Moiré Superlattice Theory Notes

Theory backup for the MSL Rust framework

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1. Overview

These notes collect the theoretical background for the *moiré superlattice (MSL)* framework implemented in Rust.

- Geometry and lattice construction
- Continuum models (e.g. Bistritzer–MacDonald)
- Envelope approximations and effective models
- Numerical aspects and scaling limits

For quick jumps, see Section 3 and Section 4.

2. Motivation and context

The MSL framework targets problems where a twisted bilayer (or multilayer) structure leads to emergent long-wavelength degrees of freedom. The effective description often lives on a moiré superlattice in real or reciprocal space.

A prototypical example is the continuum model for twisted bilayer graphene (cite relevant papers from exampleBib.bib as needed).

We often work in a Hilbert space of layer, sublattice, and valley degrees of freedom and use operators like

$$H$$

acting on k-dependent spinors.

Example usage of the shared math helpers:

- Real-space coordinate

  $$r \in \boldsymbol{R}^2$$
- Bloch wavevector

  $$k \in \boldsymbol{R}^2$$
- State vector

  $$|\psi\rangle$$
- Overlap

  $$\langle \varphi \mid \psi \rangle$$

The actual BM model details are in Section 3.

3. Bistritzer–MacDonald model

The Bistritzer–MacDonald (BM) model describes twisted bilayer graphene in the continuum limit. The Hamiltonian acts on a four-component spinor representing layer (top/bottom) and sublattice (A/B) degrees of freedom.

3.1. Model structure

The model consists of:

- Intralayer Dirac cones for each layer
- Interlayer tunneling terms with moiré modulation
- Valley degree of freedom (K, K')

3.2. Key parameters

Using our shared macros:

Moiré parameters:

$$\theta = \theta,\ a = a,\ t = t_\perp$$

.

Where:

- θ

  : twist angle (typically

$\approx 1^\circ$

for magic angle)

- a

: graphene lattice constant (≈ 2.46 Å)

- $t_\perp$

: interlayer hopping amplitude

3.3. Hamiltonian structure

The continuum Hamiltonian in momentum space:

$$H(\boldsymbol{k}) = \begin{pmatrix} H_0(\boldsymbol{k}) & T(\boldsymbol{k}) \\ T^{\dagger(\boldsymbol{k})} & H_0(R_\theta \boldsymbol{k}) \end{pmatrix}$$

where

H_0

is the single-layer Dirac Hamiltonian and

T

encodes the moiré-modulated interlayer coupling.

3.4. Envelope approximation connection

This model connects to the envelope approximation framework discussed in Section 4, where we project onto low-energy subspaces.

4. Envelope approximation

The envelope approximation (EA) is a systematic method to derive effective low-energy models for moiré systems by projecting the full Hamiltonian onto slowly-varying envelope functions.

4.1. Physical picture

In a moiré system with length scale

L_m

, the physics separates into:

- **Fast** oscillations at the monolayer lattice scale

a

- **Slow** modulations at the moiré scale

$$L_m \approx \frac{a}{\theta}$$

The EA systematically captures the slow physics while averaging over fast oscillations.

4.2. Mathematical framework

Starting from the full tight-binding Hamiltonian

$$H_{\mathrm{TB}}$$

, we:

1. Expand wavefunctions as Bloch-modulated envelopes:

$$\psi(\boldsymbol{r}) = \sum_n \varphi_{n(\boldsymbol{r})} u_{\boldsymbol{k}_n}(\boldsymbol{r})$$

2. Project onto a low-energy subspace (e.g., states near Dirac points)
3. Derive an effective Hamiltonian

$$\widehat{H_{\mathrm{eff}}}$$

for the envelopes

4.3. Implementation in MSL

The MSL framework implements EA through several stages:

- **Lattice setup**: Define monolayer and moiré lattices
- **Local Bloch functions**: Compute monolayer eigenstates at each moiré site
- **EA operator construction**: Build effective coupling matrices
- **Envelope solver**: Solve the effective eigenvalue problem

For details on the numerical pipeline, see the `research/envelope_approximation/` directory in the MSL repository.

4.4. Validity regime

The EA is valid when:

- θ

  is small (

  $$\theta \ll 10°$$

)
- Interlayer coupling

  $$t_\perp$$

  is moderate
- Energy scales separate:

  $$\varepsilon_{\text{moiré}} \ll \varepsilon_{\text{monolayer}}$$

These conditions ensure clean separation between fast and slow degrees of freedom.

5. References

Bibliography