Real Space and Momentum Space Methods for 2D Heterostructures

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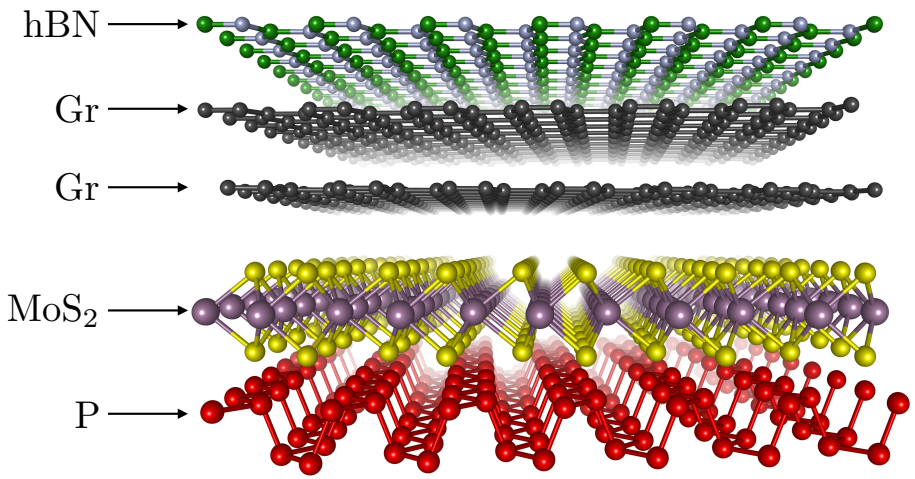
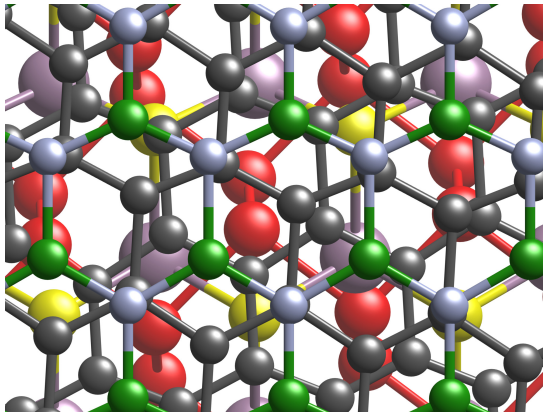
Stacked 2D Heterostuctures: No Periodic Structure



Example of heterostructure with five monolayers



Top view of the atomic structure

- Mechanical properties (relaxation, defects, etc.)
- Diffraction, dark field imaging
- Electronic structure (density of states, Kubo transport, scattering)
- Quantum, kinetic, hydrodynamic models of transport
- Plasmonics, edge states, topological properties

2D Lattices

A Bravais lattice, $\mathcal{R}$, and its unit cell, Γ, is defined for non-singular $A \in \mathbb{R}^{2\times 2}$ by

$$\mathcal{R} := \{An : n \in \mathbb{Z}^2\}, \qquad \Gamma = \{A\beta : \beta \in [0,1)^2\}.$$

$\mathcal{A}$: set of m orbitals associated with the unit cell. $|\mathcal{A}| = m$.

The orbitals in $\mathcal{A}$ can correspond to basis functions centered at the lattice points of $\mathcal{R}$ or can be centered at other basis atoms in the unit cell.

$\Omega = \mathcal{R} \times \mathcal{A}$: total degrees of freedom.

The reciprocal lattice to $\mathcal{R}$ and its unit cell (the Brillouin zone) is given by

$$\mathcal{R}^* := \{2\pi A^{-T} n : n \in \mathbb{Z}^2\}, \qquad \Gamma^* = \{2\pi A^{-T} \beta : \beta \in [0,1)^2\}.$$

2D bilayer geometry

For sheet $j \in \{1, 2\}$, we define the Bravais lattice

$$\mathcal{R}_j := \{A_j n : n \in \mathbb{Z}^2\}$$

where A_j is a 2×2 invertible matrix. We define the *unit cell* for sheet j as

$$\Gamma_j := \{A_j x : x \in [0, 1)^2\}.$$

Each individual sheet is trivially periodic, since

$$\mathcal{R}_j = A_j n + \mathcal{R}_j \qquad \text{for } n \in \mathbb{Z}^2.$$

The combined system $\mathcal{R}_1 \cup \mathcal{R}_2$ need not be periodic, though.

We represent multilattices by $\Omega_1 := \mathcal{R}_1 \times \mathcal{A}_1$ and $\Omega_2 := \mathcal{R}_2 \times \mathcal{A}_2$, and

$$\Omega := \Omega_1 \cup \Omega_2 = \mathcal{R}_1 \times \mathcal{A}_1 \cup \mathcal{R}_2 \times \mathcal{A}_2.$$

The orbitals in $\mathcal{A}_j$ can correspond to basis functions centered at the lattice points of $\mathcal{R}_j$ or can be centered at other basis atoms in the unit cell.

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2D multilayer geometry

For sheet $j \in \{1, \ldots, p\}$, we define the Bravais lattice

$$\mathcal{R}_j := \{A_j n : n \in \mathbb{Z}^2\}$$

where A_j is a 2×2 invertible matrix. We define the *unit cell* for sheet j as

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Each individual sheet is trivially periodic, since

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The combined system $\mathcal{R}_1 \cup \cdots \cup \mathcal{R}_p$ need not be periodic, though.

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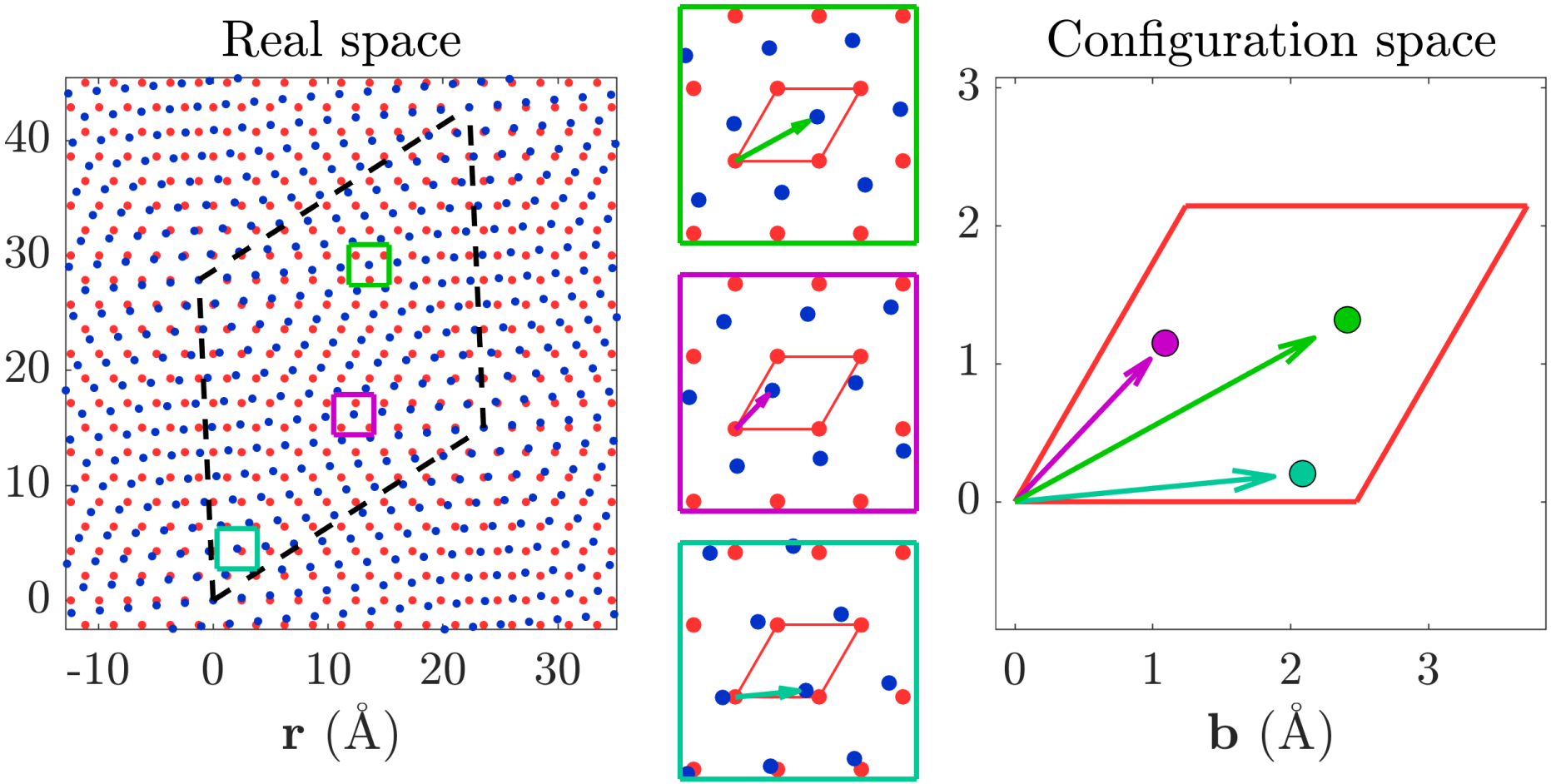
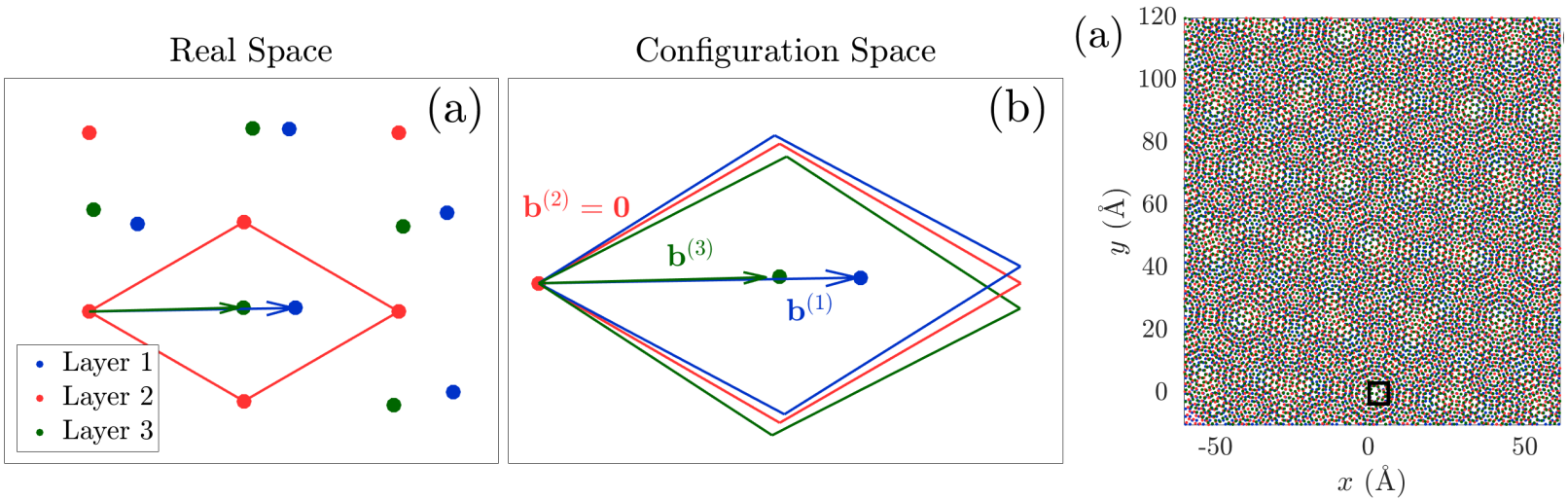


Isomorphism between real space and configuration (disregistry) space for incommensurate systems. Configuration space is uniformly sampled (Ergodicity).

Red-orbital's local environment described completely by the "$\vec{b}$-shift" between the blue and red unit-cells.

Our configuration space approach gives a unified and computationally efficient approach to mechanics, electronic structure, transport, diffraction.

Twisted Trilayer Configuration Space



The local configuration (disregistry) of layer j in a twisted trilayer is given by the $2 \cdot 2 = 4$ dimensional torus $X_j = \Gamma_i \times \Gamma_k$ where $i \neq j \neq k$.

There is no $2D$ periodic moiré domain for $p > 2$. Moiré of moiré.

The local configuration (disregistry) of layer j in a p layer heterostructure is given by the $2(p-1)$ dimensional torus $X_j = \times_{i \neq j} \Gamma_i$.

