A first-principles-based multi-scale model for moiré phonons

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Physical Review B 106 (14), 144305 (2022)

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**Twisted bilayer graphene**

- Superconductivity in moiré systems

**Background**

- Evidence for nodal superconductivity:
  - X. Liu, J. Li et al., Science 371, 6535 (2021); 1731-1735.

- Lack of comprehensive microscopic theory
  - First-principles calculations are insensitive to screening.
  - Continuum model (neglecting out-of-plane relaxation)
  - Large system size: difficult to obtain force fields
  - Aperiodicity: cannot use first-principles approach

**Model validation**

- Developed a first-principles-based continuum model for moiré phonons based on configuration spaces, bypassing expensive force fields calculations and generic to all twist angles and materials.
- Benchmarking against first-principles calculations, showing good agreement.

**Phonons?**

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**Model challenges**

- Feasible to obtain force fields
- Generic to all twist angles and materials
- First-principles based continuum model

**Configuration space continuum model**

- Phonon moiré equations of motion

\[
\sum_{\mu \neq \nu} \mathbf{D}_{\mu \nu}((\mathbf{r}, \omega), \mathbf{R}, \omega_{\text{out}}) \mathbf{G}_{\mu \nu} = \omega^2 \mathbf{G}_{\mu \nu}
\]

- Phonon scattering selection rule

\[
\mathbf{D}_{\text{scat}}(\mathbf{k}) = \mathbf{D}_{\text{dyn}}(\mathbf{k}) - \mathbf{G}_{\text{scat}}(\mathbf{k}) = (\mathbf{G}_{\text{scat}} - \mathbf{G}_{\text{scat}}^\ast) = \mathbf{G}_{\text{scat}} - \mathbf{G}_{\text{scat}}^\ast
\]

- Moiré reciprocal lattice

**Electrons?**

- In analogy to the electronic structure selection rule (Bistritzer and MacDonald model)

**Obtaining the matrix element: configuration space**

- \( \mathbf{b}(\mathbf{r}) = (1 - A_2 A_1^{-1}) \mathbf{r} \)

**Twisted bilayer graphene band structure**

- ∆ point phonon

**Summary**

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\textsuperscript{1} J.Z.L. acknowledges support from the NSF under Award No. DMR-1922172 and the Army Research Office under Award No. W911NF-17-D-0001. M.A. acknowledges support from the NSF under Award Nos. DMR-1922172 and the Army Research Office under Award No. W911NF-17-D-0001. E.K. acknowledges support from the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, NSF Award No. DMR-1922172, and the Army Research Office under Award No. W911NF-17-D-0001. Z.Z. is supported by a Stanford Science fellowship. J.L. acknowledges funding support from the Harvard Herchel-Smith and PRISE fellowships.

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Twisted bilayer graphene \( \theta = 7.34^\circ \)