Exact real space formulation and efficient computation of the electronic properties of 2D heterostructures

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2D bilayer geometry

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

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

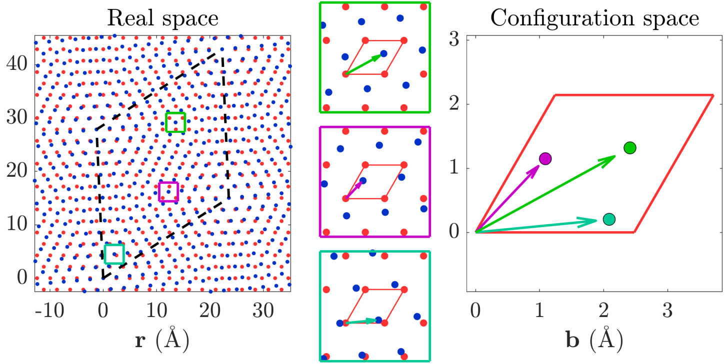
where A_j is a 2×2 invertible matrix whose columns are primitive lattice vectors. We define the *unit cell* for layer j as

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

Reciprocal lattice: $\mathcal{R}_j^* := \{2\pi A^{-T} n : n \in \mathbb{Z}^2\}$.
Brillouin Zone: $\Gamma_j^* = \{2\pi A^{-T} x : x \in [0, 1)^2\}$.

Represent multilattices by $\mathcal{R}_1 \times \mathcal{A}_1$ and $\mathcal{R}_2 \times \mathcal{A}_2$
where $\mathcal{A}_i$ denotes the set of orbitals associated with each lattice point in layer i.

Let $B_r := \{x \in \mathbb{R}^2 : |x| \leqslant r\}$, so that $\mathcal{R}_j \cap B_r = \{R_j \in \mathcal{R}_j : |R_j| \leqslant r\}$ are the set of lattice points in layer j with magnitude less than or equal to r.



Blue lattice points' ($\mathcal{R}_1$) local environment (Γ_2) described completely by the disregistry between the red and blue unit-cells.

Isomorphism (one-to-one mapping) between $\mathcal{R}_1$ and configurations (disregistries) (Γ_2) of incommensurate systems.

Configuration space approach gives a unified theoretical and computational approach to mechanics, electronic structure, transport, and diffraction.

[Generalized Kubo formulas for the transport properties of incommensurate 2D atomic heterostructures. E. Cancés, P. Cazeaux, and M. Luskin. Journal of Mathematical Physics, 58:063502, 2017.]

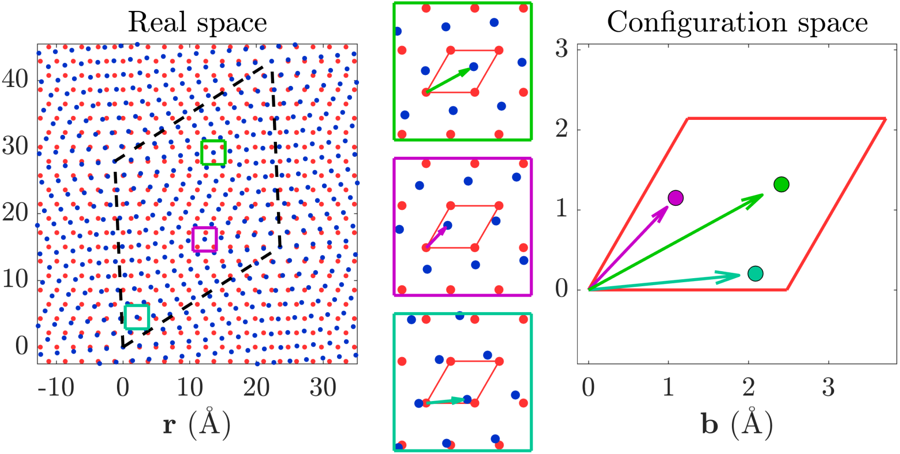
Disregistry

The disregistry of an atom R_1 of layer 1 with respect to layer 2 is given by

$$b_{1\to 2}(R_1) = \mathrm{mod}_{\Gamma_2}(R_1), \qquad R_1 \in \mathcal{R}_1.$$

Since $A_2 A_1^{-1} R_1 \in \mathcal{R}_2$, we can smoothly interpolate to $\mathbb{R}^2$ by

$$b_{1\to 2}(x) = \mathrm{mod}_{\Gamma_2}\big[(I - A_2 A_1^{-1})x\big].$$



Moiré Unit Cell and Superlattice

$b_{1\to 2}(x)$ and $b_{2\to 1}(x)$ are isomorphisms

$$b_{1\to 2} : \begin{cases} \Gamma_{\mathcal{M}} \to \Gamma_2, \\ \quad x \mapsto (I - A_2 A_1^{-1})x = A_2(A_2^{-1} - A_1^{-1})x, \end{cases}$$
$$b_{2\to 1} : \begin{cases} \Gamma_{\mathcal{M}} \to \Gamma_1, \\ \quad x \mapsto (I - A_1 A_2^{-1})x = A_1(A_1^{-1} - A_2^{-1})x, \end{cases}$$

where $\Gamma_{\mathcal{M}}$ is the periodic moiré cell:

$$\Gamma_{\mathcal{M}} := \mathbb{R}^2/\mathcal{R}_{\mathcal{M}} \equiv (A_1^{-1} - A_2^{-1})^{-1}[0,1)^2,$$

and $\mathcal{R}_{\mathcal{M}}$ is the moiré superlattice given by

$$\mathcal{R}_{\mathcal{M}} := (A_1^{-1} - A_2^{-1})^{-1}\mathbb{Z}^2.$$

Reciprocal moiré lattice is then given by

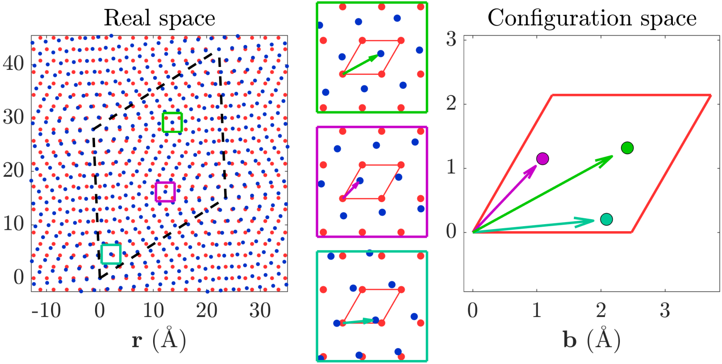
$$\mathcal{R}^*_{\mathcal{M}} := 2\pi(A_1^{-T} - A_2^{-T})\mathbb{Z}^2.$$

Ergodicity of Disregistries for Incommensurate 2D Layers

For $h \in C_{\text{per}}(\Gamma_2)$, we thus have that $h(R_1) = h(b_{1\to 2}(R_1))$ and

$$\frac{1}{\#\mathcal{R}_1 \cap B_r} \sum_{R_1 \in \mathcal{R}_1 \cap B_r} h(R_1) = \frac{1}{\#\mathcal{R}_1 \cap B_r} \sum_{R_1 \in \mathcal{R}_1 \cap B_r} h(b_{1\to 2}(R_1)) \to \frac{1}{|\Gamma_2|} \int_{\Gamma_2} h(b)\,db.$$

Replace integrals (traces) over $BZ_{\text{supercell}}$ by disregistries Γ_2



[Generalized Kubo formulas for the transport properties of incommensurate 2D atomic heterostructures. E. Cancés, P. Cazeaux, and M. Luskin. Journal of Mathematical Physics, 58:063502, 2017.]