grid; the operator is the compact one of Section 5.1.1 with the pair blocks in the parallel-transport gauge and the eight remote bands in the Löwdin mass tensor. The per-mode bandwidth is the spread of each eigenvalue over the nine $\mathbf{q}$ -points, and the RMS bandwidth averages over the twenty modes.

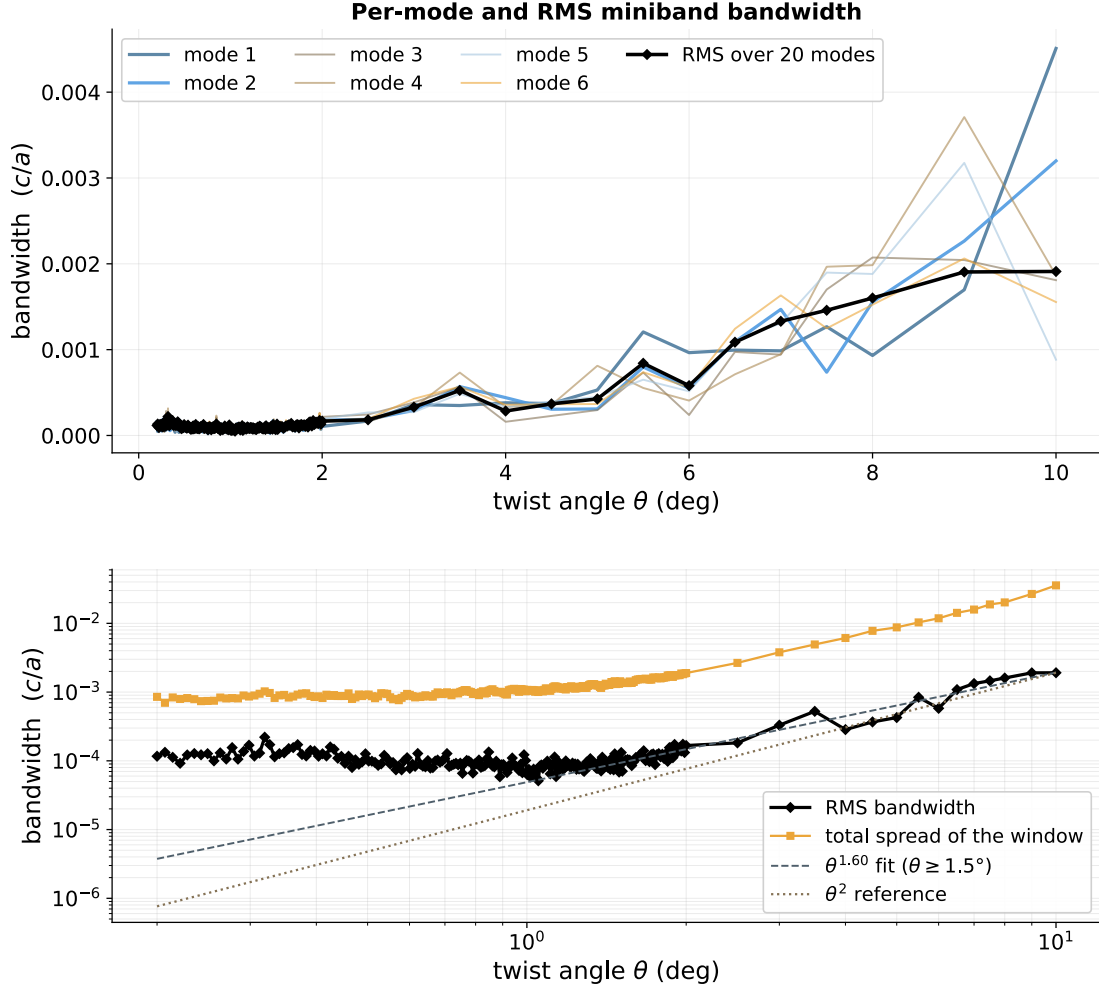


Figure 53: Moire miniband bandwidth against the twist angle for the honeycomb TM Dirac pair at K (237 angles, nine $\mathbf{q}$ -points, twenty modes around the Dirac energy). **Top**: per-mode bandwidth of the six lowest modes and the RMS over all twenty. **Bottom**: RMS bandwidth and total spread of the window on logarithmic axes, with the power law fitted above 1.5° and a θ^2 reference.

Figure 53 shows the result. Above 1.5° the RMS bandwidth follows a power law $\theta^{1.6}$, between the linear scaling of a velocity-dominated Dirac envelope and the quadratic scaling of a mass-dominated one, which is what the coexistence of both terms in the effective Hamiltonian predicts. Below 1.5° the bandwidth stops decreasing. It settles on a plateau between 5×10^{-5} and 2×10^{-4} in frequency, fluctuates from angle to angle, and reaches its shallowest value of 5×10^{-5} at 1.05° , a factor of three below the plateau's upper edge and not a collapse. The origin of the plateau is not a magic angle: as the angle shrinks at a fixed number of moire grid points, the twenty modes nearest the Dirac energy sample an ever denser ladder of minibands, and their individual widths fall below the level spacing of the ladder and below the resolution that a 48×48 envelope grid can provide for

the ever finer registry structure. A search for a flat band in this regime needs an angle-adapted grid and a velocity criterion rather than a bandwidth criterion.

No magic angle is found for this crystal, and the reason is structural. In the Bistritzer–MacDonald model the magic angle is reached when the interlayer coupling matches the Dirac velocity, so that the two cancel and the lowest bands flatten. In the photonic honeycomb crystal studied here, the two sublattices of one layer play the roles of the two layers, and the coupling that the twist modulates is the registry dependence of the local band data, which is weak compared with the Dirac velocity at every angle inside the validity window of the two-atomic approximation (Figure 18). Matching the two would require angles at which the local-periodicity picture has already broken down. Whether a bilayer of two honeycomb crystals, with a genuine interlayer coupling, has a photonic magic angle within reach of the envelope framework is a question this thesis leaves open; the ingredients to answer it, the velocity, the mass tensor and the registry potential as functions of the registry, are exactly the ones the pipeline delivers.

The envelope framework is not restricted to the moire Γ' point. Varying the moire Bloch momentum $\mathbf{q}$ across the moire Brillouin zone traces out the moire miniband structure, the dispersion of the moire-scale eigenstates as a function of $\mathbf{q}$, which is the two-scale analogue of the monolayer band diagram. Figure 54 shows it for the Dirac pair at 1° along the full high-symmetry path.

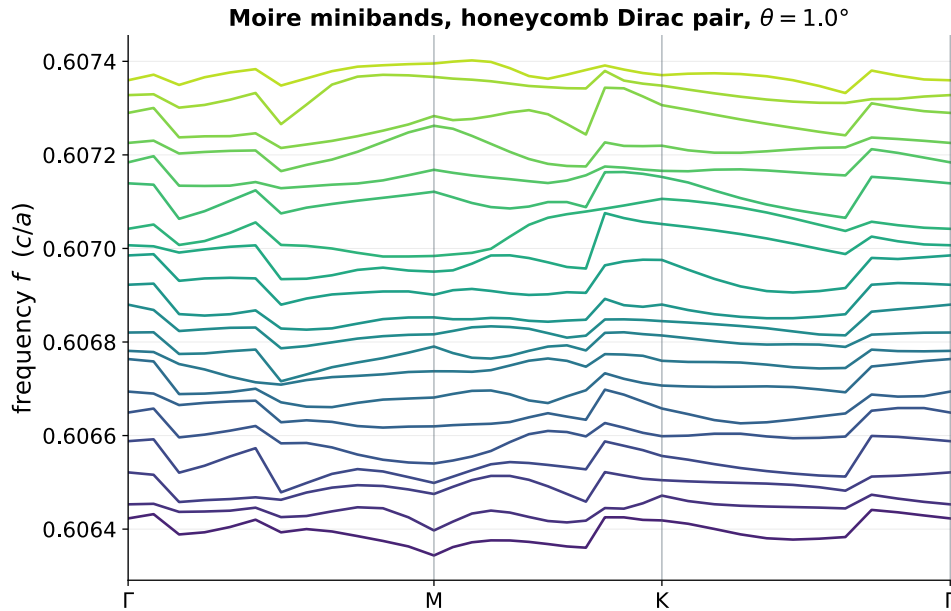


Figure 54: Moire minibands of the honeycomb TM Dirac pair at $\theta = 1^\circ$ along Γ – M – K – Γ of the moire Brillouin zone, twelve points per segment, the twenty eigenvalues nearest the Dirac energy. Each curve is one miniband.

This chapter walked through the full arc of the envelope framework in practice: the pipeline, the reference solvers, the requirements of an honest comparison and the two crystals on which it was carried out, the internal consistency of the pipeline, the geometric physics of the Dirac crystal, and the spectral predictions. What is established is this. On an isolated manifold with a weak interlayer coupling the envelope approximation is exact to the precision of the best full-Maxwell solvers, with measured error laws in the angle and in the coupling. On the strongly coupled thesis crystal it reproduces the manifold floor within MPB’s own error and is the only solver below 2° , while the symmetry of its tower awaits a covariant gauge. The geometric data, in a consistent gauge, decompose the moire physics in a way no supercell solver can. And the honeycomb Dirac crystal has no magic angle inside the window where the theory applies.

6 Conclusion

Photonic moire crystals arise when two periodic dielectric layers are stacked with a small relative twist, producing a superlattice whose period far exceeds the monolayer lattice constant. This simple construction confronts conventional solvers with two compounding obstacles: at generic twist angles the bilayer is incommensurate and no periodic unit cell exists at all, while at the special commensurate angles where periodicity is restored, the supercells grow so rapidly that brute-force computation becomes infeasible precisely where the moire physics is richest.

This thesis addresses both problems through a single pipeline built from three interlocking pieces.