The Tight-Binding Model for 2D Multilayers

Construct a basis of *(Wannier) orbitals* defined on a lattice $\mathcal{R}_j$ of $\mathbb{R}^2$:

$$(\phi_{\alpha,R})_{\substack{R\in\mathcal{R}_j \\ \alpha\in\mathcal{A}_j}} \qquad \text{where} \qquad \phi_{\alpha,R}(x) = \phi_\alpha(x-R).$$

Denote the (tight-binding) hamiltonian operator H by

$$[H]_{R\alpha,R'\alpha'} := \langle \phi_{\alpha,R} | \mathcal{H} | \phi_{\alpha',R'} \rangle = h_{\alpha,\alpha'}(R-R')$$

where $\mathcal{H} = -\hbar^2/(2m_e)\Delta + V_{ion}(x)$ is a Schrödinger operator with periodic potential and the mass operator is

$$[S]_{R\alpha,R'\alpha'} := \langle \phi_{\alpha,R} | \phi_{\alpha',R'} \rangle = s_{\alpha,\alpha'}(R-R').$$

When the basis of crystal orbitals is obtained from a Wannier orbital construction, it is usually orthonormal, i.e., S is the identity operator.

The operator H does not have translation symmetry and thus cannot be diagonalized by a Bloch-Fourier transform if $\mathcal{R}_1 \cup \cdots \cup \mathcal{R}_p$ is not periodic.

Density of States Approximation

Finite domain Hamiltonian: for $\Omega_r := \bigcup_{j=1}^{p} \{[\mathcal{R}_j \cap B_r] \times \mathcal{A}_j\}$, $r > 0$,

$$H^r := (H_{R\alpha,R'\alpha'})_{R\alpha,R'\alpha' \in \Omega_r}.$$

The density of states, $\mathcal{D}[H^r]$, can be defined as linear functional on test functions:

$$\mathcal{D}[H^r](g) := \frac{1}{|\Omega_r|} \mathrm{Tr}[g(H^r)] = \frac{1}{|\Omega_r|} \sum_{R\alpha \in \Omega_r} g(H^r)_{R\alpha,R\alpha} = \frac{1}{|\Omega_r|} \sum_{i=1}^{|\Omega_r|} g(\epsilon_{r,i}),$$

where $\epsilon_{r,i}$ are the eigenvalues of H^r.
Represent the linear functional by the density of states, $\rho_r(E)$,

$$\mathcal{D}[H^r](g) = \int g(E)\rho_r(E)\, dE.$$

Approximate $\rho_r(\epsilon)$ by setting $g(E) = \frac{1}{\sqrt{2\pi}\kappa} \exp -\frac{(E-\epsilon)^2}{2\kappa^2}$.
The local density of states distribution is defined as the linear functional

$$\mathcal{D}_{R\alpha}[H^r](g) := [g(H^r)]_{R\alpha,R\alpha}, \qquad R\alpha \in \Omega_r.$$

Note that

$$\frac{1}{|\Omega_r|} \sum_{R\alpha \in \Omega_r} \mathcal{D}_{R\alpha}[H^r] = \mathcal{D}[H^r].$$

Equidistribution of lattice shifts (Ergodicity)

Let $\mathcal{R}_1, \ldots, \mathcal{R}_p$ be incommensurate lattices embedded in $\mathbb{R}^2$:

$$v + \mathcal{R}_1^* \cup \cdots \cup \mathcal{R}_p^* = \mathcal{R}_1^* \cup \cdots \cup \mathcal{R}_p^* \quad \Leftrightarrow \quad v = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

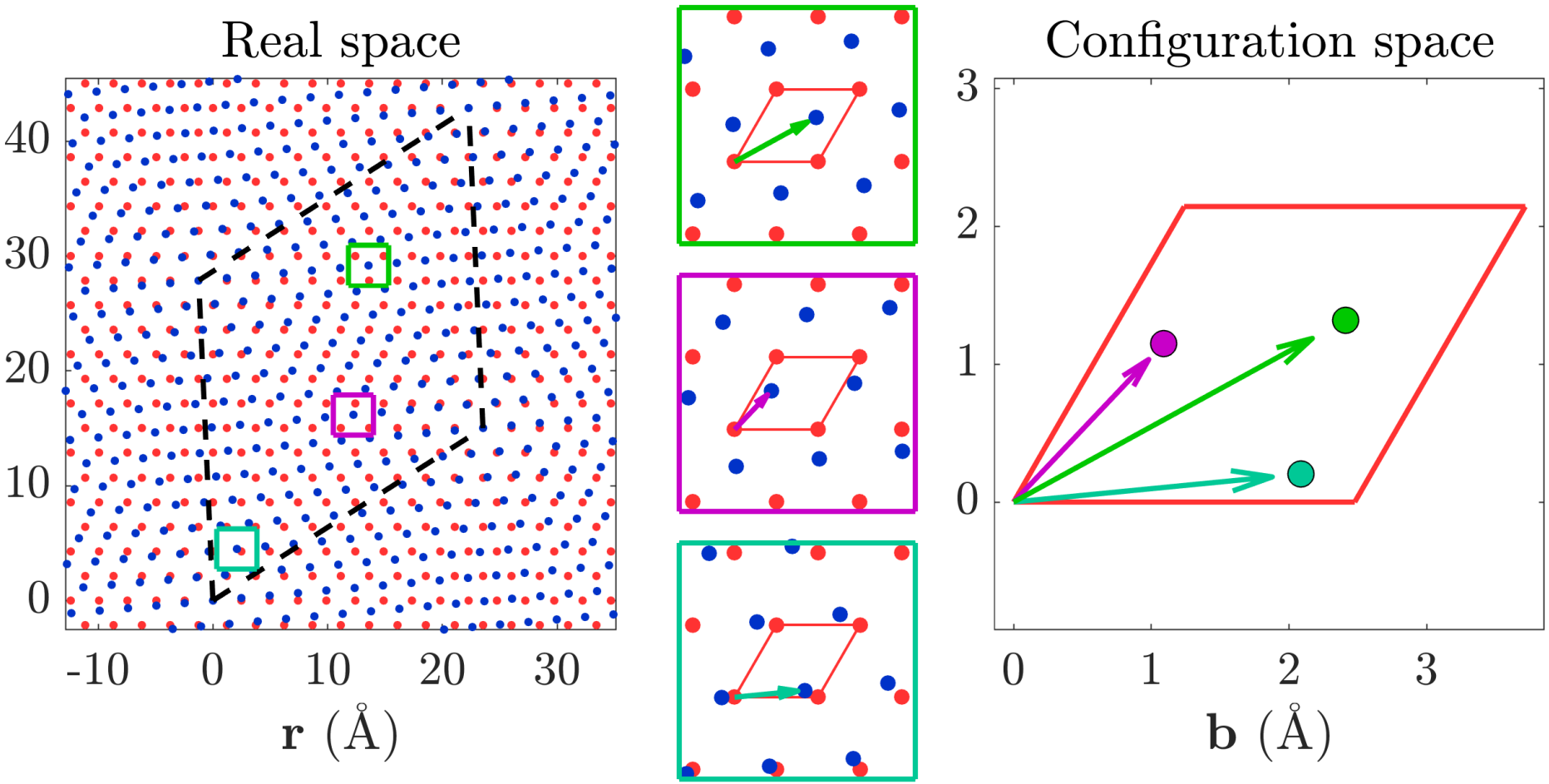
where $\mathcal{R}_j^*$ is the reciprocal lattice to $\mathcal{R}_j$.

Theorem

For $h \in C_{per}(X_j)$ where $X_j = \times_{i \neq j} \Gamma_i$, we have

$$\frac{1}{\#\mathcal{R}_j \cap B_r} \sum_{R_j \in \mathcal{R}_j \cap B_r} h(R_j) \to \frac{1}{|X_j|} \int_{X_j} h(b) db.$$

Local geometries around sites of sheet j can be parameterized by the local configurations X_j.



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Red-orbital's local environment described completely by the "$\vec{b}$-shift" between the blue and red unit-cells.

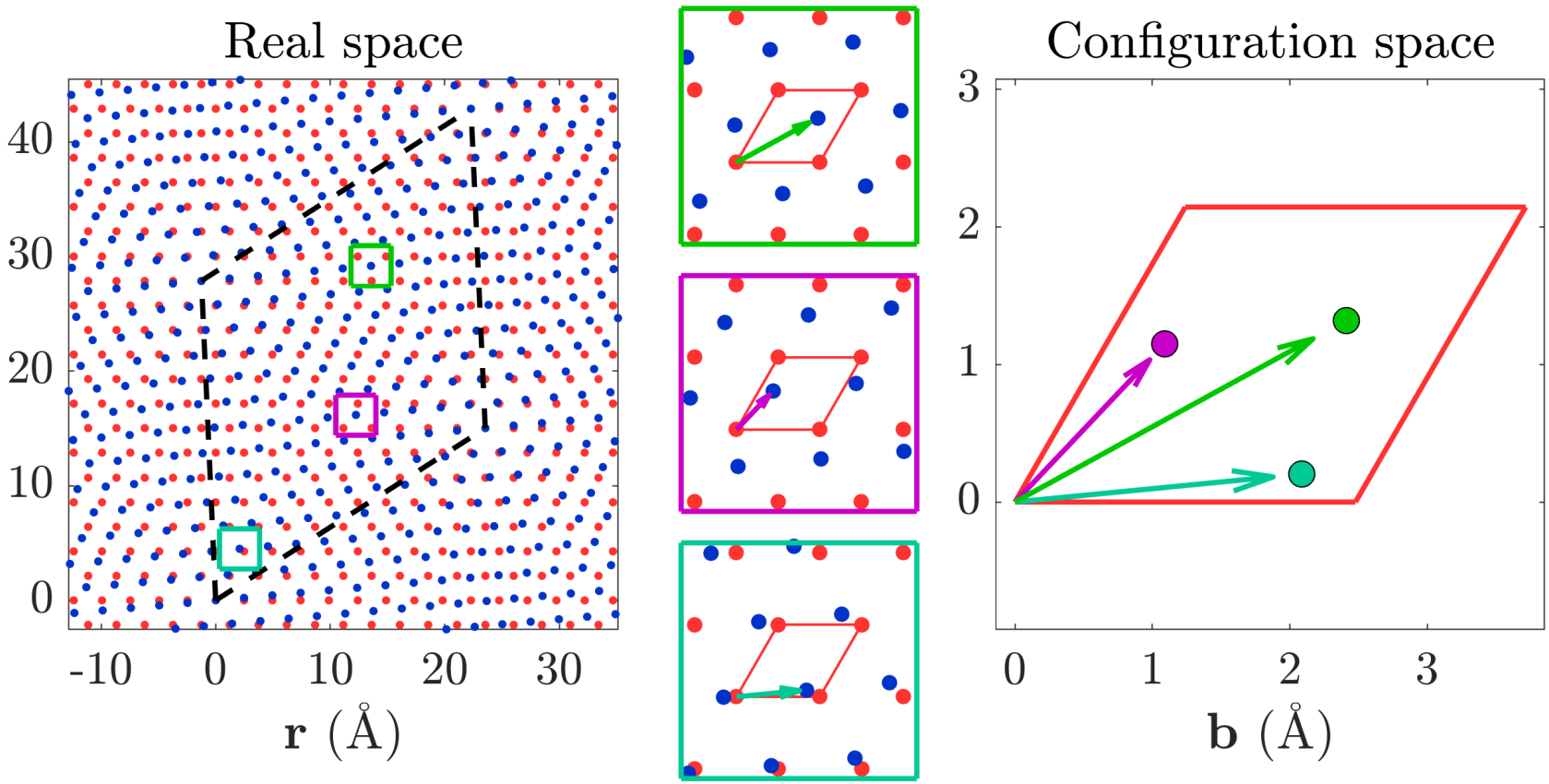
Shifted Hamiltonian and Local DoS

Define the Hamiltonian for a cluster of radius r in which the sheet i is shifted by $b_i \in \Gamma_i$ for $i \neq j$

$$[H_{r,j}(b)]_{R\alpha,R'\alpha'}, \quad R\alpha, R'\alpha' \in \Omega_r.$$

We can then approximate

$$\mathcal{D}_{R\alpha}[H^r] \approx \mathcal{D}_{0\alpha}[H_{r,j}(\mathrm{mod}_{X_j}(R))], \quad R\alpha \in \mathcal{R}_j \times \mathcal{A}_j.$$



Formal Derivation of Disregistry-Based DoS

Since

$$\mathcal{D}_{R\alpha}[H^r] \approx \mathcal{D}_{0\alpha}[H_{r,j}(\mathrm{mod}_{X_j}(R))], \quad R\alpha \in \mathcal{R}_j \times \mathcal{A}_j,$$

and $\mathrm{mod}_{X_j}(R)$ for $R \in \mathcal{R}_j$ uniformly samples X_j, we can formally derive by the ergodic property of incommensurate lattices

$$\frac{1}{|\Omega_r|} \sum_{R\alpha \in \Omega_r} \mathcal{D}_{R\alpha}[H^r] \approx \frac{1}{|\Omega_r|} \sum_{R\alpha \in \Omega_r} \mathcal{D}_{0\alpha}[H_{r,j}(\mathrm{mod}_{X_j}(R))]$$

$$\to \nu \sum_{j=1}^{p} \sum_{\alpha \in \mathcal{A}_j} \int_{X_j} \mathcal{D}_{0\alpha}[H_{r,j}(b)]db,$$

where

$$\nu = \frac{1}{\sum_{j=1}^{p} |X_j|\,|\mathcal{A}_j|}.$$

Global method $\mathcal{D}[H^r](g)$ gives linear convergence.

