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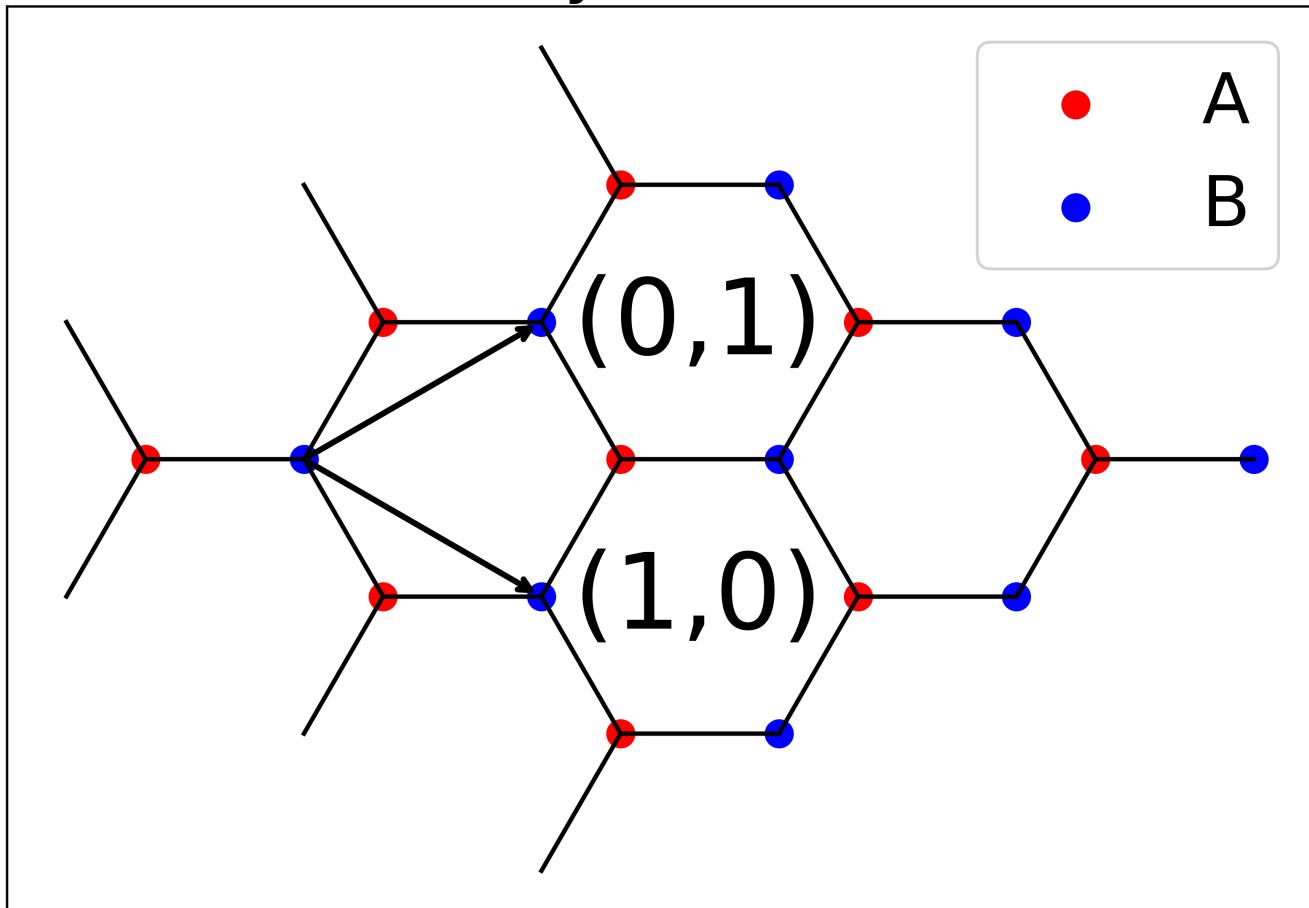
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Atomic corrugation and electron localization due to Moiré patterns in twisted bilayer graphenes