The first piece is the *two-atomic crystal approximation* (Section 3.1). At small twist angles, every local patch of the bilayer closely resembles a periodic crystal with a two-atom basis. The inter-layer shift varies smoothly from patch to patch, parametrised by the registry map $\delta(\mathbf{R})$. This formulation replaces the global incommensurability problem with a family of periodic local problems, one for each registry, connected by a slowly varying envelope. A quality parameter $\beta = \theta/\gamma$ quantifies when the approximation is reliable and provides accuracy zones that can be checked before any calculation.

The second piece is the *multiband envelope approximation* (Section 3). Starting from the local Bloch modes of the two-atomic crystal, a systematic two-scale expansion separates the fast monolayer-scale oscillations from the slow moire-scale modulations. Projecting the full Maxwell operator onto a retained band subspace yields an effective Hamiltonian whose ingredients, local band energies, interband velocities, inverse mass tensors, Berry connections, and Born-Huang leakage potentials, are all defined on the registry domain and are independent of the twist angle. The moire eigenproblem then reduces to solving this effective Hamiltonian on a moire-scale grid, with the twist angle entering only through a single scaling parameter $\eta = a/L$.

The third piece is *Blaze2D* (Section 4), a two-dimensional plane-wave eigensolver written in Rust. The envelope approximation requires full Bloch eigenvector data at every registry point, not just eigenfrequencies, and existing solvers either lack the necessary output or are too slow for the thousands of local problems that a dense registry sweep requires. Blaze2D was built to fill this gap. It solves the local Bloch eigenproblem with full eigenvector extraction and feeds the results directly into the envelope pipeline.

With these three components assembled, we applied the pipeline to concrete photonic moire crystals and tested its outputs against independent references (Section 5). The reference is a finite-difference frequency-domain (FDFD) eigensolver, validated against the established plane-wave code MPB. A surprising finding emerged during this comparison: FDFD at just one pixel per lattice constant already reproduces the low-frequency moire spectrum, because the coarse grid naturally performs the same scale separation that the envelope theory formalises. This observation provides both a cheap reference for validation and an independent confirmation that the moire-scale modulation, not the sub-cell geometry, determines the low-lying eigenvalues.

The comparison was carried to the level of individual eigenvalues. Section 5 states what such an agreement requires and then reaches it. On the thesis crystal, a strongly coupled square bilayer whose registry potential is as deep as the band gap that isolates it, the completed envelope model reproduces the manifold floor within MPB's own discretisation error at every angle where a reference exists and runs at 1° and 0.5° , where no brute-force solver fits in memory; the symmetry of its tower on that crystal is the one item left open, with its cause identified. On a smooth single-valley crystal built to the requirements, the envelope model, the plane-wave reference and FDFD agree on the manifold state to 8×10^{-7} in frequency with a measured convergence law $\eta^{3.8}$, and the resummed-frame model matches all 51 states of a declared domain on a supercell of 8911 cells to within the reference's own discretisation error, with the counts fixed before the comparison. The order-by-order ladder shows that the η^2 remote-band term the theory already contained recovers two to three decades, and the remaining error of the completed model follows the a_2^2 law of the next order. The derivation was audited alongside by exact algebra and machine-precision identity checks, from the registry map and the exact lift to the first-order remainder, the remote-band term and the second-order bookkeeping, and the operator that was validated is the one stated in Section 3 and displayed in full in Appendix A.

The honeycomb Dirac crystal, the platform on which the geometric content of the effective Hamiltonian was displayed, was extracted at the zone corner with the Dirac pair as the retained manifold. The registry-domain

maps of band energies, velocities, mass tensors, Born-Huang potential and Berry geometry, the latter in a parallel-transport gauge, provide a spatially resolved decomposition of the moire physics that no supercell solver offers, and the magic-angle scan is reported as it came out.

The main contribution of this thesis is merging these components into an open-source, end-to-end research pipeline that takes a crystal specification and a twist angle as input and produces moire eigenvalues, envelope mode profiles, miniband dispersions, and the full set of geometric Hamiltonian data as output, together with the demonstration, on a crystal where every solver can be over-converged, that the envelope approximation is exact where it claims to be.

Several directions remain open. The registry-adapted frames of the completed model need a gauge that is covariant under the point group before the strongly coupled thesis crystal's tower can be reproduced with its degeneracies. The next order of the theory, registry-dependent frames at every moire harmonic, is defined and unneeded in the materials studied here; a material with a stronger second layer will need it. The current treatment is restricted to strictly two-dimensional photonic crystals, while most experimental moire photonics operates in the slab geometry, where interlayer coupling is mediated by evanescent fields across a finite gap rather than by direct dielectric superposition. Extending the two-scale formalism to three-dimensional slab systems is a natural next step, and Blaze2D is structured in a way that makes a three-dimensional extension feasible. Even in its current form, the framework demonstrates that the two-scale envelope approach, well established in electronic moire systems, can be carried through rigorously for the photonic case and validated to the precision of the best full-Maxwell solvers. We hope that it adds a useful theoretical tool to the photonic moire crystal toolbox and serves as a starting point for further extensions.

Appendix A: The Effective Hamiltonians at a Glance

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**

$$\mathcal{H}_{\text{eff}} = \left[\underbrace{\Lambda}_{\text{band energies}} \right] + \eta \left[\underbrace{\frac{1}{2} (v^{(i)} \Pi_i + \Pi_i v^{(i)})}_{\text{group velocity} \cdot \text{covariant momentum}} + \underbrace{\Xi_{\text{sc}}^{(1)} + \frac{i}{2} \partial_{R_i} v^{(i)} + \frac{1}{2} [A_i, v^{(i)}]}_{\text{first-order remainder} + U_{\text{BH}}^{(1)}} \right] \\ + \eta^2 \left[\underbrace{\frac{1}{2} \Pi_i M_{ij}^{-1} \Pi_j}_{\text{inverse mass tensor} + (\text{Löwdin downfolded})} + \underbrace{\Xi_i^\dagger \varepsilon^{-1} \Xi_i}_{\text{Born-Huang}} + \underbrace{K_i^\dagger \mathcal{D}_i - \mathcal{D}_i K_i}_{\text{direct 1-deriv. remainder}} + \underbrace{\mathcal{D}_i \mathcal{T}_i^\dagger R_Q \mathcal{R} - \mathcal{R}^\dagger R_Q \mathcal{T}_i \mathcal{D}_i}_{\text{Löwdin 1-deriv. cross}} - \underbrace{\mathcal{R}^\dagger R_Q \mathcal{R}}_{\text{Löwdin scalar}} \right] + O(\eta^3)$$

slow derivatives act on everything to their right, coefficient fields included; the second-order bracket is the flux form of the direct term plus $-S^\dagger R_Q S$ for the remote-band excursion (equivalent to the raw split with $\Gamma^{(2)}$, not additional to it)

where

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

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

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

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

direct one-derivative coefficient (flux form of $-D_{R_i} \varepsilon^{-1} D_{R_i}$ projected on U)

$$K_i = U^\dagger \varepsilon^{-1} \Xi_i, \quad \mathcal{H}_{\text{dir}}^{(2)} = -\mathcal{D}_i (G \mathcal{D}_i + K_i) + K_i^\dagger \mathcal{D}_i + \Xi_i^\dagger \varepsilon^{-1} \Xi_i$$

remote-band excursion (manifestly Hermitian; expanded into the three Löwdin pieces above)

$$S = \mathcal{T}_i \mathcal{D}_i + \mathcal{R}, \quad \mathcal{H}_{\text{remote}}^{(2)} = -S^\dagger R_Q S$$

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

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

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

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

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

$$\mathcal{T}_i = -i Q \mathcal{V}_i U, \quad R_Q = [Q (\mathcal{L}_{\text{TE}}^{(0)} - \lambda_{\text{ref}}) Q]^{-1}, \quad \mathcal{R} = -Q [i \mathcal{V}_i \Xi_i + (\partial_{R_i} \varepsilon^{-1}) D_{r_i} U]$$

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) $U(\mathbf{R})$: retained Bloch frame, columns u_n $D_{r_i} = \partial_{r_i} + i k_{0,i}$ (fast cov. deriv.) $D_{R_i} = \partial_{R_i} + i q_i$ (slow cov. deriv.) φ : smooth test field $\langle \cdot, \cdot \rangle_\Omega$: fast-cell inner product

Figure 55: The complete TE effective Hamiltonian of Section 3.5.5 with every term written out. Bracket colours mark the order in η ; term colours mark the five named ingredients and the Löwdin remote-band pieces. The second-order bracket is the flux form Equation 59 plus the remote-band excursion $-S^\dagger R_Q S$ of Equation 91; slow derivatives act on everything to their right.