Local method $\mathcal{D}_{0\alpha}[H_{r,j}(b)]$ gives exponential convergence.

Thermodynamic Limit

Let $S(H)$ be an interval containing the spectrum of H.

Theorem

There exists a bounded linear functional $\mathcal{D}[H] : C(S(H)) \to \mathbb{C}$ *such that*

$$\mathcal{D}[H_{r,j}(0)] \to \mathcal{D}[H] \quad \text{as } r \to \infty, \quad \text{for } j = 1, \ldots, p,$$

and

$$\mathcal{D}[H] = \nu \sum_{j=1}^{p} \sum_{\alpha \in \mathcal{A}_j} \int_{X_j} \mathcal{D}_{0\alpha}[H(b)] db,$$

where

$$\nu = \frac{1}{\sum_{j=1}^{p} |X_j| \, |\mathcal{A}_j|}.$$

If g *is analytic for* $d(z, S[H]) < d$, *we have the explicit error bound*

$$\left| \mathcal{D}[H](g) - \nu \sum_{j=1}^{p} \sum_{\alpha \in \mathcal{A}_j} \int_{X_j} \mathcal{D}_{0\alpha}[H_{r,j}(b)](g) db \right| \leqslant C d^{-6} \sup_{d(z,S[H]) < d} |g(z)| e^{-\gamma d r}.$$

If g is analytic for $d(z, S[H]) < d$, we have the explicit error bound

$$\left| \mathcal{D}[H](g) - \nu \sum_{j=1}^{p} \sum_{\alpha \in \mathcal{A}_j} \int_{X_j} \mathcal{D}_{0\alpha}[H_{r,j}(b)](g) db \right| \leqslant C d^{-6} \sup_{d(z,S[H])<d} |g(z)| e^{-\gamma d r}.$$

Algorithmic approximations:

- Sample from torus X_j.
- Cut-off Hamiltonian at radius r to obtain $H_{r,j}(b)$.
- Approximate DOS $\rho(\epsilon)$ by setting $g(E) = \frac{1}{\sqrt{2\pi}\kappa} \exp - \frac{(E-\epsilon)^2}{2\kappa^2}$. Then

$$\sup_{d(z,S[H])<d} |g(z)| \leqslant \frac{1}{\sqrt{2\pi}\kappa} \exp\left(\frac{d^2}{2\kappa^2}\right).$$

Solution by Kernel (Chebyshev) polynomial method.

Representation of LDoS by Cauchy Integral Formula

We can write for $\Omega_r \subset \Omega$, , $R\alpha \in \Omega_r$, and g analytic

$$[g(H^r)]_{R\alpha R\alpha} = \frac{1}{2\pi i} \oint_{\mathbb{C}} g(z)[(z - H^r)^{-1}]_{R\alpha R\alpha} dz,$$

where $\mathbb{C}$ is a contour around $S[H]$ which contains the spectrum.

Assume that

$$|h_{\alpha\alpha'}(x)| \leqslant Ce^{-\gamma|x|}.$$

Extend Combes–Thomas decay estimate for $[(z - H^r)^{-1}]_{R\alpha R'\alpha'}$:

There exists $C > 0$ and $\kappa > 0$ such that for all $z \in \mathbb{C}$, $\mathrm{dist}(z, S(H^r)) \geqslant d$,

$$\left|[(z - H^r)^{-1}]_{R\alpha R'\alpha'}\right| \leqslant Ce^{-\kappa\gamma d|R-R'|}.$$

Exponential Convergence of LDOS

For simplicity, consider a 1D lattice with lattice constant $a = 1$. Assume

$$H_{\ell,m} \leqslant C \exp\left(-\gamma|\ell - m|\right), \qquad (z - H^r)^{-1}_{\ell,m} \leqslant C \exp\left(-\gamma|\ell - m|\right),$$

for $\mathrm{dist}(z, S[H]) \geqslant d$. For $r' > r$, we then estimate

$$[g(H_{r'})]_{00} - [g(H_r)]_{00} = \frac{1}{2\pi i} \oint_{\mathbb{C}} g(z)[(z - H_{r'})^{-1} - (z - H^r)^{-1}]_{00}\, dz.$$

We thus need to estimate

$$\begin{aligned}[(z - H_{r'})^{-1} - (z - H^r)^{-1}]_{00} &= [(z - H_{r'})^{-1}(H_{r'} - H^r)(z - H_r)^{-1}]_{00} \\ &= \left(\sum_{\ell \in \Omega_{r'} \setminus \Omega_r} \sum_{m \in \Omega_r} + \sum_{\ell \in \Omega_r} \sum_{m \in \Omega_{r'} \setminus \Omega_r} + \sum_{\ell \in \Omega_{r'} \setminus \Omega_r} \sum_{m \in \Omega_{r'} \setminus \Omega_r} \right) \\ &\qquad (z - H_{r'})^{-1}_{0\ell}(H_{r'} - H^r)_{\ell m}(z - H_r)^{-1}_{m0}.\end{aligned}$$

Exponential Convergence of LDOS

Estimate

$$\left| \sum_{\ell \in \Omega_{r'} \setminus \Omega_r} \sum_{m \in \Omega_r} (z - H_{r'})^{-1}_{0\ell} (H_{r'} - H^r)_{\ell m} (z - H_r)^{-1}_{m0} \right|$$

$$\leqslant 2C^2 \sum_{\ell=r+1}^{r'} \sum_{m=0}^{r} \exp\left(-\gamma(\ell + (\ell - m) + m)\right) = 2C^2 \sum_{\ell=r+1}^{r'} \sum_{m=0}^{r} \exp\left(-2\gamma\ell\right)$$

$$\leqslant 2C^2 \int_r^{r'} x \exp\left(-2\gamma x\right) dx \leqslant 2C^2 \frac{r \exp\left(-2\gamma r\right)}{2\gamma} + 2C^2 \frac{\exp\left(-2\gamma r\right)}{(2\gamma)^2}$$

$$\leqslant C_1 \exp\left(-\gamma r\right).$$

Local Method $g(H^r)_{00}$ converges exponentially.
(periodic chain has only one configuration)

Global Method $\frac{1}{2r} \operatorname{Tr} g(H^r)$ converges linearly:

$$\text{Global Method Error } \approx \frac{1}{2r} \int_0^r \exp\left(-\gamma(r - s)\right) ds = \frac{1}{2r\gamma} \left(1 - \exp\left(\gamma r\right)\right).$$

Twisted Bilayer Graphene Calculation

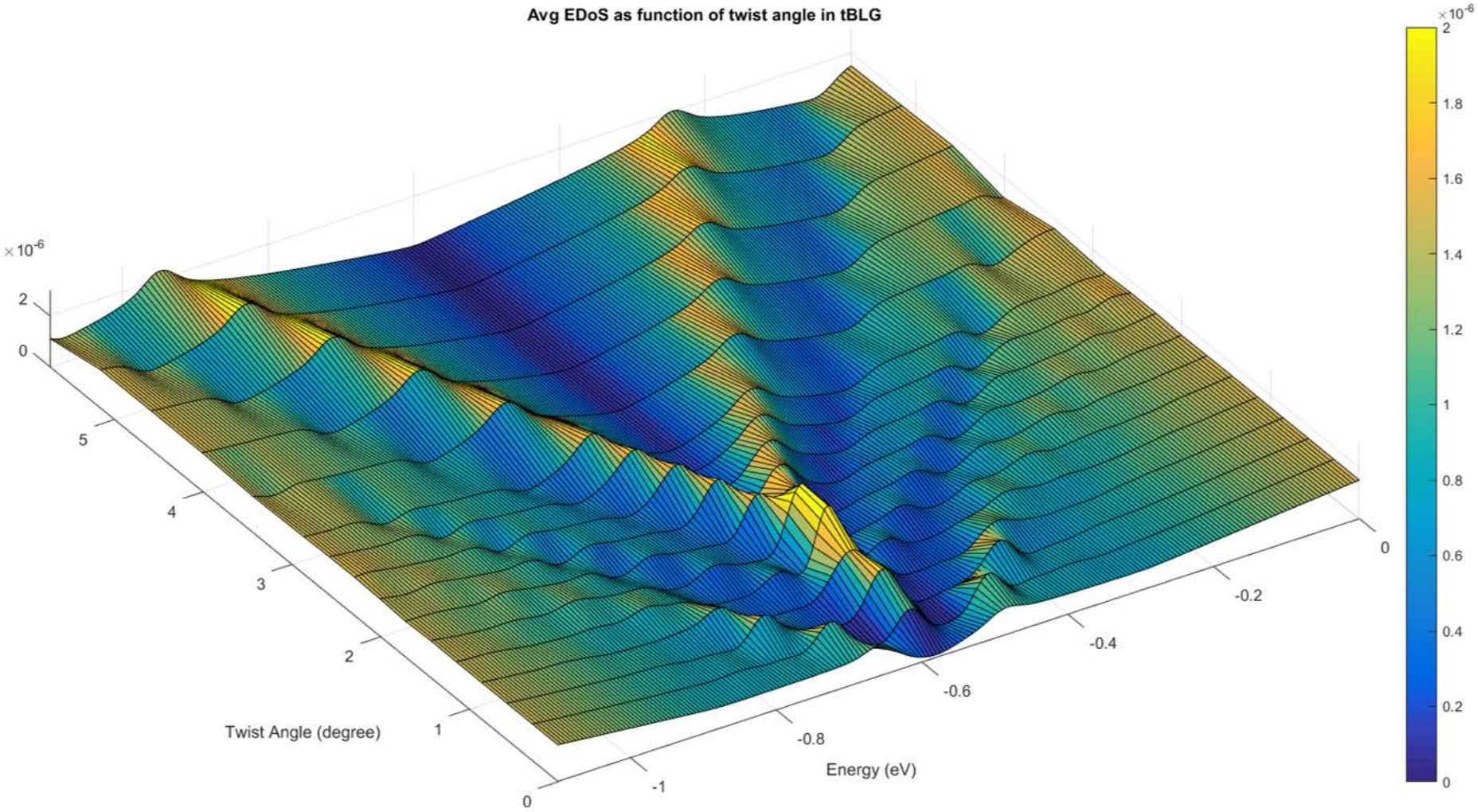


Figure: 500 Angstrom radius disk (600,000 atoms in total)

