MSL Quick Reference

Key formulas and definitions

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1. Key scales

- Moiré length scale

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

- Twist angle

$$\theta$$

(typically

$$0.5°$$

to

$$10°$$

)
- Interlayer coupling parameters

$$t_\perp$$

,

$$t_\parallel$$

- Energy scales:

$$\varepsilon_{\text{Dirac}} \approx v_F \, |\boldsymbol{k}|$$

,

$$\varepsilon_{\text{moiré}} \approx \frac{v_F}{L_m}$$

2. Core objects

- Real-space coordinate:

$$r \in \boldsymbol{R}^2$$

- Momentum-space coordinate:

$$k \in \boldsymbol{R}^2$$

- State vectors:

$$|\psi\rangle$$

,

$$\langle\psi|$$

- Operators:

$\hat{H}$

,

$\hat{T}$

- Inner products:

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

3. Lattice vectors

For triangular monolayer lattice:

$$\boldsymbol{a}_1 = a\begin{pmatrix}1\\0\end{pmatrix}, \quad \boldsymbol{a}_2 = a\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix}$$

Reciprocal lattice:

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1\\ -\frac{1}{\sqrt{3}}\end{pmatrix}, \quad \boldsymbol{b}_2 = \frac{2\pi}{a}\begin{pmatrix}0\\ \frac{2}{\sqrt{3}}\end{pmatrix}$$

Moiré reciprocal lattice vectors (small angle approximation):

$$\boldsymbol{G}_m \approx \theta \, |\boldsymbol{G}_{\text{mono}}|$$

4. Common Hamiltonians

4.1. Single-layer Dirac Hamiltonian

$$H_0(\boldsymbol{k}) = v_F \boldsymbol{\sigma} \cdot \boldsymbol{k}$$

where

$$\boldsymbol{\sigma} = \left(\sigma_x, \sigma_y\right)$$

are Pauli matrices for sublattice.

4.2. Interlayer coupling (BM model)

$$T(\boldsymbol{r}) = \sum_{j=0}^{2} T_j e^{i\boldsymbol{q}_j \cdot \boldsymbol{r}}$$

with

$$\boldsymbol{q}_j$$

the moiré reciprocal vectors.

5. MSL Framework components

5.1. Rust core modules

- `lattice`: Bravais lattice construction and operations
- `reciprocal`: Reciprocal space calculations
- `symmetry`: Point group and space group operations
- `bloch`: Bloch eigensolvers and band structures

5.2. Python bindings

Import via: `from msl import Lattice, ReciprocalLattice, ...`

5.3. Key functions

- `Lattice::new(a1, a2)`: Create 2D Bravais lattice
- `generate_moire_lattice(theta)`: Construct moiré superlattice
- `compute_band_structure(kpath)`: Calculate energy bands

6. Numerical considerations

- **k-point sampling**: Use

$$N_k \approx 100$$

  points per moiré BZ edge for convergence
- **Truncation**: Include

$$\approx 3$$

  shells of moiré reciprocal vectors
- **Energy cutoffs**: Typically

$$E_{\text{cut}} \approx 10 \times t_{\perp}$$

7. References

For detailed theory, see the main MSL theory notes and relevant literature in the shared bibliography.

Bibliography