Full TM Effective Hamiltonian

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

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

$$+ \eta^2 \left[\underbrace{\frac{1}{2} \Pi_i \tilde{M}_{ij}^{-1} \Pi_j}_{\text{inverse mass tensor} + (\text{Löwdin downfolded})} + \underbrace{Y_i^\dagger Y_i}_{\text{Born-Huang (TM)}} + \underbrace{\tilde{K}_i^\dagger \mathcal{D}_i - \mathcal{D}_i \tilde{K}_i}_{\text{direct 1-deriv. remainder}} + \underbrace{\mathcal{D}_i \tilde{\mathcal{T}}_i^\dagger R_Q \tilde{\mathcal{R}} - \tilde{\mathcal{R}}^\dagger R_Q \tilde{\mathcal{T}}_i \mathcal{D}_i}_{\text{Löwdin 1-deriv. cross}} - \underbrace{\tilde{\mathcal{R}}^\dagger R_Q \tilde{\mathcal{R}}}_{\text{Löwdin scalar}} \right] + O(\eta^3)$$

acts on the hermitized envelope $\tilde{f}$ of $\tilde{\psi} = \varepsilon^{1/2} \psi$; slow derivatives act on everything to their right; same flux-form and $-\tilde{S}^\dagger R_Q \tilde{S}$ bookkeeping as the TE poster, every coefficient dressed by ρ

where

gauge-covariant slow momentum, slow covariant derivative, and Berry connection of the hermitized frame

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

Löwdin-corrected inverse mass tensor; weighted metric $\tilde{G}_{mn} = \langle \tilde{u}_m, \varepsilon^{-1} \tilde{u}_n \rangle_\Omega$

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

direct one-derivative coefficient (flux form of $-\rho D_{R_i} D_{R_i} \rho$ projected on $\tilde{U}$)

$$\tilde{K}_i = \tilde{U}^\dagger \rho Y_i, \quad \tilde{\mathcal{H}}_{\text{dir}}^{(2)} = -\mathcal{D}_i (\tilde{G} \mathcal{D}_i + \tilde{K}_i) + \tilde{K}_i^\dagger \mathcal{D}_i + Y_i^\dagger Y_i$$

remote-band excursion (manifestly Hermitian; expanded into the three Löwdin pieces above)

$$\tilde{S} = \tilde{\mathcal{T}}_i \mathcal{D}_i + \tilde{\mathcal{R}}, \quad \tilde{\mathcal{H}}_{\text{remote}}^{(2)} = -\tilde{S}^\dagger R_Q \tilde{S}$$

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

$$\tilde{\mathcal{V}}_i \varphi = -2i \rho D_{r_i} (\rho \varphi) = -2i \varepsilon^{-1} D_{r_i} \varphi + i \varepsilon^{-2} (\partial_{r_i} \varepsilon) \varphi, \quad \tilde{v}_{mn}^{(i)} = \langle \tilde{u}_m, \tilde{\mathcal{V}}_i \tilde{u}_n \rangle_\Omega$$

frame leakage, TM leakage flux (carries the slow variation of ρ ; no TE analogue), first-order scalar remainder

$$\tilde{\Xi}_i = Q \partial_{R_i} \tilde{U}, \quad Y_i = \rho \tilde{\Xi}_i + (\partial_{R_i} \rho) \tilde{U}, \quad \tilde{\Xi}_{\text{sc}}^{(1)} = -\sum_i [i \tilde{U}^\dagger \tilde{\mathcal{V}}_i \tilde{\Xi}_i + 2 \tilde{U}^\dagger \rho D_{r_i} ((\partial_{R_i} \rho) \tilde{U})]$$

Löwdin coupling operators (P - Q channels) and reduced resolvent of the hermitized local operator

$$\tilde{\mathcal{T}}_i = -i Q \tilde{\mathcal{V}}_i \tilde{U}, \quad R_Q = [Q (\tilde{\mathcal{H}}_{\text{TM}}^{(0)} - \lambda_{\text{ref}}) Q]^{-1}, \quad \tilde{\mathcal{R}} = -Q [i \tilde{\mathcal{V}}_i \tilde{\Xi}_i + 2 \rho D_{r_i} ((\partial_{R_i} \rho) \tilde{U})]$$

TM Born-Huang potential, expanded (ε^{-1} -weighted leakage plus the hermitizing-factor terms)

$$U_{\text{BH,TM}} = Y_i^\dagger Y_i = \tilde{\Xi}_i^\dagger \varepsilon^{-1} \tilde{\Xi}_i + [\tilde{\Xi}_i^\dagger \rho (\partial_{R_i} \rho) \tilde{U} + \text{h.c.}] + \tilde{U}^\dagger (\partial_{R_i} \rho)^2 \tilde{U}$$

$$\rho = \varepsilon^{-1/2}, \quad \tilde{u}_n = \varepsilon^{1/2} u_n^{\text{TM}} \text{ (hermitized local Bloch states, plain-orthonormal)} \quad | \quad \tilde{\mathcal{H}}_{\text{TM}}^{(0)} = -\rho D_r \cdot D_r \rho \quad | \quad P = \tilde{U} \tilde{U}^\dagger, Q = 1 - P \quad | \quad D_{r_i} = \partial_{r_i} + i k_{0,i}, D_{R_i} = \partial_{R_i} + i q_i \quad | \quad \langle \cdot, \cdot \rangle_\Omega: \text{fast-cell inner product}$$

Figure 56: The complete TM effective Hamiltonian of Section 3.6.2 in the same layout. Every coefficient carries the hermitizing factor $\rho = \varepsilon^{-1/2}$, and the leakage flux Y_i of Equation 77 collects the slow variation of ρ that has no TE analogue. Coefficient identities are listed in Appendix B.

Appendix B: Downfolding and Coefficient Identities

TE Downfolding Identities

This section records the exact remainder decompositions and Löwdin split used in Section 3.5.5. The covariant frame notation $(U, P, Q, A_i, \Xi_i, \Pi_i)$ is defined in the main text at Equation 51 through Equation 54. Throughout, slow derivatives act on everything to their right, including the $\mathbf{R}$ -dependence of coefficient operators, and $\mathcal{D}_i^\dagger = -\mathcal{D}_i$ on the moire torus.

First-Order Exact Remainder

The exact first-order projected operator may be written as

$$\mathcal{H}_{\text{TE,exact}}^{(1)} = -iv^{(i)}\mathcal{D}_i + \Xi_{\text{sc}}^{(1)} \quad (85)$$

where the scalar remainder produced by slow-frame and slow-coefficient terms is

$$\Xi_{\text{sc}}^{(1)} := - \sum_{i=x,y} \left[iU^\dagger \mathcal{V}_i \Xi_i + U^\dagger (\partial_{R_i} \varepsilon^{-1}) D_{r_i} U \right] \quad (86)$$

Comparing this with the symmetrized drift gives

$$\mathcal{H}_{\text{TE,exact}}^{(1)} = \frac{1}{2} (v^{(i)} \Pi_i + \Pi_i v^{(i)}) + U_{\text{rem}}^{(1)} \quad (87)$$

with exact remainder

$$U_{\text{rem}}^{(1)} := \Xi_{\text{sc}}^{(1)} + \frac{i}{2} \partial_{R_i} v^{(i)} + \frac{1}{2} [A_i, v^{(i)}] \quad (88)$$

The three correction terms arise, respectively, from the slow variation of u_n and ε^{-1} not absorbed into the velocity coupling, from the $\mathbf{R}$ -derivative of the velocity field itself, and from the commutator with the Berry connection. The commutator is what is left when the symmetrized product is expanded with $\Pi_i = -i\mathcal{D}_i$ and $\mathcal{D}_i = D_{R_i} - iA_i$: the Berry connection enters the exact operator once, through $\mathcal{D}_i$, and the symmetrization must not count it a second time.

Löwdin Split of the Remote-Band Term

To expose the structure of the Löwdin correction in Equation 56, define

$$\mathcal{T}_i := -iQ\mathcal{V}_iU \quad (89)$$

and

$$\mathcal{R} := -Q \left[i\mathcal{V}_i \Xi_i + (\partial_{R_i} \varepsilon^{-1}) D_{r_i} U \right]. \quad (90)$$

The first-order operator restricted to the excursion into the remote sector is then $Q\mathcal{L}_{\text{TE}}^{(1)}U = \mathcal{T}_i\mathcal{D}_i + \mathcal{R} =: S$, and the remote-band term is the manifestly Hermitian form

$$-U^\dagger \mathcal{L}_{\text{TE}}^{(1)} Q R_Q Q \mathcal{L}_{\text{TE}}^{(1)} U = -S^\dagger R_Q S, \quad S := \mathcal{T}_i \mathcal{D}_i + \mathcal{R}. \quad (91)$$

Expanding with $\mathcal{D}_i^\dagger = -\mathcal{D}_i$ gives

$$-S^\dagger R_Q S = \mathcal{D}_i (\mathcal{T}_i^\dagger R_Q \mathcal{T}_j \mathcal{D}_j + \mathcal{T}_i^\dagger R_Q \mathcal{R}) - \mathcal{R}^\dagger R_Q \mathcal{T}_i \mathcal{D}_i - \mathcal{R}^\dagger R_Q \mathcal{R}. \quad (92)$$

The first term is the remote-band kinetic correction that feeds into the mass tensor: with $\Pi_i = -i\mathcal{D}_i$ it reads $-\Pi_i \mathcal{T}_i^\dagger R_Q \mathcal{T}_j \Pi_j$, and $\mathcal{T}_i^\dagger R_Q \mathcal{T}_j = \sum_{\ell \notin P} v_{m\ell}^{(i)} v_{\ell n}^{(j)} / (\lambda_\ell - \lambda_{\text{ref}})$ reproduces the Löwdin sum of Equation 58 once the reference energy is replaced by the retained band energies. The second and third terms are the one-derivative cross remainders, the last term is the scalar remainder. Because the coefficient operators depend on $\mathbf{R}$, a split with the derivatives pulled out in front of frozen coefficients is neither an operator identity nor Hermitian; the form Equation 91 is the one to implement.

Scalar Sector and Born-Huang

The direct second-order operator admits two complete bookkeepings. The raw split Equation 49 uses the coefficients G , $B^{(i)}$ and $\Gamma^{(2)}$. The flux form uses the leakage Ξ_i and

$$K_i := U^\dagger \varepsilon^{-1} \Xi_i, \quad (93)$$

and reads

$$\mathcal{H}_{\text{TE,dir}}^{(2)} = -\mathcal{D}_i(G\mathcal{D}_i + K_i) + K_i^\dagger \mathcal{D}_i + \Xi_i^\dagger \varepsilon^{-1} \Xi_i. \quad (94)$$

The two forms are equal; the scalar $\Gamma^{(2)}$ of the raw split is contained in the leakage and K terms of the flux form, so the two must never be added. Combining the metric term $-\mathcal{D}_i G \mathcal{D}_i = \Pi_i G \Pi_i$ with the Löwdin kinetic correction from Equation 92 yields the full Hermitian inverse mass tensor stated in Equation 58. The last term of Equation 94 is the exact TE Born-Huang leakage penalty, weighted by ε^{-1} . The commonly cited unweighted form $\Xi_i^\dagger \Xi_i$ is recovered only after replacing ε^{-1} by its cell-averaged value.