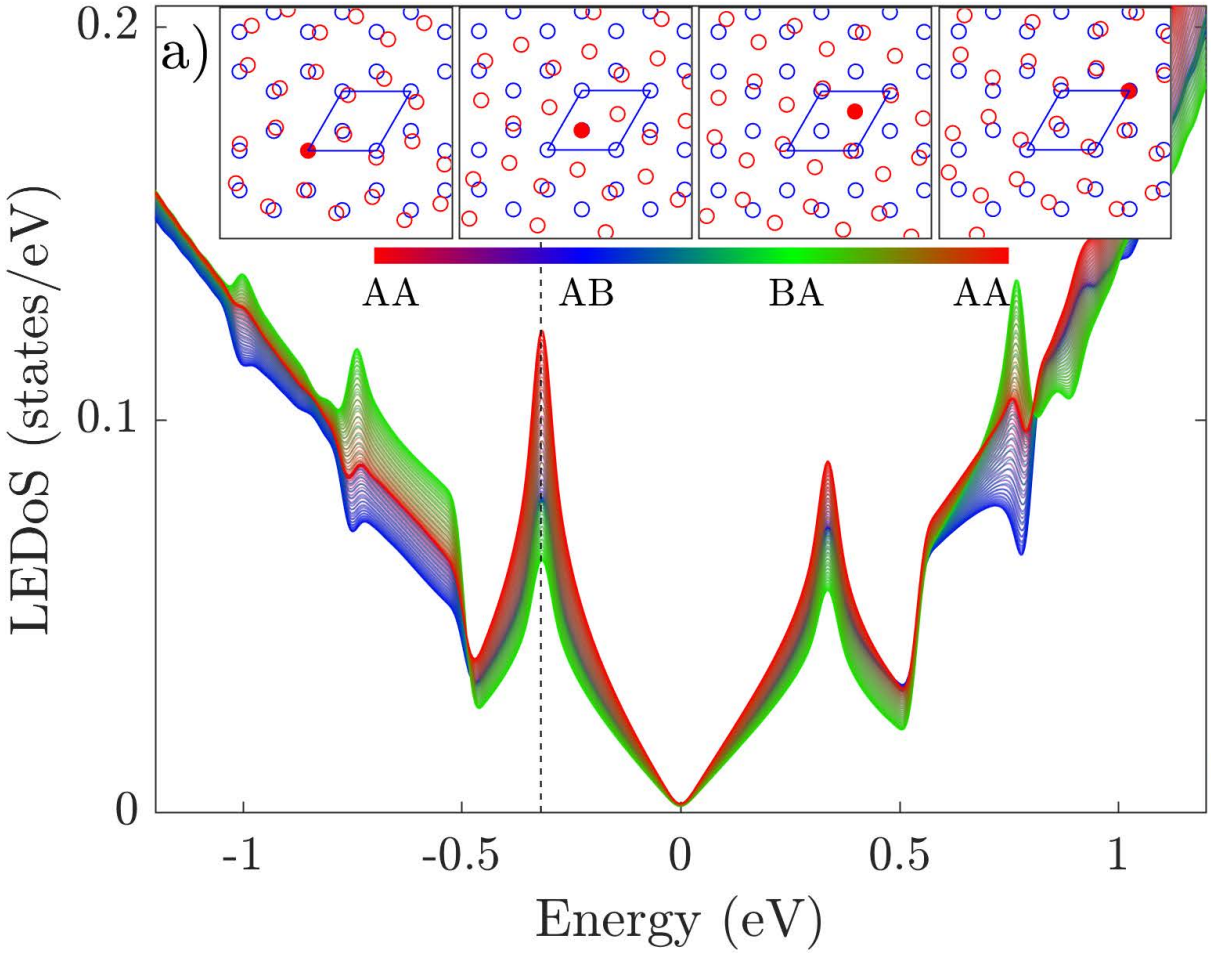


Figure: Local Electronic Density of States as a function of shift distance across the unit cell diagonal: (a) Scan of a single orbital's LEDoS with the coloring corresponding to distance across the diagonal. The insets show the real-space configurations ω for three types of stacking with the bottom layer atoms represented by blue circles and the top layer ones by red circles. The unit-cell of the bottom layer is outlined in blue and the shifted orbital is highlighted as a filled red dot.

Transform to Momentum Space

The multilayer wave function $\psi_{R,\alpha} = (\psi_{R_1\alpha_1}, \ldots, \psi_{R_p\alpha_p})$ or $\psi := (\psi_1, \ldots, \psi_p)$ is defined on $\Omega := \Omega_1 \cup \cdots \cup \Omega_p = \mathcal{R}_1 \times \mathcal{A}_1 \cup \cdots \cup \mathcal{R}_p \times \mathcal{A}_p$

Define the Bloch transform for each sheet

$$\breve{\psi}_j(q) = |\Gamma_j^*|^{-1/2} \sum_{R_j \in \mathcal{R}_j} \psi_{R_j\alpha_j} e^{-iR_j \cdot q}, \qquad q \in \mathrm{BZ}_j,\ \alpha_j \in \mathcal{A}_j.$$

Transform the Hamiltonian to momentum space

$$\widetilde{H_{jj}\psi_j}(q) = c_j \widetilde{h_{jj}}(q) \breve{\psi}_j(q), \qquad q \in \mathrm{BZ}_j,$$
$$\widetilde{H_{jk}\psi_k}(q) = \sum_{G_j \in \mathcal{R}_j^*} c_{jk} \widehat{h_{jk}}(q + G_j) \breve{\psi}_k(q + G_j), \qquad j \neq k,\ q \in \mathrm{BZ}_j,$$

where $c_j = |\Gamma_j^*|^{1/2}$, $c_{jk} = c_j \cdot c_k$, and

$$\widetilde{h_{jj}}(q) = |\Gamma_j^*|^{-1/2} \sum_{R_j \in \mathcal{R}_j} h_{\alpha_j\alpha_j}(R_j) e^{-iR_j \cdot q}, \qquad \alpha_j \in \mathcal{A}_j,\ q \in \mathrm{BZ}_j,$$

$$\widehat{h_{jk}}(q) = \frac{1}{2\pi} \int h_{\alpha\alpha'}(x) e^{-ix \cdot q} dx, \qquad j \neq k,\ \alpha_j \in \mathcal{A}_j,\ \alpha_k \in \mathcal{A}_k\ , q \in \mathbb{R}^2.$$

The proof follows from the Poisson summation formula:

$$|\Gamma_j^*|^{-1} \sum_{R_j \in \mathcal{R}_j} e^{iq \cdot R_j} = \sum_{G_j \in \mathcal{R}_j^*} \delta(q + G_j), \quad q \in \mathbb{R}.$$

Interlayer Scattering

Transform the Hamiltonian to momentum space

$$\widetilde{H_{jj}\psi_j}(q) = c_j \widetilde{h_{jj}}(q)\breve{\psi}_j(q), \qquad q \in \mathrm{BZ}_j,$$
$$\widetilde{H_{jk}\psi_k}(q) = \sum_{G_j \in \mathcal{R}_j^*} c_{jk}\widehat{h_{jk}}(q+G_j)\widetilde{\psi_k}(q+G_j), \qquad j \neq k,\ q \in \mathrm{BZ}_j.$$

We thus see that

$$\breve{\psi}_j(q) \text{ scatters to } \widetilde{\psi_k}(q+G_j) = \widetilde{\psi_k}(q+G_j-G_k), \quad G_j \in \mathcal{R}_j^*,\ G_k \in \mathcal{R}_k^*.$$

Bilayer:

$$\widetilde{\psi_1}(q) \text{ scatters to } \widetilde{\psi_2}(q+G_1-G_2), \quad G_1 \in \mathcal{R}_1^*,\ G_2 \in \mathcal{R}_2^*.$$
$$\widetilde{\psi_2}(q+G_1-G_2) \text{ scatters to } \widetilde{\psi_1}(q+(G_1-G_2)+(G_2'-G_1'))$$
$$= \widetilde{\psi_1}(q+(G_1-G_1')-(G_2-G_2')), \quad G_2' \in \mathcal{R}_2^*,\ G_1' \in \mathcal{R}_1^*.$$

Transform Bilayer Hamiltonian to Reciprocal Space

Note that if $q = \mathrm{mod}_{\mathrm{BZ}_1} G_2$,

$$\exp iq \cdot R_1 = \exp iG_2 \cdot R_1, \qquad R_1 \in \mathcal{R}_1.$$

Since the reciprocal lattice, $\mathcal{R}_2^*$, uniformly samples the torus BZ_1 by $q = \mathrm{mod}_{\Gamma_1^*} G_2$, we can equivalently formulate the Hamiltonian in reciprocal space.

The reciprocal space degrees of freedom are:

$$\begin{aligned}
\Omega_j^* &= \mathcal{R}_i^* \times \mathcal{A}_j, \\
\Omega^* &= \Omega_1^* \cup \Omega_2^*, \\
\Omega_r^* &= ((\mathcal{R}_2^* \cap B_r) \times \mathcal{A}_1) \cup ((\mathcal{R}_1^* \cap B_r) \times \mathcal{A}_2),
\end{aligned}$$

and the Hamiltonian for the bilayer can then be defined by $\widehat{H} : \Omega^* \to \Omega^*$,

$$\begin{aligned}
[\widehat{H}]_{G\alpha, G'\alpha'} &= c_j \widetilde{h_{\alpha\alpha'}}(G)\delta_{GG'}, && \text{if } G\alpha \in \Omega_j^*, G'\alpha' \in \Omega_j^*, \\
[\widehat{H}]_{G\alpha, G'\alpha'} &= c_0 \hat{h}_{\alpha\alpha'}(G + G'), && \text{if } G\alpha \in \Omega_j^*, G'\alpha' \in \Omega_i^*.
\end{aligned}$$

Shifted Configuration-Based Momentum Space Hamilton

Define the momentum Hamiltonian centered at a configuration $q \in \mathrm{BZ}_j$ by

$$[\widehat{H}(q)]_{G\alpha,G'\alpha'} = c_0 \hat{h}_{\alpha\alpha'}(q+G+G'), \qquad \text{if } \alpha \in \mathcal{A}_j, \alpha' \in \mathcal{A}_i,$$
$$[\widehat{H}(q)]_{G\alpha,G'\alpha'} = c_j \widetilde{h_{\alpha\alpha'}}(q+G)\delta_{GG'}, \qquad G\alpha, G'\alpha' \in \Omega_j^*.$$

We then have the following theorem based on the ergodicity property:

Theorem

$$Tr\, g(H) = Tr\, g(\widehat{H}) = \nu^* \sum_{j=1}^{2} \sum_{\alpha \in \mathcal{A}_j} \int_{BZ_j} [g \circ \widehat{H}(q)]_{0\alpha,0\alpha},$$

where

$$\nu^* = \Big[|BZ_2| \cdot |\mathcal{A}_1| + |BZ_1| \cdot |\mathcal{A}_2| \Big]^{-1}.$$

Multilayer Momentum Space Hamiltonian

The multi-layer momentum degrees of freedom are

$$\Omega^* = \cup_{j=1}^{p} \Omega_j^* := \cup_{j=1}^{p} \mathcal{G}_j \times \mathcal{A}_j,$$

where $\mathcal{G}_j = \{G = (G_1, \cdots G_p) \in \otimes_{k \in S} \mathcal{R}_k^* : \ G_j = 0\}$. The intralayer interaction is

$$[\widehat{H}]_{G\alpha, \tilde{G}\tilde{\alpha}} = \delta_{G\tilde{G}} \widetilde{h_{\alpha\alpha}}(\sum_k G_k), \quad G\alpha, \tilde{G}\tilde{\alpha} \in \Omega_j^*.$$

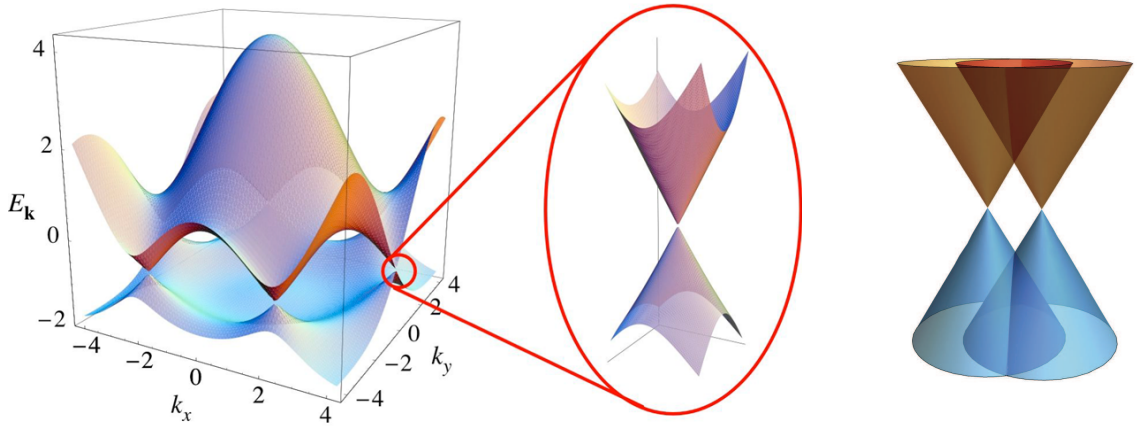
If $k \neq j$ and $G\alpha \in \Omega_k$ and $\tilde{G}\tilde{\alpha} \in \Omega_j$, we define the interlayer interaction by

$$[\widehat{H}]_{G\alpha, \tilde{G}\tilde{\alpha}}$$
$$= \delta_{\{|k-j|=1\}} \sqrt{|\mathrm{BZ}_k| \cdot |\mathrm{BZ}_j|} \left(\Pi_{s \in S \setminus \{k,j\}} \delta_{G_s \tilde{G}_s}\right) \hat{h}_{\alpha\alpha'}(G_j + \tilde{G}_k + \sum_{s \in S \setminus \{k,j\}} G_s).$$

The density of states are given in momentum space by

$$\int \rho(E) g(E)\, dE = \nu^* \sum_{j=1}^{p} \sum_{\alpha \in \mathcal{A}_j} \int_{\mathrm{BZ}_j} [g \circ \widehat{H}(q)]_{0\alpha, 0\alpha} dq, \quad \nu^* = (\sum_{j=1}^{p} |\mathrm{BZ}_j| \cdot |\mathcal{A}_j|)^{-1}.$$

Graphene Band Structure



[*The electronic properties of graphene*, Neto, Geim, et al, *Rev. Mod. Phys*]
[*Correlated insulator behaviour at half-filling in magic-angle graphene superlattices*,Cao, Jarillo-Herroro, et al, *Nature*]

Figure: L: Monolayer graphene bands at the Fermi level. The Dirac cone. R: Band structure for non-interacting twisted bilayer graphene.