TM Coefficient Identities

This section records the TM-specific coefficient definitions used in Section 3.6.2. The covariant frame identities (Berry connection, leakage operators, covariant momentum) are identical to those in the TE section above, applied to the hermitized Bloch states $\tilde{u}_n := \varepsilon^{\frac{1}{2}} u_n^{\text{TM}}$ collected in the frame $\tilde{U}$.

Hermitized TM Velocity

Setting $\rho := \varepsilon^{-1/2}$, the hermitized TM velocity operator is

$$\tilde{\mathcal{V}}_i \varphi := -2i\rho D_{r_i}(\rho\varphi) \quad (95)$$

Expanding the product rule yields the two-term form stated in Equation 75:

$$\tilde{\mathcal{V}}_i \varphi = -2i\varepsilon^{-1} D_{r_i} \varphi + i\varepsilon^{-2} (\partial_{r_i} \varepsilon) \varphi \quad (96)$$

The velocity matrix elements for any $\alpha, \beta \in P \cup Q$ are

$$\tilde{v}_{\alpha\beta}^{(i)} := \langle \tilde{u}_\alpha, \tilde{\mathcal{V}}_i \tilde{u}_\beta \rangle_\Omega \quad (97)$$

First-Order Remainder

For any $\alpha, \beta \in P \cup Q$, the exact TM first-order remainder matrix is

$$\tilde{\Gamma}_{\alpha\beta}^{(1)} = - \sum_{i=x,y} \left[i \langle \tilde{u}_\alpha, \tilde{\mathcal{V}}_i (\partial_{R_i} \tilde{u}_\beta) \rangle_\Omega + 2 \langle \tilde{u}_\alpha, \rho D_{r_i} ((\partial_{R_i} \rho) \tilde{u}_\beta) \rangle_\Omega \right] \quad (98)$$

The second term, proportional to $\partial_{R_i} \rho$, arises from the slow variation of the hermitizing factor and has no TE analogue. Compare the TE remainder in Equation 86, where the corresponding slot is occupied by the slow dielectric gradient $\partial_{R_i} \varepsilon^{-1}$ acting directly. Splitting $\partial_{R_i} \tilde{U} = -i\tilde{U} A_i + \tilde{\Xi}_i$ turns Equation 98 into the covariant form $-i\tilde{v}^{(i)} \mathcal{D}_i + \tilde{\Xi}_{\text{sc}}^{(1)}$ with

$$\tilde{\Xi}_{\text{sc}}^{(1)} := - \sum_{i=x,y} \left[i\tilde{U}^\dagger \tilde{\mathcal{V}}_i \tilde{\Xi}_i + 2\tilde{U}^\dagger \rho D_{r_i} ((\partial_{R_i} \rho) \tilde{U}) \right], \quad (99)$$

and the symmetrized remainder is $\tilde{U}_{\text{rem}}^{(1)} = \tilde{\Xi}_{\text{sc}}^{(1)} + (i/2) \partial_{R_i} \tilde{v}^{(i)} + \frac{1}{2} [A_i, \tilde{v}^{(i)}]$, exactly as in the TE case.

Direct Second-Order Coefficients

The metric, one-derivative, and scalar matrices entering the raw split of the direct retained-space second-order operator are

$$\begin{aligned} \tilde{G}_{mn} &= \langle \tilde{u}_m, \rho^2 \tilde{u}_n \rangle_\Omega = \langle \tilde{u}_m, \varepsilon^{-1} \tilde{u}_n \rangle_\Omega \\ \tilde{B}_{mn}^{(i)} &= 2 \langle \tilde{u}_m, \varepsilon^{-1} \partial_{R_i} \tilde{u}_n \rangle_\Omega - \langle \tilde{u}_m, \varepsilon^{-2} (\partial_{R_i} \varepsilon) \tilde{u}_n \rangle_\Omega \\ \tilde{\Gamma}_{mn}^{(2)} &= - \sum_{i=x,y} \langle \tilde{u}_m, \rho \partial_{R_i}^2 (\rho \tilde{u}_n) \rangle_\Omega \end{aligned} \quad (100)$$

The one-derivative coefficient $\tilde{B}^{(i)}$ differs from the TE case by the explicit dielectric-gradient correction $\varepsilon^{-2}\partial_{R_i}\varepsilon$, while $\tilde{\Gamma}^{(2)}$ acquires slow second derivatives of ρ through the product rule. The equivalent flux form uses the TM leakage flux $Y_i = \rho\tilde{\Xi}_i + (\partial_{R_i}\rho)\tilde{U}$ of Equation 77 and $\tilde{K}_i := \tilde{U}^\dagger\rho Y_i$,

$$\tilde{\mathcal{H}}_{\text{TM,dir}}^{(2)} = -\mathcal{D}_i(\tilde{G}\mathcal{D}_i + \tilde{K}_i) + \tilde{K}_i^\dagger\mathcal{D}_i + Y_i^\dagger Y_i, \quad (101)$$

whose last term is the TM Born-Huang penalty.

Löwdin Split

With $\tilde{\mathcal{T}}_i := -iQ\tilde{\mathcal{V}}_i\tilde{U}$, $\tilde{\mathcal{R}} := -Q[i\tilde{\mathcal{V}}_i\tilde{\Xi}_i + 2\rho D_{r_i}((\partial_{R_i}\rho)\tilde{U})]$, $\tilde{S} := \tilde{\mathcal{T}}_i\mathcal{D}_i + \tilde{\mathcal{R}}$ and the reduced resolvent $R_Q = [Q(\tilde{\mathcal{H}}_{\text{TM}}^{(0)} - \lambda_{\text{ref}})Q]^{-1}$ of the hermitized local operator, the TM remote-band term is $-\tilde{S}^\dagger R_Q \tilde{S}$, with the same expansion as Equation 92. Its kinetic part, combined with $\tilde{G}$, gives the TM mass tensor: the structural formula Equation 58 with $\tilde{v}$ and $\tilde{G}$ in place of v and G .

Appendix C: Computational Hardware

All numerical results, benchmarks, and timing measurements reported in this thesis were obtained on a single desktop workstation. The hardware specifications are listed below for reproducibility of the performance data discussed in Section 4, in particular the memory-bandwidth bottleneck identified in Section 4.6 and the single-core and multi-core benchmarks in Section 4.8. The computations of Section 5 ran on the same machine under WSL2 with 40 GB of memory available to the Linux guest.

Reproducibility and Software

The custom open-source ecosystem developed for this thesis is divided into two primary projects: **MSL (Moire SuperLattice)**, available as a repository [49] with full documentation [50], and **Blaze2D**, published as a repository [39], a Python package [40], and a technical report [51]. Every figure of Section 5 from Section 5.4 on is produced by a script under `assets/python/second_edition/` of the thesis repository from small result snapshots under `assets/data/second_edition/`; each script header names the MSL command and commit that produced its data.

Icons from the preface were taken from The Noun Project.

Processor

Model	Intel Core i9-13900K (Raptor Lake, 13th Gen)
Cores	24 total: 8 Performance-cores + 16 Efficiency-cores
Threads	32 (Hyper-Threading on P-cores)
P-core clock	3.0 GHz base / 5.8 GHz turbo (non-overclocked)
E-core clock	2.2 GHz base / 4.3 GHz turbo
L1 data cache	48 KB per P-core, 32 KB per E-core
L1 instruction cache	32 KB per P-core, 64 KB per E-core
L2 cache	2 MB per P-core, 4 MB per E-core cluster (4 cores)
L3 cache (shared)	36 MB Intel Smart Cache

For multi-threaded benchmarks all *physical* cores were utilized.

Memory

The memory-bandwidth ceiling relevant to the mixed-precision discussion in Section 4.6 is set by the product of channel count, bus width, and effective data rate. Because the LOBPCG solver is memory-bandwidth-bound rather than compute-bound (Section 4.6), halving the storage precision from f64 to f32 translates almost directly into a $2 \times$ throughput gain.

Type	DDR5
Total capacity	64 GB
Channel configuration	4 $\times$ 32-bit channels
NB frequency	4500 MHz
DRAM frequency	2100 MHz
FSB : DRAM ratio	1 : 21
CAS latency	CL 36

Appendix D: Additional Figures

This appendix collects supplementary figures from the EA–FDFD comparison studies discussed in Section 5. The hexagonal-rod crystal at the M point ($\varepsilon = 12$, $r/a = 0.22$, TM polarisation) was used as an early multi-band test case with an earlier implementation of the envelope operator, before the defects listed in Section 5.4 were repaired. The FDFD lanes are unaffected; the EA lanes carry that earlier operator (fermion-doubled kinetic stencil, non-Hermitian Löwdin term, single-precision solve) and are kept as a record of that stage, not as a validation.

EA vs FDFD: Hexagonal Crystal at the M Point

Figure 57 shows the mode-by-mode eigenfrequency comparison. At each angle, sorted FDFD eigenfrequencies are plotted for resolutions from 1 to 16 px/ a , alongside the EA prediction of the earlier operator. The EA eigenvalues track the converged FDFD reference closely at small angles (1° – 2°), where the scale-separation parameter η is small. At larger angles (4° – 8°), the EA spectrum is systematically narrower than the FDFD spectrum.

Hex rods $\varepsilon = 12$, $r/a = 0.22$, TM at M — 50 lowest modes

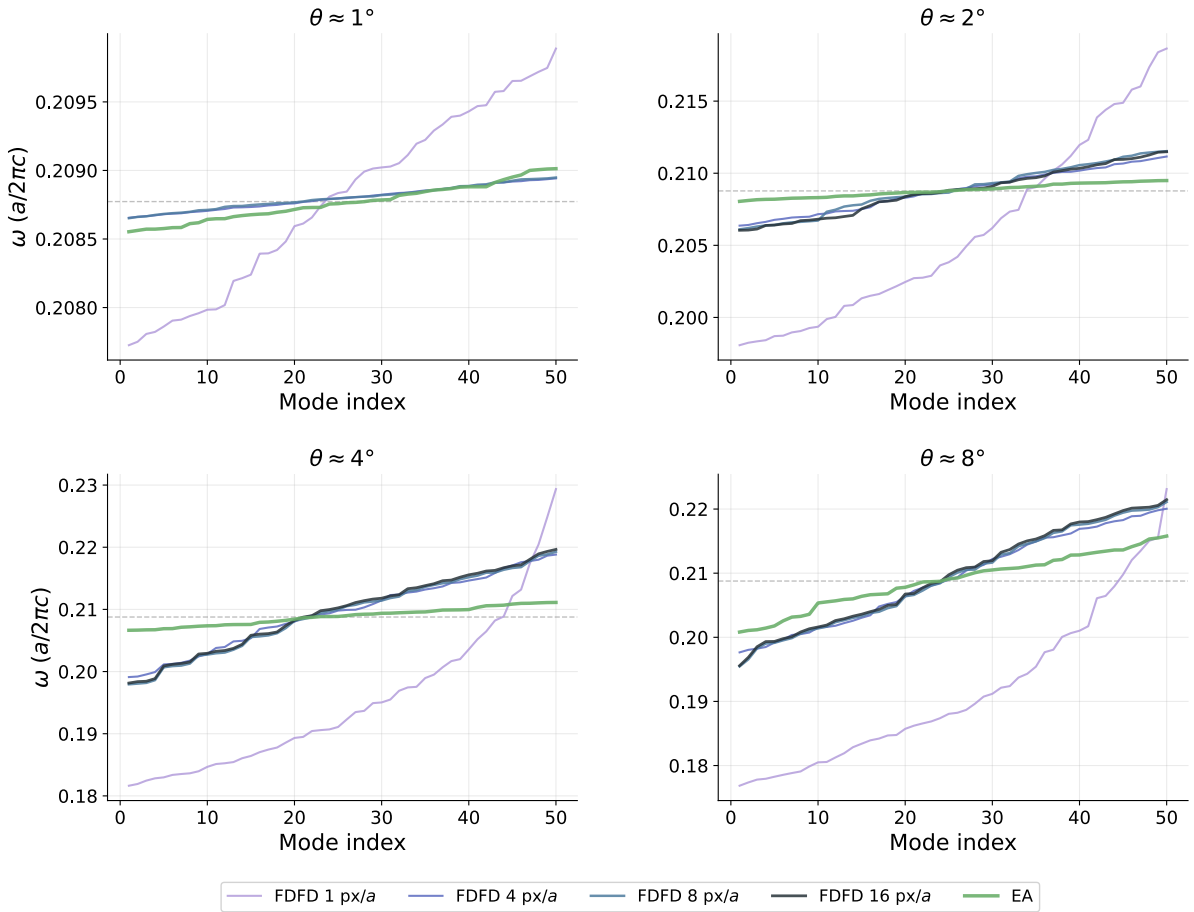


Figure 57: Mode-by-mode eigenfrequency comparison for the hexagonal-rod crystal ($\varepsilon = 12$, $r/a = 0.22$, TM at M) at four twist angles. Each panel shows sorted eigenfrequencies vs. mode index for FDFD at several resolutions (purple–charcoal) and the EA prediction of the earlier operator (green). The dashed line marks the monolayer M -point frequency $\omega \approx 0.2088$. At small angles the EA and converged FDFD curves nearly coincide; at larger angles the EA bandwidth is systematically narrower.



Figure 58: Eigenvalue-stripe overview for the same four configurations as Figure 57. Each horizontal lane shows the 50 lowest eigenfrequencies as vertical lines. The two FDFD lanes (1 px/a and best available resolution) are compared against the EA lane of the earlier operator. The dotted vertical line marks the monolayer M -point frequency.

Figure 59 displays the spatial structure of the EA envelope eigenvectors. The normalised envelope intensity $|F|^2$ is shown for the six lowest modes at each twist angle. At large angles the envelopes show clear moire-scale nodal patterns; at small angles the extreme band flatness ($\Delta\omega < 10^{-3}$) yields dense, noisy patterns on the coarse envelope grid.

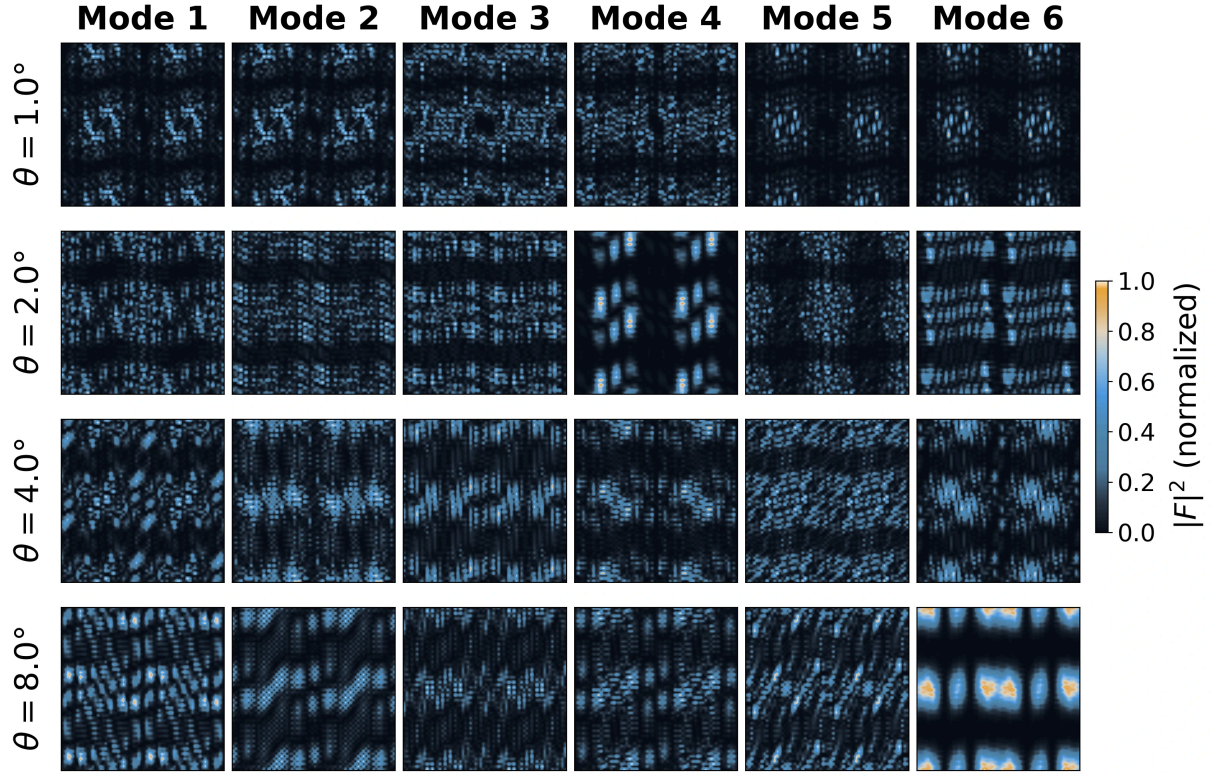


Figure 59: EA envelope mode profiles $|F|^2$ (normalised) for the six lowest modes at Γ , hexagonal TM crystal at M , at four twist angles, earlier operator. Columns: mode index 1–6; rows: $\theta = 1^\circ, 2^\circ, 4^\circ, 8^\circ$. At large angles the modes show clear moiré-scale structure; at small angles the extreme band flatness yields dense, noisy patterns on the coarse envelope grid.

Figure 60 shows the bandwidth scaling. The converged FDFD data follows the expected θ^2 law in this kinetic-dominated crystal. The EA bandwidth tracks the same trend but sits consistently below, reflecting the narrower spectral coverage seen in the line plots.

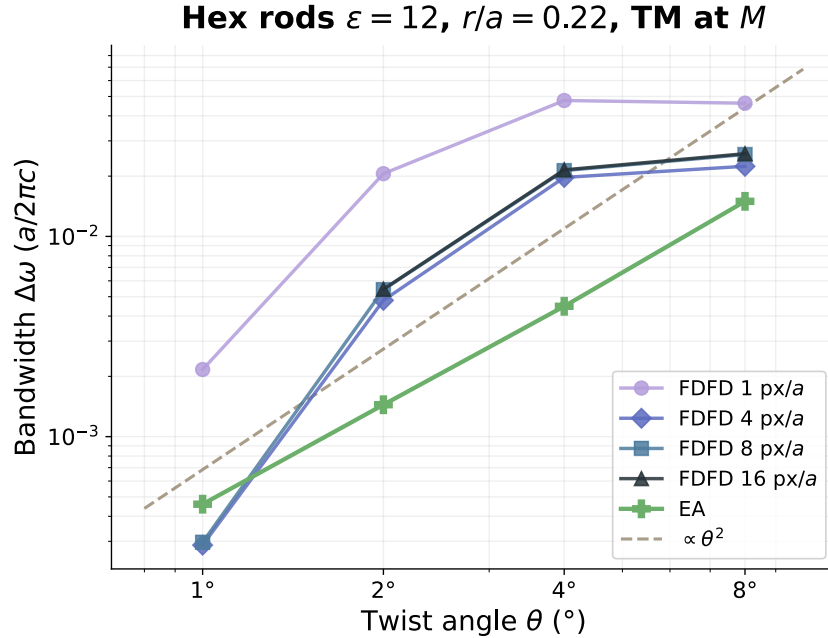


Figure 60: Bandwidth $\Delta\omega$ of the 50 lowest TM modes at M vs. twist angle θ for the hexagonal-rod crystal ($\varepsilon = 12$, $r/a = 0.22$). FDFD at four resolutions (purple–charcoal) and the EA prediction of the earlier operator (green) are shown on log-log axes; the dashed line is a θ^2 reference. The converged FDFD data follows $\Delta\omega \propto \theta^2$. The EA bandwidth tracks the same scaling law but is systematically narrower.