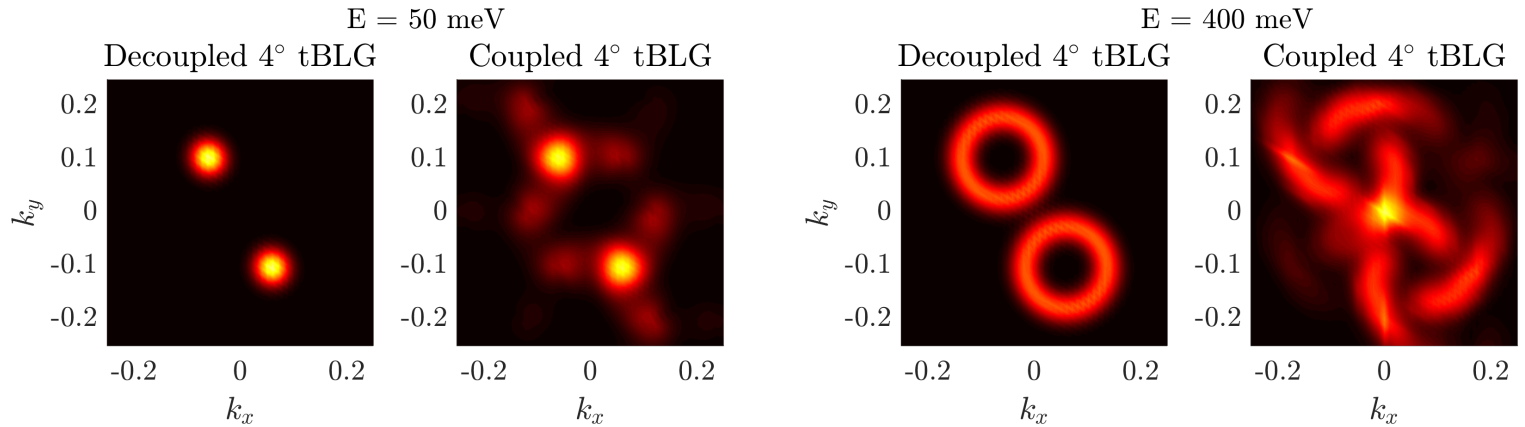


Figure: Twisted bilayer graphene momentum local DoS

Momentum Space Hamiltonian Domain Reduction

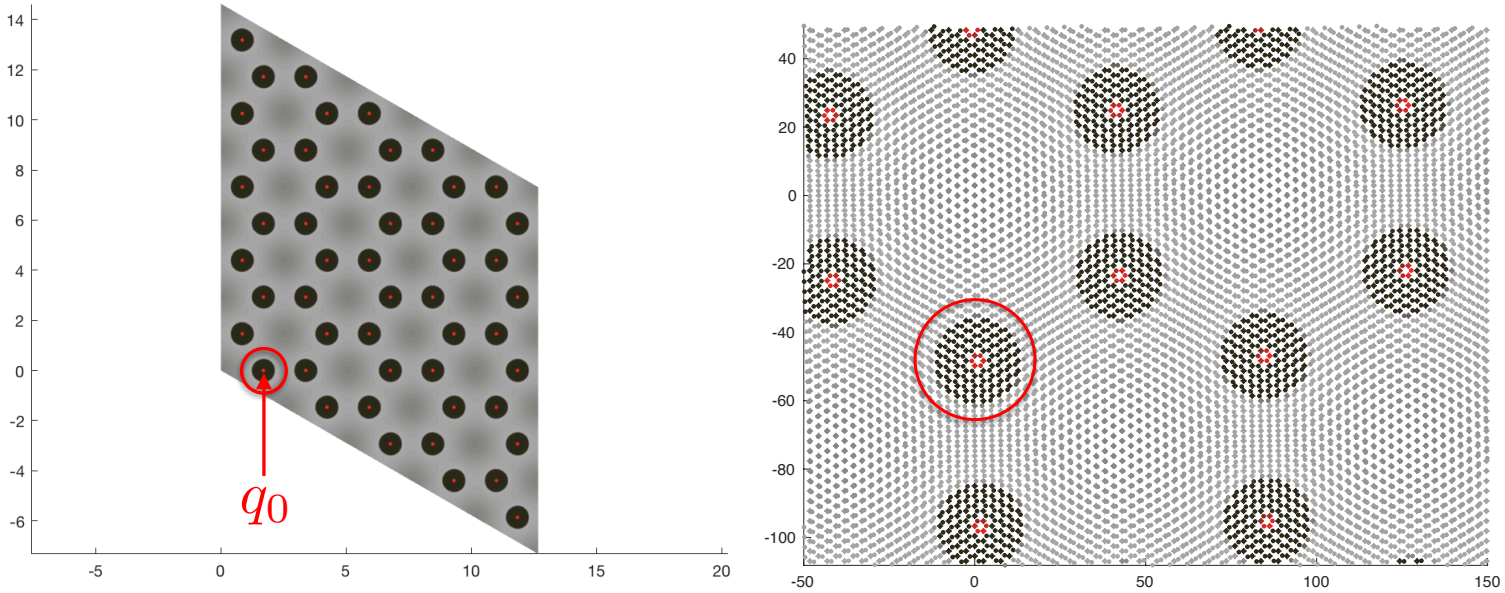


Figure: Strongly interacting DoF in momentum q space (left) and reciprocal space (right).

Can approximate $\widehat{H}(q)$ by $\widehat{H}|_{\Omega_r^*}(q)$ in

$$\text{Tr } g(H) = \text{Tr } g(\widehat{H}) \approx \nu^* \sum_{j=1}^{2} \sum_{\alpha \in \mathcal{A}_j} \int_{\text{BZ}_j} [g \circ \widehat{H}|_{\Omega_r^*}(q)]_{0\alpha,0\alpha},$$

More efficient to approximate $\widehat{H}(q)$ by $\widehat{H}(q)|_{\Omega_{j\epsilon r}^*(q)}$
where $\Omega_{j\epsilon r}^*(q) \subset \Omega_r^*(q)$ are the strongly interacting degrees of freedom at energy ϵ.

Error Estimates for Hamiltonian Domain Reduction

Let $\phi_{\epsilon\kappa}(E) = \frac{1}{\sqrt{2\pi}\kappa} e^{-\frac{(E-\epsilon)^2}{2\kappa^2}}$. Then

$$\left| \text{Tr } \phi_{\epsilon\kappa}(H) - \nu^* \sum_{j=1}^{2} \sum_{\alpha \in \mathcal{A}_j} \int_{\text{BZ}_j} [\phi_{\epsilon\kappa} \circ \widehat{H}|_{\Omega_r^*}(q)]_{0\alpha,0\alpha} \right| \lesssim \kappa^{-7} e^{-\gamma\kappa r}.$$

For ϵ with compact and connected strongly interacting sets $\Omega^*_{j\epsilon r}(q)$, we have the improved convergence rate

$$\left| \text{Tr } \phi_{\epsilon\kappa}(H) - \nu^* \sum_{j=1}^{2} \sum_{\alpha \in \mathcal{A}_j} \int_{\text{BZ}_j} [\phi_{\epsilon\kappa} \circ \widehat{H}|_{\Omega^*_{j\epsilon r}}(q)]_{0\alpha,0\alpha} \right| \lesssim \kappa^{-3} e^{-\gamma r}.$$

To obtain comparable error as $\kappa \to 0$, $\frac{r_2}{r_1} \approx \kappa$ where r_1 for Ω_r^* and r_2 for $\Omega^*_{j\epsilon r}$.
Can do direct solution for eigenvalue problem for $\Omega^*_{j\epsilon r}$.

Smoothness of Real Space LDos

Can we improve the efficiency of the real space approach?

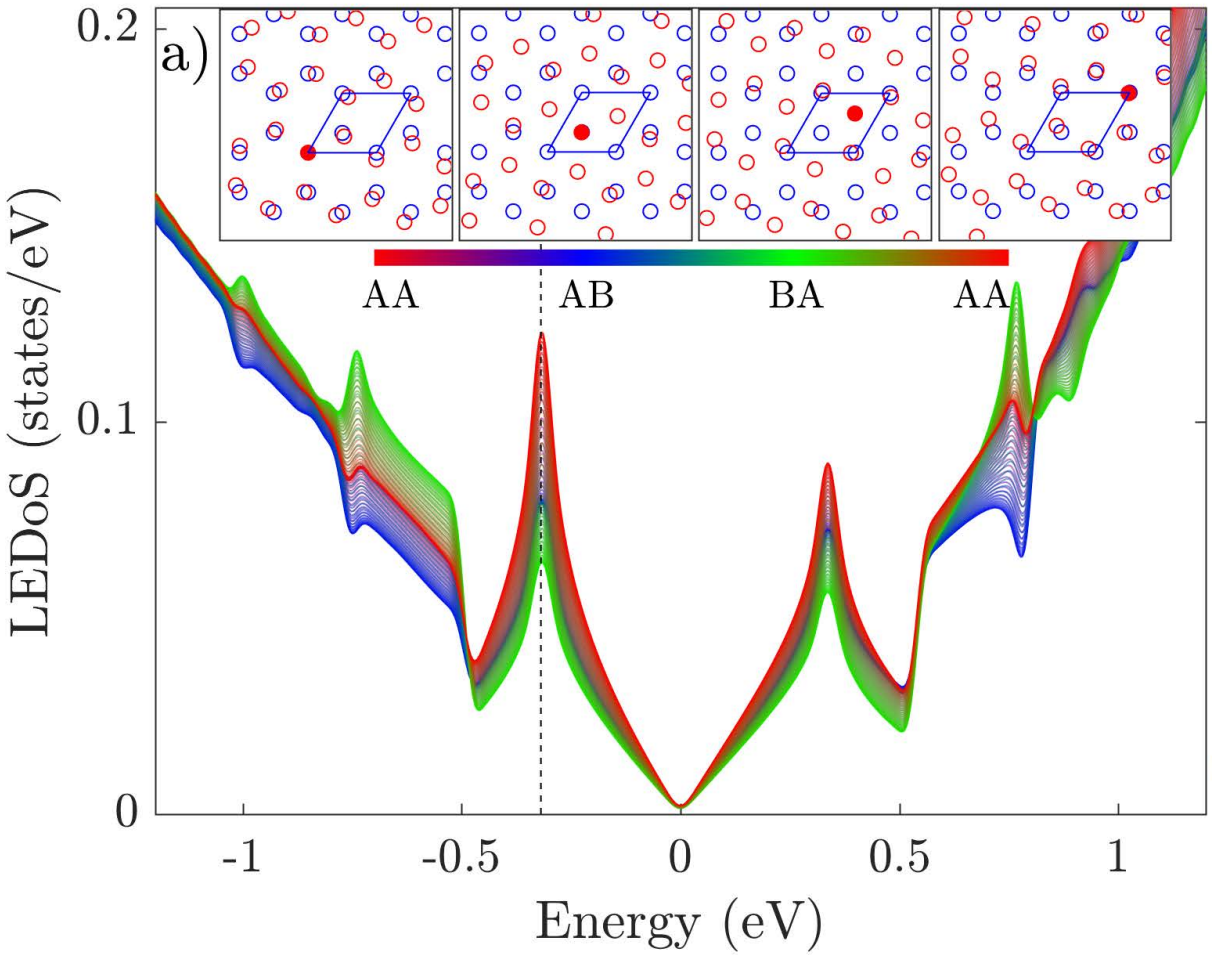
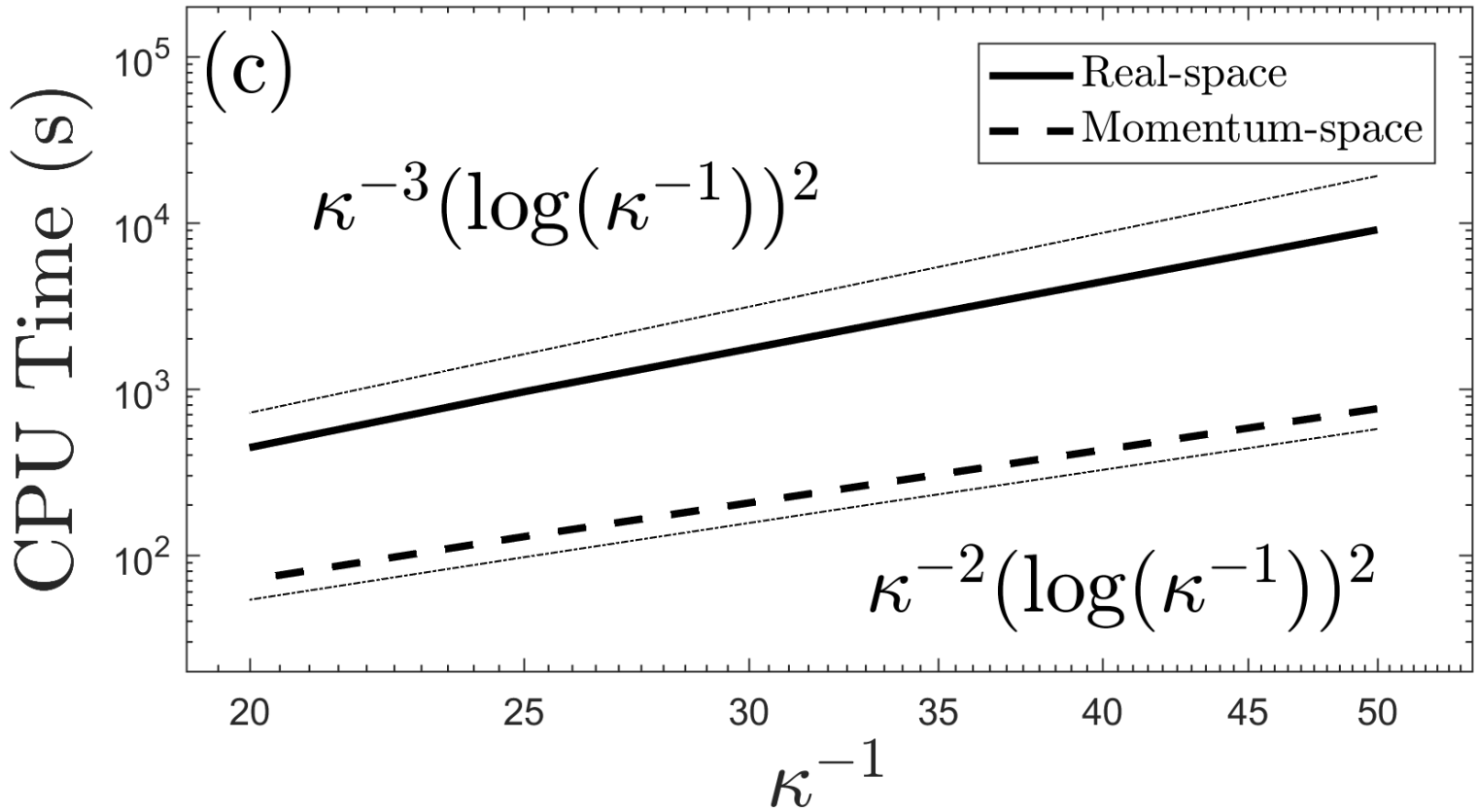