Honeycomb TM Dirac Stack at K

Figure 61 shows the full ten-layer EA ingredient stack for the honeycomb TM crystal at K , and Figure 62 shows the same registry-domain data mapped onto moire cells of three twist angles. Both are produced from the extraction at the K corner, $\mathbf{k}_0 = (2/3, 1/3)$, with the Dirac pair in bands 1 and 2 (zero-based) and a parallel-transport gauge across the registry grid (Section 5.8).

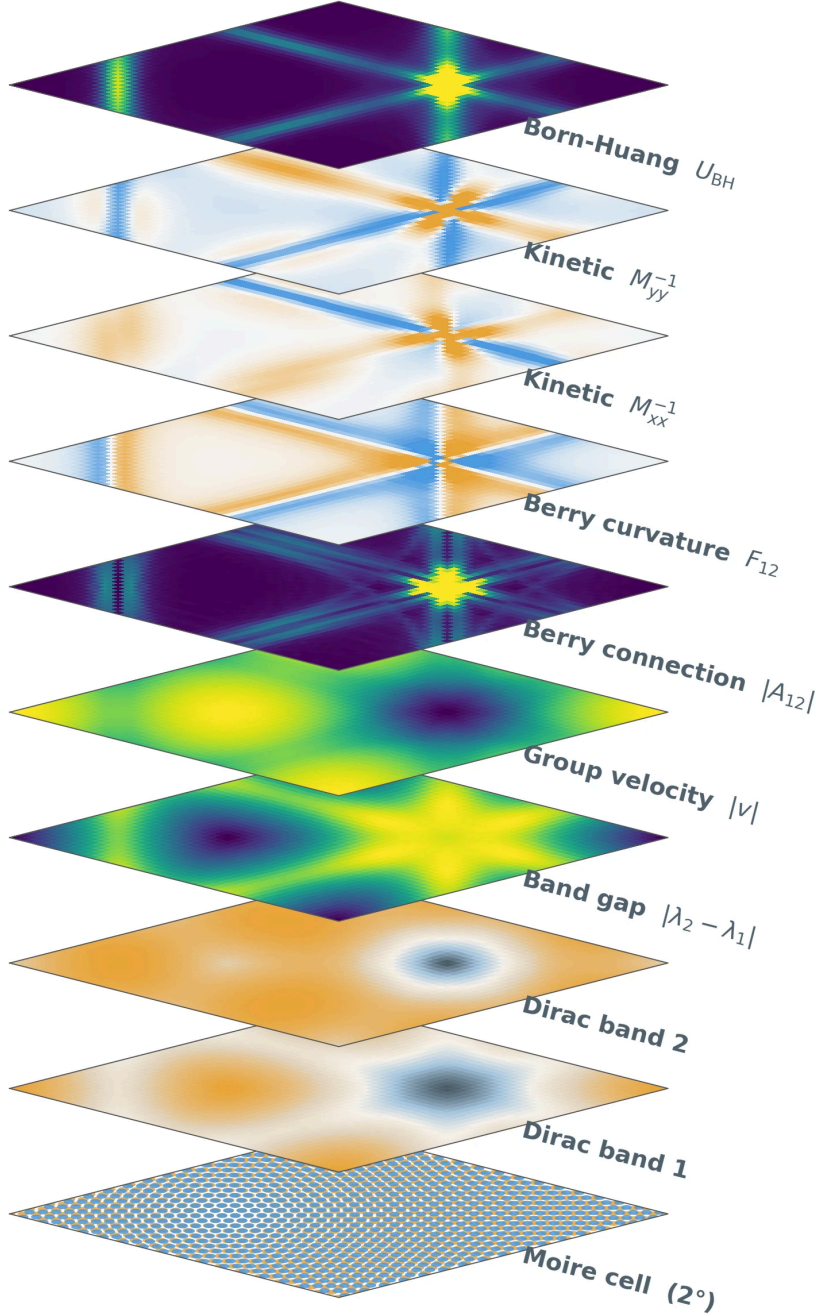


Figure 61: Full EA ingredient stack for the honeycomb TM photonic crystal at the K -point Dirac cone. Ten layers spanning the complete set of envelope Hamiltonian ingredients: crystal unit cell, eigenvalue maps for the two Dirac bands, group-velocity norm, kinetic mass tensors, Born-Huang correction, Berry curvature of the Dirac pair, Berry connection $|A_{12}|$ in the parallel-transport gauge, and the inter-band gap $\Delta\lambda$ between the two Dirac bands. The 48×48 registry sweep resolves the full spatial structure across the moire unit cell.

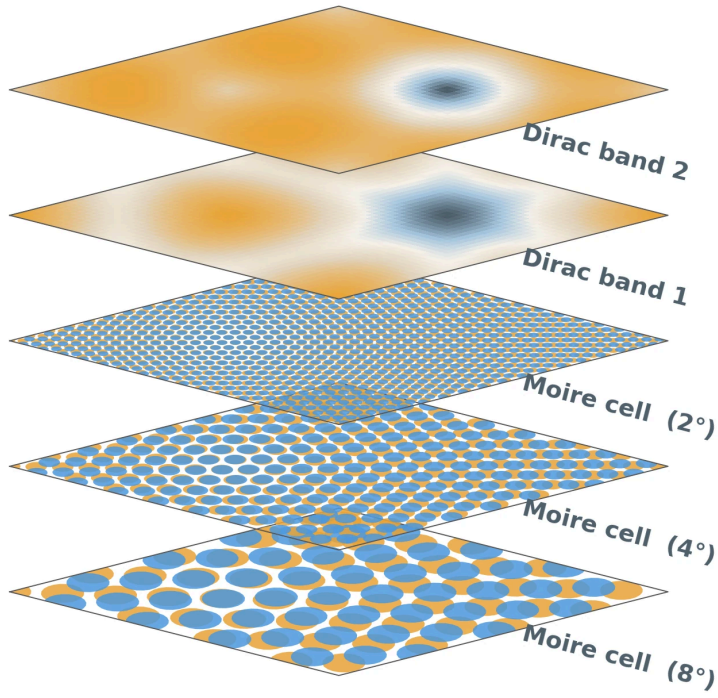


Figure 62: Registry-domain landscapes of the two Dirac bands (bands 1 and 2, zero-based) of the honeycomb TM crystal, stacked above the moire cells at 8° , 4° , and 2° . The registry data are independent of the twist angle; only the moire cell they are mapped onto changes with θ , which is the Phase 1 invariance of Section 5.1.1 made visible.

Appendix E: Errata to the First Edition

The first edition of this thesis was submitted on March 27, 2026. The corrections below were established by the post-submission audit of the derivation and of the numerical pipeline, each by a direct test (exact algebra, machine-precision identity checks on band-limited test spaces, or controlled reruns). The list gives the first-edition statement, its location, and where the second edition treats the corrected form. Figures whose underlying data were regenerated are marked as such.

Location (1st ed.)	First-edition statement	Second edition
Sec. 3.1, registry map	$\delta_{\text{raw}}(\mathbf{R}) = (R_{-\frac{\theta}{2}} - R_{+\frac{\theta}{2}})\mathbf{R}$, short by one factor of $1/\eta$; the literal map never traverses the registry torus and contradicts the drift estimate of the same section.	$\delta_{\text{raw}}(\mathbf{R}) = (R_{-\frac{\theta}{2}} - R_{+\frac{\theta}{2}})x/a = -J\mathbf{R}$ with constant Jacobian $-J$ (Equation 12, Equation 22).
Sec. 3.2, two-scale lift	The diagonal restriction of the lifted proxy was called “the actual moire permittivity”.	It differs from the exact bilayer by a $\cos(\theta/2)$ dilation of the fast frame, an $O(\eta^2)$ effect; the exact layer-locked lift is Equation 20.
Sec. 3.5, gauge freedom	Unrestricted frame rotations $U \rightarrow UW(\mathbf{R})$ were said to leave the assembled operator gauge-meaningful.	Admissible W are phases, permutations, and rotations inside degenerate blocks, because Λ is kept diagonal and the Löwdin denominators carry band labels (Section 3.5.3).
App. A, first-order remainder	$U_{\text{rem}}^{(1)}$ contained the anticommutator $\frac{1}{2}(A_i v^{(i)} + v^{(i)} A_i)$, which counts the Berry connection twice.	Commutator $\frac{1}{2}[A_i, v^{(i)}]$ (Equation 88).
App. A, Löwdin split	The displayed expansion of the remote-band term was sign-flipped and non-Hermitian, and inconsistent with the (correct) mass tensor of the main text.	Manifestly Hermitian form $-S^\dagger R_Q S$ with $S = \mathcal{T}_i \mathcal{D}_i + \mathcal{R}$ and its expansion (Equation 91, Equation 92).
Sec. 3.5 and the TE Hamiltonian figure	The scalar $\Gamma^{(2)}$ was added on top of the leakage and K terms it already contains, and the Löwdin cross term was shown without its slow derivative.	Flux form Equation 59; corrected TE poster and new TM poster in Appendix A.
Sec. 3.6, TM operator	No expanded TM operator and no TM leakage identity were given.	TM leakage flux Y_i (Equation 77), TM flux form and Löwdin split (Appendix B), TM poster.
Sec. 3.7 (new)	The expansion was not related to its all-orders limit.	The resummed-frame model (Section 3.7, Equation 79).
Sec. 5.1, 5.6–5.8, App. C, all honeycomb data	The honeycomb TM extraction used $\mathbf{k}_0 = (1/3, 1/3)$, an interior point on the Γ – K line at 58 % of the corner distance, and retained bands 2–3 (zero-based), which are only accidentally near-degenerate there. Berry-connection maps were gauge-blind and showed noise.	All honeycomb figures regenerated at $K = (2/3, 1/3)$ with the Dirac pair in bands 1–2 ($\omega_D = 0.6394$), a parallel-transport gauge, and gauge-invariant metrics; the magic-angle scan was rerun on the same angle set (Section 5.8, Section 5.9).
Sec. 5.4.2, square comparison	Three bands near X of the equal-rod square crystal were said to pass the isolation criterion, and the EA–FDFD spectra were compared on that basis.	The equal-rod crystal has no registry-common gap; its X manifold dissolves into the folded band-0 continuum, so no eigenvalue comparison is possible there for any method (Section 5.4). The comparison moved to the asymmetric bilayer (Section 5.5).

Location (1st ed.)	First-edition statement	Second edition
Sec. 5.4.2, bandwidth scaling	Both FDFD and EA were said to follow $\Delta\omega \propto \theta^2$; only EA data were shown.	Quadratic scaling holds in the kinetic-dominated regime; the thesis crystal is potential-dominated and does not follow it (Section 5.5).
Sec. 5.4.3, deficient single-band case	A single retained band was diagnosed as too simple to reproduce a supercell spectrum.	Withdrawn: a single band with exact frames is reference-limited on every state of its domain; the failure was the fixed-frame dispersion error (Section 5.6).
Sec. 5.5	Whether eigenvalue-by-eigenvalue agreement is “even the right metric” was left open.	It is the right metric and it is reached under the protocol of Section 5.4.
Ch. 5, pipeline	The first-edition envelope operator carried a fermion-doubled kinetic stencil, a non-Hermitian Löwdin term, grid-divergent boundary fields, and a single-precision eigensolve.	All four repaired before any second-edition run (Section 5.4).
App. C, Fig. 58 caption	Described “five Hamiltonian layers on three moire grids”.	The figure shows the two Dirac-band landscapes above three moire cells (Figure 62).

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] J. W. (L. R. Strutt, On the manufacture and theory of diffraction-gratings, *Philosophical Magazine* **47**, 81 (1874).
- [4] R. S. Sirohi and F. S. Chau, *Optical Methods of Measurement: Wholefield Techniques* (Marcel Dekker, 1999).
- [5] S. Dufresne, *Using Moiré Patterns To Guide Ships*, <https://hackaday.com/2018/04/07/using-moire-patterns-to-guide-ships/>.
- [6] R. Bistritzer and A. H. MacDonald, Moiré bands in twisted double-layer graphene, *Proceedings of the National Academy of Sciences* **108**, 12233 (2011).
- [7] Y. Cao et al., Correlated insulator behaviour at half-filling in magic-angle graphene superlattices, *Nature* **556**, 80 (2018).
- [8] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, Unconventional superconductivity in magic-angle graphene superlattices, *Nature* **556**, 43 (2018).
- [9] J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, *Photonic Crystals: Molding the Flow of Light*, 2nd ed. (Princeton University Press, 2008).
- [10] P. Wang, Y. Zheng, X. Chen, C. Huang, Y. V. Kartashov, L. Torner, V. V. Konotop, and F. Ye, Localization and delocalization of light in photonic moiré lattices, *Nature* **577**, 42 (2020).
- [11] H. Tang, F. Du, S. Carr, C. DeVault, O. Mello, and E. Mazur, Modeling the optical properties of twisted bilayer photonic crystals, *Light: Science & Applications* **10**, 157 (2021).
- [12] K. Dong, T. Zhang, J. Li, Q. Wang, F. Yang, Y. Rho, D. Wang, C. P. Grigoropoulos, J. Wu, and J. Yao, Flat Bands in Magic-Angle Bilayer Photonic Crystals at Small Twists, *Physical Review Letters* **126**, 223601 (2021).
- [13] B. Lou, N. Zhao, M. Minber, C. Guo, J. Vuckovic, and S. Fan, Theory for Twisted Bilayer Photonic Crystal Slabs, *Physical Review Letters* **126**, 136101 (2021).
- [14] X.-R. Mao, Z.-K. Shao, H.-Y. Luan, S.-L. Wang, and R.-M. Ma, Magic-angle lasers in nanostructured moiré superlattice, *Nature Nanotechnology* **16**, 1099 (2021).
- [15] C.-H. Yi, H. C. Park, and M. J. Park, Strong interlayer coupling and stable topological flat bands in twisted bilayer photonic Moiré superlattices, *Light: Science & Applications* **11**, 289 (2022).
- [16] L. Huang, W. Zhang, and X. Zhang, Moiré Quasibound States in the Continuum, *Physical Review Letters* **128**, 253901 (2022).
- [17] H. Tang, X. Ni, F. Du, V. Srikrishna, and E. Mazur, Experimental probe of twist angle-dependent band structure of on-chip optical bilayer photonic crystal, *Science Advances* **9**, eadh8498 (2023).
- [18] H. Qin et al., Optical moiré bound states in the continuum, *Nature Communications* **15**, 9080 (2024).
- [19] Z. Yan, Y. Wang, X. Liu, and others, Cavity quantum electrodynamics with moiré photonic crystal nanocavity, *Nature Communications* **16**, 765 (2025).
- [20] M. Oudich, X. Kong, T. Zhang, C. Qiu, and Y. Jing, Engineered Moiré Photonic and Phononic Superlattices, *Nature Materials* **23**, 1169 (2024).
- [21] J. M. Luttinger and W. Kohn, Motion of Electrons and Holes in Perturbed Periodic Fields, *Physical Review* **97**, 869 (1955).
- [22] M. V. Berry, Quantal Phase Factors Accompanying Adiabatic Changes, *Proceedings of the Royal Society of London. Series A* **392**, 45 (1984).

- [23] F. Wilczek and A. Zee, Appearance of Gauge Structure in Simple Dynamical Systems, *Physical Review Letters* **52**, 2111 (1984).
- [24] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, 1954).
- [25] S. G. Johnson and J. D. Joannopoulos, Block-iterative frequency-domain methods for Maxwell's equations in a planewave basis, *Optics Express* **8**, 173 (2001).
- [26] J. D. Joannopoulos, P. R. Villeneuve, and S. Fan, Photonic crystals: putting a new twist on light, *Nature* **386**, 143 (1997).
- [27] K. Yee, Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media, *IEEE Transactions on Antennas and Propagation* **14**, 302 (1966).
- [28] A. Taflov and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, 3rd ed. (Artech House, 2005).
- [29] D. Gratias and M. Quinquandon, Crystallography of homophase twisted bilayers: coincidence, union lattices and space groups, *Acta Crystallographica Section A: Foundations and Advances* **79**, 301 (2023).
- [30] L. Zou, H. C. Po, A. Vishwanath, and T. Senthil, Band structure of twisted bilayer graphene: Emergent symmetries, commensurate approximants, and Wannier obstructions, *Physical Review B* **98**, 85435 (2018).
- [31] P. Yeh, A. Yariv, and C.-S. Hong, Electromagnetic propagation in periodic stratified media. I. General theory, *Journal of the Optical Society of America* **67**, 423 (1977).
- [32] A. Bensoussan, J.-L. Lions, and G. Papanicolaou, *Asymptotic Analysis for Periodic Structures* (North-Holland, 1978).
- [33] G. Allaire, Homogenization and two-scale convergence, *SIAM Journal on Mathematical Analysis* **23**, 1482 (1992).
- [34] P.-O. Löwdin, A Note on the Quantum-Mechanical Perturbation Theory, *The Journal of Chemical Physics* **19**, 1396 (1951).
- [35] R. Winkler, *Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems*, Vol. 191 (Springer, Berlin, 2003).
- [36] K. Sakoda, *Optical Properties of Photonic Crystals*, 2nd ed., Vol. 80 (Springer, Berlin, 2005).
- [37] P. Virtanen et al., SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python, *Nature Methods* **17**, 261 (2020).
- [38] M. Minkov, I. A. D. Williamson, M. Aggarwal, D. Gerini, S. Lou, Z. Song, T. W. Hughes, and S. Fan, Legume: an open-source Python solver for photonic crystal slabs, *Computer Physics Communications* **253**, 107198 (2020).
- [39] R.-M. Lehner, *Repository: Blaze2D - A Rust-based 2D PWE Maxwell Solver*, <https://github.com/RnLe/blaze2d>.
- [40] R.-M. Lehner, *PyPI: blaze2d*, <https://pypi.org/project/blaze2d/>.
- [41] A. V. Knyazev, Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method, *SIAM Journal on Scientific Computing* **23**, 517 (2001).
- [42] A. Farjadpour, D. Roundy, A. Rodriguez, M. Ibanescu, P. Bermel, J. D. Joannopoulos, S. G. Johnson, and G. W. Burr, Improving accuracy by subpixel smoothing in the finite-difference time domain, *Optics Letters* **31**, 2972 (2006).
- [43] A. Stathopoulos and K. Wu, A Block Orthogonalization Procedure with Constant Synchronization Requirements, *SIAM Journal on Scientific Computing* **23**, 2165 (2002).
- [44] J. Woo, S. Kim, and W. Y. Kim, Dynamic Precision Approach for Accelerating Large-Scale Eigenvalue Solvers in Electronic Structure Calculations on Graphics Processing Units, *Journal of Chemical Theory and Computation* **19**, 1457 (2023).