Figure: LDoS is smooth for real space shift (disregisty, configuration). No strongly interacting compact connected set of shifts.

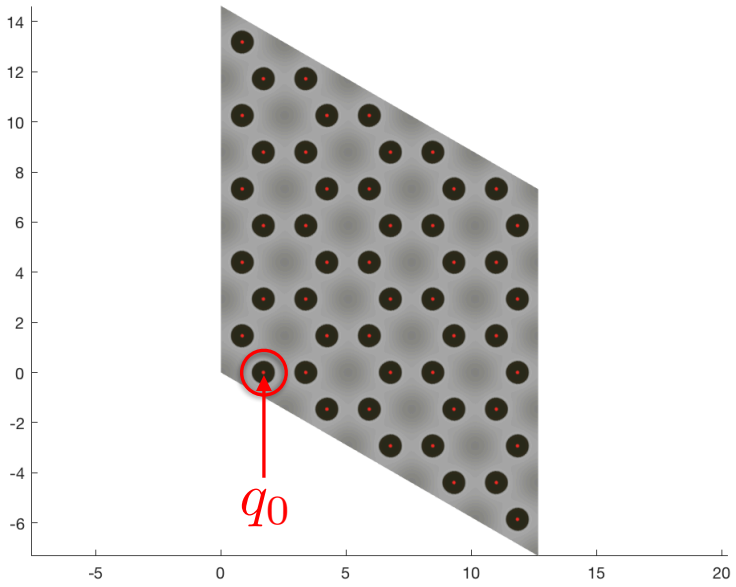
Improved Computational Efficiency for Momentum Space versus Real Space

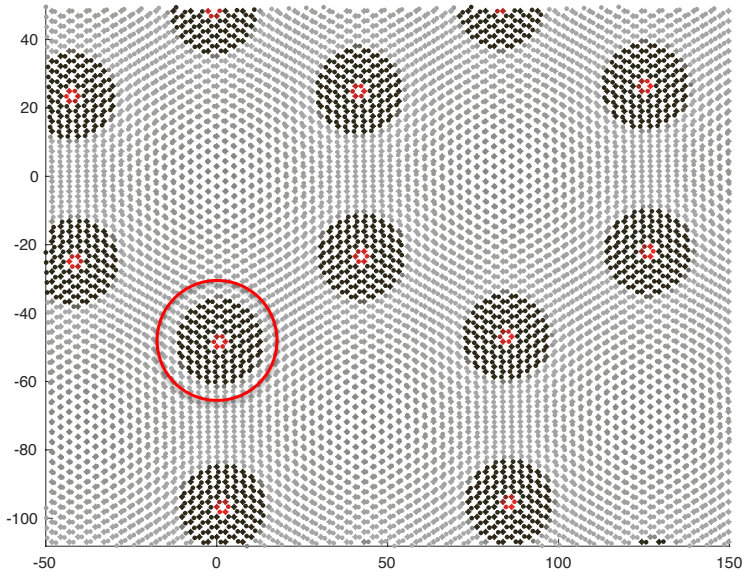


Multilayer Challenge

For $p = 2$, $\widehat{H}(q)$ can be reduced by restricting the Hamiltonian to DOF $q + K_1$ that lie in the a compact dark region of in the figure below.

For $p > 2$ the reduced Hamiltonian must retain the DOF in the cylinder $q + K_1 + K_3$ that lies in the dark region.





Kubo Formula for Conductivity on a Periodic Supercell

The Kubo formula for the linear response of charge to an applied field is

$$\sigma^r_{jk} = \frac{e^2}{\hbar^2}\frac{1}{|\Omega_r|}\mathrm{Tr}[\partial_j H^r (i\omega + \eta + \mathcal{L}_{H^r})^{-1}\partial_k f_\beta(H^r)],$$

where the current operator, Liouvillian operator, and Fermi-Dirac distribution are

$$\partial_j H = i[\mathbf{R}_j, H] = i(\mathbf{R}_j H - H\mathbf{R}_j), \qquad \mathcal{L}_H(A) = \frac{i}{\hbar}[H, A],$$

$$f_\beta(E) = \left(1 + e^{\beta(E-E_F)}\right)^{-1}$$

with ω the frequency, η the dissipation, E_F the Fermi-level.

The Hamiltonian H^r now denotes H restricted to wave functions that are periodic on a supercell of period r on $\mathcal{R}$.

Kubo Formula for Conductivity on a Periodic Supercell

The Kubo formula can equivalently be given by

$$\sigma_{jk}^r = \frac{1}{|\Omega_r|} \sum_{m,\, n} F_\xi(E_m, E_n) \langle v_n | \partial_j H^r | v_m \rangle \langle v_m | \partial_k H^r | v_n \rangle,$$

where (E_m, v_m) are the eigenvalue, eigenvector pairs of H^r, $\xi = (\beta, \eta, \omega, E_F)$, and the *conductivity function* is given by

$$F_\xi(E, E') = \frac{ie^2}{\hbar^2} \frac{f_\beta(E - E_F) - f_\beta(E' - E_F)}{(E - E')(E - E' + \omega + i\eta)}.$$

The current-current correlation measure is given by

$$\langle v_n | \partial_j H^r | v_m \rangle \langle v_m | \partial_k H^r | v_n \rangle.$$

Kubo Formula for Periodic Structure

The limit $\sigma_{kl} = \lim_{r\to\infty} \sigma_{kl}^r$ can be formally derived by replacing the sum of the states indexed by m, n by integrals over the Brillouin zone, Γ^*, to obtain

$$\sigma_{kl} = \lim_{r\to\infty} \sigma_{kl}^r = \fint_{\Gamma*} \fint_{\Gamma*} \sum_{m,\,n} F_\xi(\varepsilon_{q,m}, \varepsilon_{q',n}) \langle v_{q',n} | \partial_j H | v_{q,m} \rangle \langle v_{q,m} | \partial_k H | v_{q',n} \rangle \, dq \, dq',$$

where $(\varepsilon_{q,m}, v_{q,m})$ are the eigenvalue-eigenvalue pairs of H.

How to generalize to incommensurate multilayers?

Current-current Correlation Measure

The *velocity operator* $\partial_p H^r \in \mathbb{R}^{\Omega_r \times \Omega_r}$ is given by

$$[\partial_p H^r]_{R\alpha,R'\alpha'} = i[H^r, \mathbf{R}_p]_{R\alpha,R'\alpha'} = -i(R' - R)_p H^r_{R\alpha,R'\alpha'}, \qquad R\alpha, R'\alpha' \in \Omega_r,$$

where $\mathbf{R}_p$ is understood as a diagonal matrix

$$[\mathbf{R}_p]_{R\alpha,R'\alpha'} = \delta_{\alpha\alpha'}\delta_{RR'}R_p.$$

The matrix-valued current-current correlation measure $\bar{\mu}^r$ on the finite system Ω_r is

$$\int_{\mathbb{R}^2} \phi(E, E')\, d\bar{\mu}^r(E, E')$$

$$= \left[\frac{1}{|\Omega_r|} \sum_{i,i'} \phi(E_i, E_{i'}) \operatorname{Tr}\Big[|v_i\rangle\langle v_i| \partial_p H^r |v_{i'}\rangle\langle v_{i'}| \partial_{p'} H^r \Big] \right]_{p,p'=1,2}$$

where (E_i, v_i) denote the eigenpairs of the Hamiltonian H^r.

Current-current Correlation Measure

$$\int_{\mathbb{R}^2} \phi(E, E')\, d\bar{\mu}^r(E, E')$$

$$= \left[\frac{1}{|\Omega_r|} \sum_{i,i'} \phi(E_i, E_{i'})\, \mathrm{Tr}\Big[|v_i\rangle\langle v_i| \partial_p H^r |v_{i'}\rangle\langle v_{i'}| \partial_{p'} H^r | \Big] \right]_{p,p'=1,2}$$

Approximate general functions $\phi(E, E')$ by sums of products of univariate functions

$$\phi(E, E') \approx \sum_{i,j} \phi_i(E)\phi_j(E').$$

We can then rewrite the current-current correlation measure as

$$\int_{\mathbb{R}^2} \phi(E, E')\, d\bar{\mu}^r(E, E') = \frac{1}{|\Omega_r|} \sum_{i,j} \mathrm{Tr}\big[\phi_i(H^r)\partial_p H^r \phi_j(H^r)\partial_{p'} H^r\big].$$

Conductivity Tensor for Finite System

The conductivity tensor for the finite system Ω_r can now be defined by

$$\bar{\sigma}^r = \frac{1}{|\Omega_r|} \int_{\mathbb{R}^2} F_\zeta(E, E') d\bar{\mu}^r(E, E'),$$

where the *conductivity function* F_ζ is defined as follows: if e is the elementary charge, $\hbar$ the Planck constant, E_F the Fermi-level of the system, and $f_\beta(E) = (1 + e^{\beta(E-E_F)})^{-1}$ the Fermi-Dirac distribution, then

$$F_\zeta(E, E') = \frac{ie^2}{\hbar^2} \frac{f_\beta(E - E_F) - f_\beta(E' - E_F)}{(E - E')(E - E' + \omega + i\eta)}.$$

Can we show that the thermodynamic limit

$$\sigma := \lim_{r \to \infty} \bar{\sigma}^r$$

exists and establish a rate of convergence?

Local Current-current Correlation Measure

We can write the current-current correlation measure as

$$\int_{\mathbb{R}^2} \phi(E,E')\, d\bar{\mu}^r(E,E') = \frac{1}{|\Omega_r|}\sum_{i,i'} \phi(E_i,E_{i'})\mathrm{Tr}\big[|v_i\rangle\langle v_i|\partial_p H^r|v_{i'}\rangle\langle v_{i'}|\partial_{p'}H^r|\big]$$

$$= \frac{1}{|\Omega_r|}\sum_{R\alpha\in\Omega_r}\left[\sum_{i,i'}\phi(E_i,E_{i'})\langle e_{R\alpha}|v_i\rangle\langle v_i|\partial_p H^r|v_{i'}\rangle\langle v_{i'}|\partial_{p'}H^r|e_{R\alpha}\rangle\right]$$

where

$$[e_{R\alpha}]_{R'\alpha'} = \delta_{\alpha\alpha'}\delta_{RR'}, \quad R'\alpha' \in \Omega_r,$$

and (E_i, v_i) are the eigenpairs of H^r.

Transform discretized integral over Ω_r to an integral over configuration space by introducing the shifted Hamiltonian

$$[H_\ell(b)]_{R\alpha,R'\alpha'} = h_{\alpha\alpha'}\big(b(\delta_{\alpha\in\mathcal{A}_{\tau(\ell)}} - \delta_{\alpha'\in\mathcal{A}_{\tau(\ell)}}) + R - R'\big), \quad R\alpha, R'\alpha' \in \Omega,$$

and $H^r_\ell(b) = H_\ell(b)|_{\Omega_r}$.

Local Current-current Correlation Measure

We can use the shifted Hamiltonian to approximate

$$\langle e_{R\alpha}|v_i\rangle\langle v_i|\partial_p H^r|v_{i'}\rangle\langle v_{i'}|\partial_{p'} H^r|e_{R\alpha}\rangle \approx \langle e_{0\alpha}|v_i\rangle\langle v_i|\partial_p H^r_\ell(b)|v_{i'}\rangle\langle v_{i'}|\partial_{p'} H^r_\ell(b)|e_{0\alpha}\rangle$$

where $b = \mathrm{mod}_i(R_j)$. Define the local current-current correlation measure $\mu^r_\ell[b]$ for a finite system Ω_r, at configuration b, in layer ℓ, via

$$\int_{\mathbb{R}^2} \phi(E,E')\, d\mu^r_\ell[b] = \sum_{\substack{i,i' \\ \alpha\in\mathcal{A}_\ell}} \phi(E_i,E_{i'})\,\langle e_{0\alpha}|v_i\rangle\langle v_i|\partial_p H^r_\ell(b)|v_{i'}\rangle\langle v_{i'}|\partial_{p'} H^r_\ell(b)|e_{0\alpha}\rangle,$$

where (E_i, v_i) are the eigenpairs of $H^r_\ell(b)$, and the configuration-based approximate current-current correlation measure and conductivity by

$$\mu^r = \nu\left(\int_{\Gamma_2} \mu^r_1[b]\, db + \int_{\Gamma_1} \mu^r_2[b]\, db\right), \qquad \text{and}$$

$$\sigma^r = \int F_\zeta\, d\mu^r(E,E').$$

Exponential Convergence of Current-current Correlation Measure

We define a strip in the complex plane

$$S_a = \{z \mid (z) \in [-a-1, a+1], (z) \in [-a, a]\}.$$

Lemma

There exist unique measures $\mu_\ell[b]$ such that for all F that are analytic on $S_a \times S_a$,

$$\int_{\mathbb{R}^2} F(E,E')d\mu_\ell^r[b](E,E') \to \int_{\mathbb{R}^2} F(E,E')d\mu_\ell[b](E,E')$$

with the rate

$$\left|\int_{\mathbb{R}^2} F(E,E')d\mu_\ell^r[b](E,E') - \int_{\mathbb{R}^2} F(E,E')d\mu_\ell[b](E,E')\right| \lesssim \sup_{z,z' \in S_a \setminus S_{a/2}} |F(z,z')| e^{-\gamma a r - c\log(a)},$$

for some $c, \gamma > 0$.

Exponential Convergence of Conductivity

Theorem

We have

$$\bar{\sigma}^r \to \sigma \qquad \text{and} \qquad \sigma^r \to \sigma \qquad \text{as } r \to \infty.$$

If $\lambda = \min\{\eta, \beta^{-1}\}$, *then there exist constants* $c, \gamma > 0$ *independent of* λ *and* r, *such that*

$$|\sigma - \sigma^r| \lesssim e^{-\gamma\lambda r - c\log(\lambda)}.$$

The global conductivity approximation only converges linearly

$$|\sigma - \bar{\sigma}^r| \lesssim \frac{1}{\eta r}.$$

Numerical Evaluation of the Approximate Conductivity:

Evaluate

$$\sigma^r[b] := \int F_\zeta(E_1, E_2)\, d\mu_\ell^r[b](E_1, E_2)$$

and integrate over local configurations b.

Computing eigenpairs E_i, v_i of H^r takes $\mathcal{O}\big(|\Omega_r|^3\big)!$ Can we do better?

A Linear-Scaling Local Conductivity Algorithm

Alternatively, assume we have an approximation

$$\tilde{F}_\zeta(E_1, E_2) := \sum_{(k_2,k_2)\in K} c_{k_1 k_2}\, T_{k_1}(E_1)\, T_{k_2}(E_2) \approx F_\zeta(E_1, E_2)$$

where $K \subset \mathbb{N}^2$ is a finite set of indices and $T_k(E)$ denotes the kth Chebyshev polynomial defined through the three-term recurrence relation

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_{k+1}(x) = 2x\, T_k(x) - T_{k-1}(x).$$

Define an approximate local conductivity

$$\tilde{\sigma}^r[b] = \sum_{\ell=1}^{2} \sum_{\alpha\in\mathcal{A}_\ell} \sum_{(k_1,k_2)\in K} c_{k_1 k_2}\, [T_{k_1}(H_{r,\ell}(b))\, \partial_j H_{r,\ell}(b)\, T_{k_2}(H_{r,\ell}(b))\, \partial_k H_{r,\ell}(b)]_{0\alpha,0\alpha}$$

which satisfies the error bound

$$\left|\sigma^r[b] - \tilde{\sigma}^r[b]\right| \leqslant C\, \|F_\zeta - \tilde{F}_\zeta\|_{[-1,1]^2}.$$

Local Conductivity Via Tensor-Product Chebyshev Approximation

1. $v_{k_1} := \partial_j H \, T_{k_1}(H) \, e_{0\alpha}$ for all $k_1 \in K_1 := \{k_1 \mid \exists k_2 : (k_1, k_2) \in K\}$
2. $w_{k_2} := T_{k_2}(H) \, \partial_k H \, e_{0\alpha}$ for all $k_2 \in K_2 := \{k_2 \mid \exists k_1 : (k_1, k_2) \in K\}$
3. $\tilde{\sigma}^r[b] := \sum_{(k_1,k_2)\in K} v_{k_1}^T w_{k_2}$

Lines 1 and 2 take $|K_1|$ and $|K_2|$, respectively, matrix-vector products when evaluated using the Chebyshev recurrence relation.

Line 3 requires $|K|$ inner products.

Due to the sparsity of $H \in \mathbb{R}^{n\times n}$, both types of products take $\mathcal{O}(|\Omega_r|)$ floating-point operations, and since $|K_1|, |K_2| \leqslant |K|$ we conclude that the computational cost is dominated by the cost of line 3 which is $\mathcal{O}(|K| \, |\Omega_r|)$.

The runtime of the algorithm is thus minimized by choosing $|K|$ as small as possible subject to the constraint that $\|F_\zeta - \tilde{F}_\zeta\|_{[-1,1]^2}$ is less than some error tolerance.

Optimal Choice For The Index Set K

The optimal choice for the index set K is to truncate the infinite Chebsyhev series

$$F_\zeta(E_1, E_2) := \sum_{k_1,k_2=0}^{\infty} c_{k_1 k_2}\, T_{k_1}(E_1)\, T_{k_2}(E_2)$$

using some small tolerance $\tau > 0$,

$$K(\tau) := \left\{(k_1, k_2) \in \mathbb{N}^2 \mid |c_{k_1 k_2}| \leqslant \tau\right\},$$

thus the size of K is linked to the decay of the Chebyshev coefficients $c_{k_1 k_2}$ which in turn depends on the regularity properties of F_ζ.

Regularity of F_ζ

Split the conductivity function $F_\zeta(E_1, E_2) = g_{\beta,E_F}(E_1, E_2)\, f_{\omega,\eta}(E_1, E_2)$ into

$$g_{\beta,E_F}(E_1, E_2) := \frac{f_\beta(E_1 - E_F) - f_\beta(E_2 - E_F)}{E_1 - E_2}$$

and

$$f_{\omega,\eta}(E_1, E_2) := \frac{1}{E_1 - E_2 + \omega + \iota\eta},$$

which are analytic everywhere except on the sets

$$S_{\beta,E_F} := \left(S^{(1)}_{\beta,E_F} \times \mathbb{C}\right) \cup \left(\mathbb{C} \times S^{(1)}_{\beta,E_F}\right) \quad \text{with} \quad S^{(1)}_{\beta,E_F} := \left\{E_F + \tfrac{\iota\pi k}{\beta} \mid k \text{ odd}\right\}$$

and

$$S_{\omega,\eta} := \left\{(E_2, E_2) \in \mathbb{C}^2 \mid E_1 - E_2 + \omega + \iota\eta = 0\right\},$$

respectively.

The conductivity function F_ζ is thus analytic except on the union of these two sets.

Decay of Chebyshev Coefficients

In one dimension, the Chebyshev coefficients c_k of a function $f(x)$ analytic on a neighborhood of $[-1, 1]$ decay exponentially, $|c_k| \leqslant C \exp(-\alpha k)$.

In two dimensions, we have two decay rates α_1, α_2 and in the case of the conductivity function F_ζ we have two sets of singularities S_{β,E_F}, $S_{\omega,\eta}$ limiting the possible values of α_1 and α_2.

Increasing β renders conductivity calculations at low temperatures rather expensive. Our pole expansion of F_ζ provably reduces the cost of evaluating the local conductivity to $\mathcal{O}\left(\beta^{1/2}\,\eta^{-5/4}\right)$ inner products for all $\beta \gtrsim \eta^{-1/2}$ and whose actual scaling was empirically found to be $\mathcal{O}\left(\beta^{1/2}\,\eta^{-1.05}\right)$ inner products.

Constraint	Parameter range	# significant terms
Relaxation	$\beta \lesssim \eta^{-1/2}$	$\mathcal{O}\left(\eta^{-3/2}\right)$
Mixed	$\eta^{-1/2} \lesssim \beta \lesssim \eta^{-1}$	$\mathcal{O}\left(\beta\eta^{-1}\right)$
Temperature	$\eta^{-1} \lesssim \beta$	$\mathcal{O}\left(\beta^2\right)$

Decay of Chebyshev Coefficients

Theorem

There exist $\alpha_{diag}(\zeta), \alpha_{anti}(\zeta) > 0$ *such that the Chebyshev coefficients* $c_{k_1 k_2}$ *of* F_ζ *are bounded by*

$$|c_{k_1,k_2}| \leqslant C(\zeta)\, \exp\big(-\alpha_{diag}(\zeta)\,(k_1+k_2) - \alpha_{anti}(\zeta)\,|k_1-k_2|\big)$$

for some $C(\zeta) < \infty$ *independent of* k_1, k_2. *In the limit* $\beta \to \infty$ *and* $\omega, \eta \to 0$ *with* $|\omega| \leqslant C\eta$ *for some* $C > 0$ *and assuming* $E_F \in [-e, e]$ *for some* $e < 1$, *it holds that*

$$\alpha_{diag}(\zeta) = \begin{cases} \Theta(\eta) & \text{if } \zeta \text{ is relaxation- or mixed-constrained,} \\ \Theta(\beta^{-1}) & \text{if } \zeta \text{ is temperature-constrained,} \end{cases}$$

$$\alpha_{anti}(\zeta) = \begin{cases} \Theta(\sqrt{\eta}) & \text{if } \zeta \text{ is relaxation-constrained,} \\ \Theta(\beta^{-1}) & \text{if } \zeta \text{ is mixed- or temperature-constrained.} \end{cases}$$