- [45] H. A. Gómez-Urrea, M. C. Ospina-Medina, J. D. Correa-Abad, M. E. Mora-Ramos, and F. J. Caro-Lopera, Tunable band structure in 2D Bravais–Moiré photonic crystal lattices, *Optics Communications* **459**, 125081 (2020).
- [46] K. Alnasser, S. Kamau, N. Hurley, J. Cui, and Y. Lin, Photonic Band Gaps and Resonance Modes in 2D Twisted Moiré Photonic Crystal, *Photonics* **8**, 408 (2021).
- [47] D. X. Nguyen, X. Letartre, E. Drouard, P. Viktorovitch, H. S. Nguyen, and T. P. Nguyen, Magic configurations in moiré superlattice of bilayer photonic crystals: Almost-perfect flatbands and unconventional localization, *Physical Review Research* **4**, L032031 (2022).
- [48] Y. Chen, T. A. Davis, W. W. Hager, and S. Rajamanickam, Algorithm 887: CHOLMOD, Supernodal Sparse Cholesky Factorization and Update/Downdate, *ACM Transactions on Mathematical Software* **35**, 1 (2008).
- [49] R.-M. Lehner, *Repository: MSL - Moire SuperLattice Generation and Analysis Pipeline*, <https://github.com/RnLe/msl>.
- [50] R.-M. Lehner, *Website: MSL Documentation*, <https://rnle.github.io/msl/>.
- [51] R.-M. Lehner, *Website: Blaze2D Technical Report & Documentation*, <https://rnle.github.io/blaze2d/blaze/>.

Glossary, Symbols & Abbreviations

Abbreviations

Abbr.	Meaning
CML	Commensurate moire lattice
CSL	Coincidence-site lattice
EA	Envelope approximation
FDFD	Finite-difference frequency-domain
LOBPCG	Locally optimal block preconditioned conjugate gradient
MPB	MIT Photonic Bands (plane-wave eigensolver)
PWE	Plane-wave expansion
TE	Transverse electric ($H_z \neq 0$)
TM	Transverse magnetic ($E_z \neq 0$)

Mathematical Symbols

Symbol	Description
$\mathbf{r}$	Fast (monolayer-scale) coordinate
$\mathbf{R}$	Slow (moire-scale) coordinate
$\delta(\mathbf{R})$	Registry map, the local inter-layer shift
$\varepsilon(\mathbf{x})$	Dielectric function
$\varepsilon_{\mathbf{G},\mathbf{G}'}^{-1}$	Inverse-permittivity Fourier matrix
$u_{n\mathbf{k}}(\mathbf{r})$	Bloch-periodic part of eigenstate n at $\mathbf{k}$
$\omega_n(\mathbf{k})$	Photonic band frequency
$\lambda_{n\mathbf{k}}$	Reduced eigenvalue ω^2/c^2
$\mathbf{G}$	Reciprocal lattice vector
$\mathbf{q}$	Moire Bloch momentum
$\mathbf{k}$	Crystal momentum / Bloch wavevector
$\mathbf{k}_0$	Carrier momentum (expansion point)
θ	Twist angle between the two layers
a	Monolayer lattice constant
L, L_m	Moire period
$\eta = a/L$	Scale-separation parameter
A_i	Non-Abelian Berry connection
Π_i	Gauge-covariant momentum
$M_{nm,ij}^{-1}$	Inverse mass tensor
U_{BH}	Born-Huang leakage potential
$D_{\mathbf{r}}, D_{\mathbf{R}}$	Fast / slow covariant derivatives
P, Q	Projectors onto retained / remote manifold
Ξ_i	Frame leakage $Q\partial_{R_i}U$ into the remote manifold
K_i	Direct one-derivative coefficient $U^\dagger \varepsilon^{-1} \Xi_i$ (flux form)
S, R_Q	Remote-band excursion $\mathcal{T}_i \mathcal{D}_i + \mathcal{R}$ and reduced resolvent

Key Concepts

Term	Definition
Band gap	Frequency window without propagating Bloch modes
Berry connection	Gauge potential from parameter dependence of Bloch states
Bloch's theorem	Eigenstates factorize into a plane wave and a lattice-periodic part
Born-Huang potential	Energy penalty from virtual leakage into remote bands
Dirac point	Dispersion crossing with linear (conical) dispersion
Envelope function	Slowly varying amplitude on the moire scale
Flat band	Band with near-zero group velocity
Effective Hamiltonian	Reduced moire-scale operator encoding band energies, geometric phases, and kinetic corrections
Löwdin partition	Perturbative folding of remote-band corrections into the active subspace
Magic angle	Twist angle at which moire minibands flatten
Moire pattern	Long-wavelength interference from nearly matched periodic structures
Photonic crystal	Periodic dielectric medium with electromagnetic band structure
Registry map	Smooth field $\delta(\mathbf{R})$ of local inter-layer shifts
Registry-common gap	Frequency window that is a band gap at every registry and every $\mathbf{k}$; the isolation criterion of an envelope manifold
Resummed frame	Envelope model with the exact local Bloch state at every moire harmonic; the all-orders limit of the η -expansion
Sylvester inertia	Exact count of eigenvalues below a shift from the LDL^T factorisation of the shifted pencil; certifies state censuses
Valley	Basin of one band extremum in the monolayer zone; distinct valleys fold to distinct or degenerate supercell sectors
Two-scale ansatz	Separation of fast coordinate $\mathbf{r}$ and slow coordinate $\mathbf{R}$

Symbol	Description
ρ, Y_i	Hermitizing factor $\varepsilon^{-1/2}$ and TM leakage flux
a_2	Interlayer amplitude of the smooth candidate's second layer

Term	Definition
Twistronics	Using geometric twist as a tuning parameter for band structure

Index

A

Avoided crossing 35

B

Band gap 5
 Band structure 5
 Berry connection 24
 Blaze2D 32
 Bloch function 6, 32
 Bloch s theorem 5
 Born-Huang potential 24
 Bragg penetration depth 14
 Brillouin zone 4, 18

C

Coincidence-site lattice 8
 Commensurate moire lattice 8
 Covariant derivative 21

D

Dielectric function 4, 32
 Downfolding 23

E

Effective Hamiltonian 24
 Eigenproblem 5, 32
 Envelope function 12

F

FDFD 6
 Flat band 5

H

High-symmetry point 5
 Homogenization theory 16

I

Incommensurate 8
 Inverse mass tensor 25

L

LOBPCG 32
 Local periodicity 12
 Löwdin partition 25

M

Maxwell s equations 4
 Moire lattice 6
 MPB 6

P

Permittivity matrix 32
 Perturbation theory 25
 Photonic crystal 4
 Plane-wave expansion 6, 32

R

Reciprocal lattice 7, 32
 Registry map 13
 Registry sweep 30, 36
 Registry-common gap 50

Resolution problem 9

S

Scale-separation parameter 16
 Spectral gap 24
 Subpixel smoothing 32
 Supercell 8

T

TE polarization 4
 TM polarization 4
 Twist angle 6
 Twisted bilayer 6
 Two-scale ansatz 12
 Two-scale lift v, 16

V

Velocity operator 22

Acknowledgements

On this page, I wish to take a brief moment to acknowledge the people who have made this work and the journey leading up to it possible.

Studying physics has been one of the best choices of my life. Yet a degree, and the thesis that concludes it, only truly gains meaning in the context of the people who shaped the journey: those who became friends, offered guidance, and carried me through stretches I could not have managed alone. My path to this point has been anything but linear, which makes the trajectory I leave with all the more significant to me. It is a privileged one, and many people deserve my gratitude for it.

First and foremost, I thank my supervisor, **Doris Reiter**. Of all the people I have met in academia, few combine scientific talent and human intuition as naturally as she does. She brings a rare dedication to supervision, one that was present at every stage of this work. She had a way of seeing potential in me where I saw uncertainty, and of giving me room to take on ambitious challenges while quietly making sure I did not lose my footing. The way I close this chapter of my life owes more to her guidance than I can properly express. I sincerely hope that Doris continues to be seen and recognized for her exceptional character, and that she receives back what she so generously gives.

I also want to express my gratitude to my second supervisor, **Moritz Cygorek**. His intrinsic enthusiasm for physics and his passion for sharing knowledge make him an exceptional talent in his own right. He exemplifies how academic discourse should be conducted at the highest level, consistently transforming our group into a rigorous, high-quality scientific environment.

Naturally, my thanks extend to the entire working group. While it is impossible to do justice to everyone in order and scope here, special thanks go to my three closest peers. To my office partner, **Anita**, whose office I graced with my presence far too rarely, but whose conversations I have always deeply valued. To **Quentin**, an exceptional scientific talent himself, who has always been incredibly helpful and reliable. I owe both Anita and Quentin my gratitude for proofreading this thesis. And to **Jana**, who continuously fosters a welcoming and open atmosphere within our group. Furthermore, I would like to mention our core team, **Thomas, Jan, and Zahra**, along with the many others who shared this space with us before moving on.

In the wider university context, countless individuals have shaped my studies. I am especially grateful to the friends who have been there since my very first days: **Christian, Lars, Antonia, Willy, Joel, and Selin**. I also owe a great deal to my fellow campaigners from the student council (Fachschaftsrat), including **Robin, Natalie, Lukas, Jack, Ramona, Froch, Kai, and Mirjam**, as well as **Joshua, Marie, Kevin, Max, Lena, and Jan-Peter** from PeP.

Outside university, there is one friend whose presence is closely tied to my studies: **Florian**. He consistently encouraged me to see this degree through to the end and gave me the confidence to believe I was truly capable of doing so.

I am endlessly grateful to my **family** for giving me the freedom, time, and space to pursue and complete this degree over the years. In particular, I owe a massive debt of gratitude to my aunt **Regina**. She is the one person without whom I would never have made it this far.

The final mention is reserved for a very special person: **Lara**. She is my partner and my second half, and I can say with absolute certainty that I would not be standing where I am today without her. It is nearly impossible for me to imagine navigating the last four years without her by my side. Everything I am and have achieved, I owe to her. She is the person who believed in me unwaveringly and who gives me the unconditional acceptance to simply be who I am.

Even though my name alone appears on the cover, I view this thesis fundamentally as a group effort. It is only through its social context that this work gains its true meaning. Therefore, I want to say it explicitly one last time: thank you, to everyone who supported and accompanied me along the way.

This thesis bears your names, too. A sincere and heartfelt **thank you**.