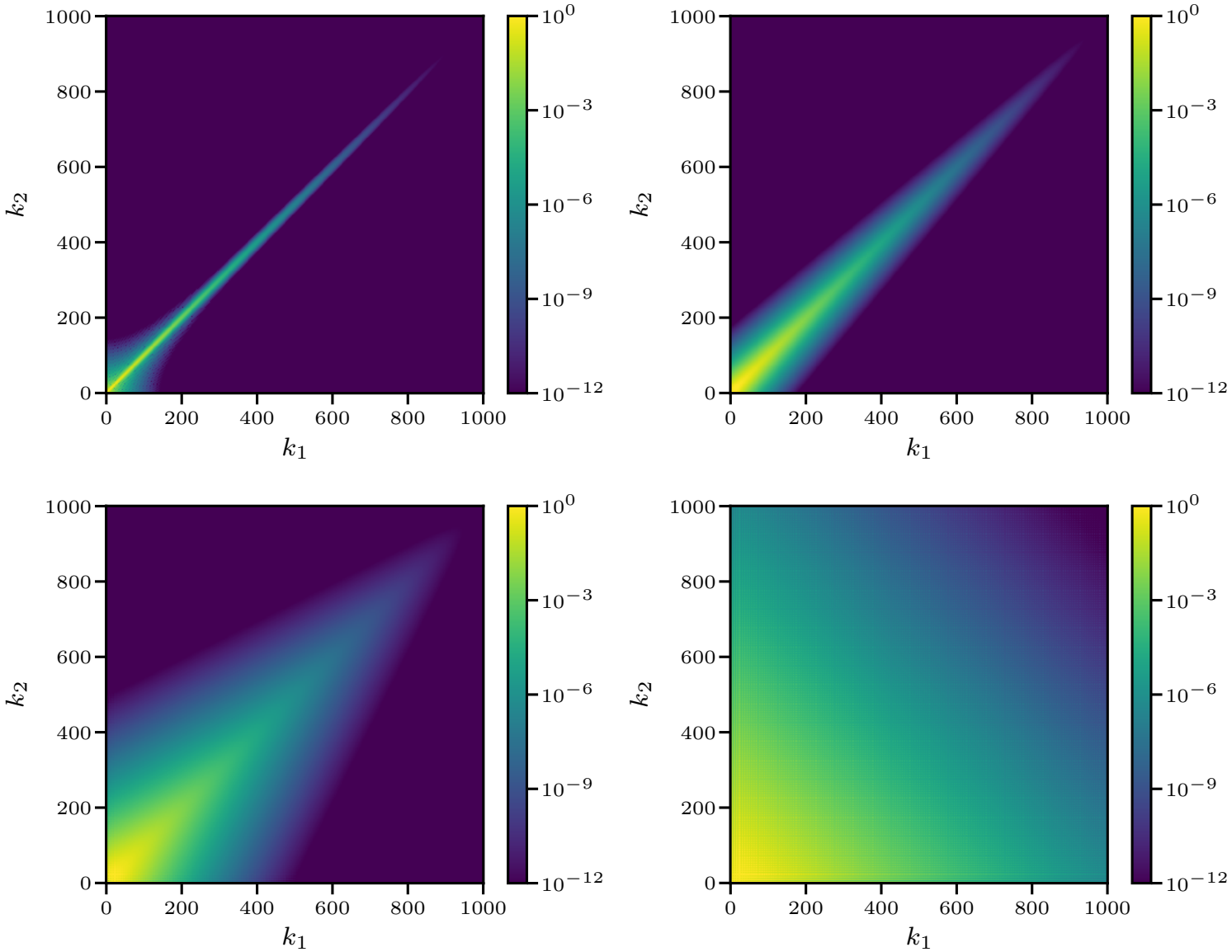


Figure: Normalized Chebyshev coefficients $\hat{c}_{k_1 k_2} := |c_{k_1 k_2}|/|c_{00}|$ of the conductivity function F_ζ with increasing temperature for fixed relaxation η.

The Chebyshev Decay Theorem suggests to truncate the infinite Chebyshev series to

$$F_{\zeta,\tau}(E_1, E_2) := \sum_{(k_1,k_2)\in K(\tau)} c_{k_1 k_2}\, T_{k_1}(E_1)\, T_{k_2}(E_2)$$

where

$$K(\tau) := \Big\{(k_1, k_2) \in \mathbb{N}^2 \mid \exp\big(-\alpha_{diag}(\zeta)\,(k_1 + k_2) - \alpha_{anti}(\zeta)\,|k_1 - k_2|\big) \leqslant \tau\Big\}.$$

It then follows from the Chebyshev Decay Theorem that

$$\|F_\zeta - F_{\zeta,\tau}\|_{[-1,1]^2} = \mathcal{O}\Big(\alpha_{diag}(\zeta)^{-1}\,\alpha_{anti}(\zeta)^{-1}\,\tau\,|\log(\tau)|\Big).$$

The $|\log(\tau)|$-factor above varies very little over a large range of τ such that one may approximate it by a constant without losing much in accuracy. Doing so yields that we need to choose the truncation tolerance $\tau_\varepsilon := \alpha_{diag}(\zeta)\,\alpha_{anti}(\zeta)\,\varepsilon$ to guarantee an error $\|F_\zeta - F_{\zeta,\tau}\|_{[-1,1]^2} \leqslant \varepsilon$, which in turn yields

$$|K(\tau_\varepsilon)| = \mathcal{O}\left(\frac{|\log(\alpha_{diag}(\zeta)\,\alpha_{anti}(\zeta)\,\varepsilon)|^2}{\alpha_{diag}(\zeta)\,\alpha_{anti}(\zeta)}\right).$$

Pole Expansion For Low-Temperature Calculations

The number of coefficients eventually scales as $\mathcal{O}\left(\beta^2\right)$ so that the Chebyshev algorithm becomes expensive at low temperatures.

To avoid these high costs at low temperatures, we propose to expand F_ζ into a sum over the poles in S_{β,E_F}.

Theorem

The conductivity function F_ζ can be written as

$$F_\zeta(E_1,E_2) = \frac{\sum_{z\in Z_{k,\beta,E_F}} \frac{1}{\beta}\frac{1}{(E_1-z)(E_2-z)} + R_{k,\beta,E_F}(E_1,E_2)}{E_1-E_2+\omega+\iota\eta}$$

where

$$Z_{k,\beta,E_F} := \left\{E_F + \tfrac{\ell\pi\iota}{\beta} \mid \ell \in \{-2k+1,-2k+3,\ldots,2k-3,2k-1\}\right\} \subset S_{\beta,E_F}$$

and the remainder R_{k,β,E_F} is analytic on the larger biellipse $E\left(\alpha_{k,\beta,E_F}\right)^2 \supset E\left(\alpha_{0,\beta,E_F}\right)^2$ with α_{k,β,E_F} the parameter of the ellipse through $E_F \pm \frac{(2k+1)\pi\iota}{\beta}$.

Pole Expansion For Low-Temperature Calculations

For k large enough, the remainder term becomes relaxation constrained such that the Chebyshev Algorithm becomes fairly efficient. For the pole terms, we propose to employ the Chebyshev Algorithm using the weighted Chebyshev approximation

$$\frac{1}{(E_1 - z)(E_2 - z)(E_1 - E_2 + \omega + \iota\eta)} \approx \sum_{k_1 k_2 \in K_z} c(z)_{k_1 k_2} \frac{T_{k_1}(E_1)}{E_1 - z} \frac{T_{k_2}(E_2)}{E_2 - z}.$$

This leads to dominant computational cost:

$$\mathrm{nip} = \mathcal{O}\left(k\,\eta^{-3/2}\right) + \begin{cases} \mathcal{O}\left(\frac{\beta^2}{k^2}\right) & \text{if } k \leqslant \left\lfloor \frac{\beta\eta - \pi}{2\pi} \right\rfloor \\ \mathcal{O}\left(\frac{\beta\eta^{-1}}{k}\right) & \text{if } \left\lceil \frac{\beta\eta - \pi}{2\pi} \right\rceil \leqslant k \leqslant \left\lfloor \frac{\beta y_\zeta - \pi}{2\pi} \right\rfloor \\ \mathcal{O}\left(\eta^{-3/2}\right) & \text{if } \left\lceil \frac{\beta y_\zeta - \pi}{2\pi} \right\rceil \leqslant k \end{cases}$$

inner products if we assume that solving a single linear system of the form $(H - zI)^{-1} v$ is less expensive than $\mathcal{O}(\eta^{-3/2})$ inner products. This cost is minimized if we choose $k = \mathcal{O}\left(\beta^{1/2}\,\eta^{1/4}\right)$ which yields $\mathrm{nip} = \mathcal{O}\left(\beta^{1/2}\,\eta^{-5/4}\right)$.

Convergence of Local versus Naive Conductivity

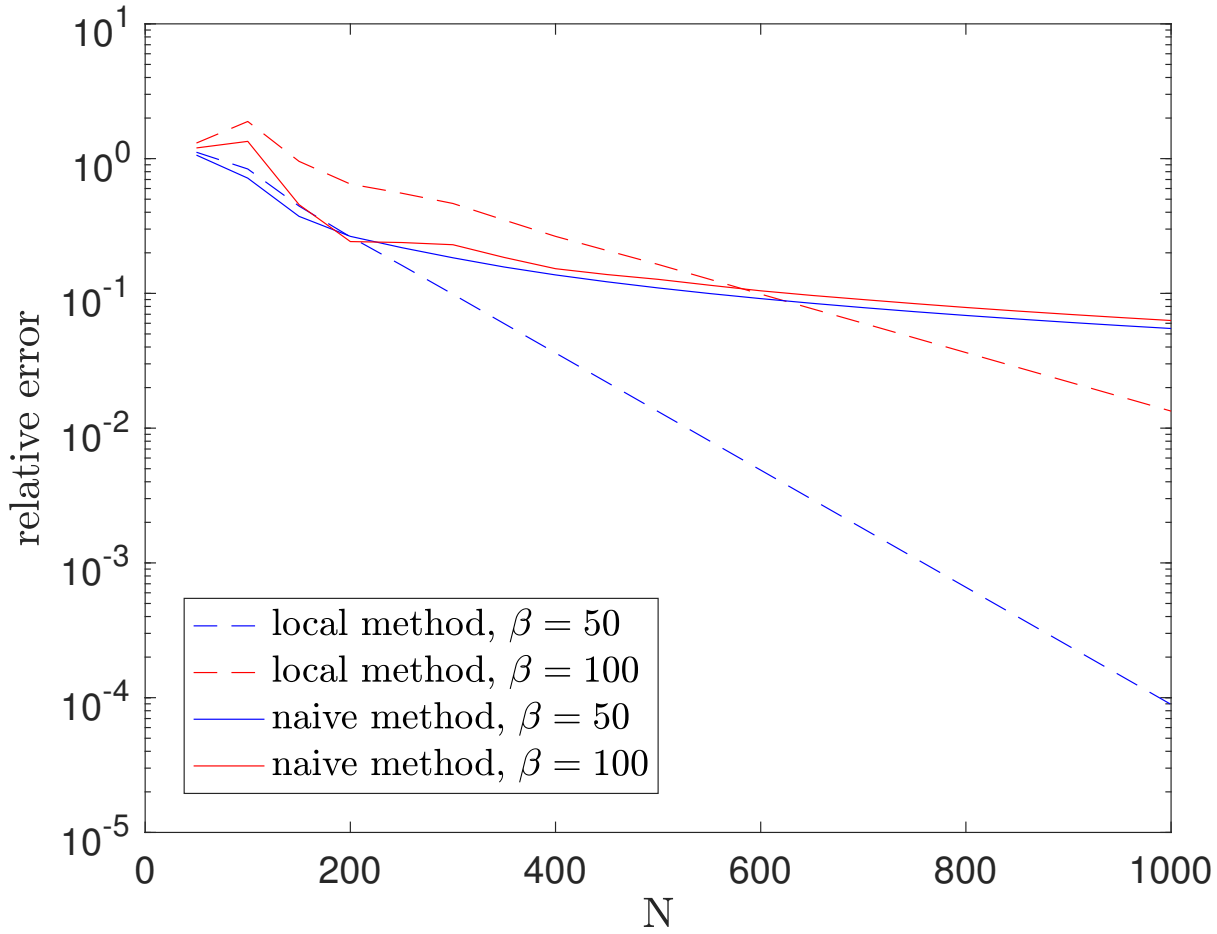


Figure: We let $\eta = \beta^{-1}$, and look at convergence for $\beta = 50$ and $\beta = 100$. The local technique converges exponentially, while the naive computation of conductivity is far weaker. Also as expected, larger β and smaller η gives a slower rate of decay.

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