Kazuyuki Uchida, Shinnosuke Furuya, Jun-Ichi Iwata, and Atsushi Oshiyama

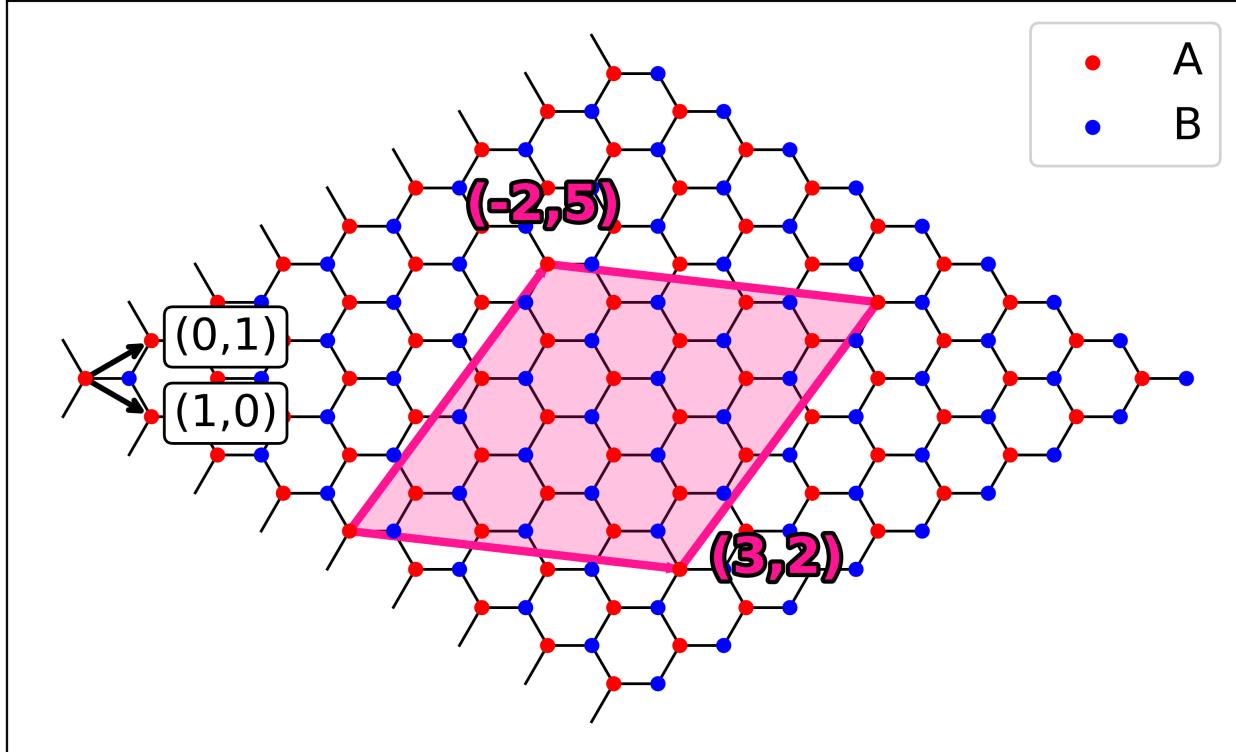
Unitcell plot

2D Honeycomb Lattice

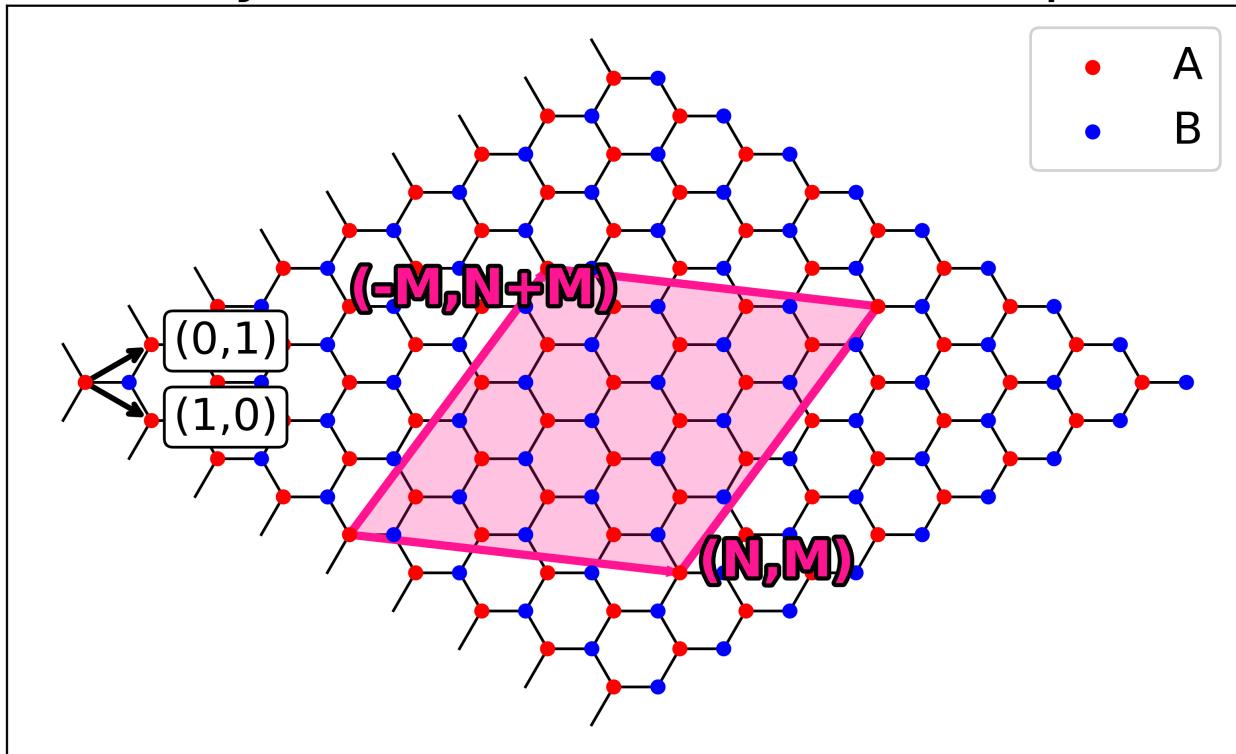


Supercell plot

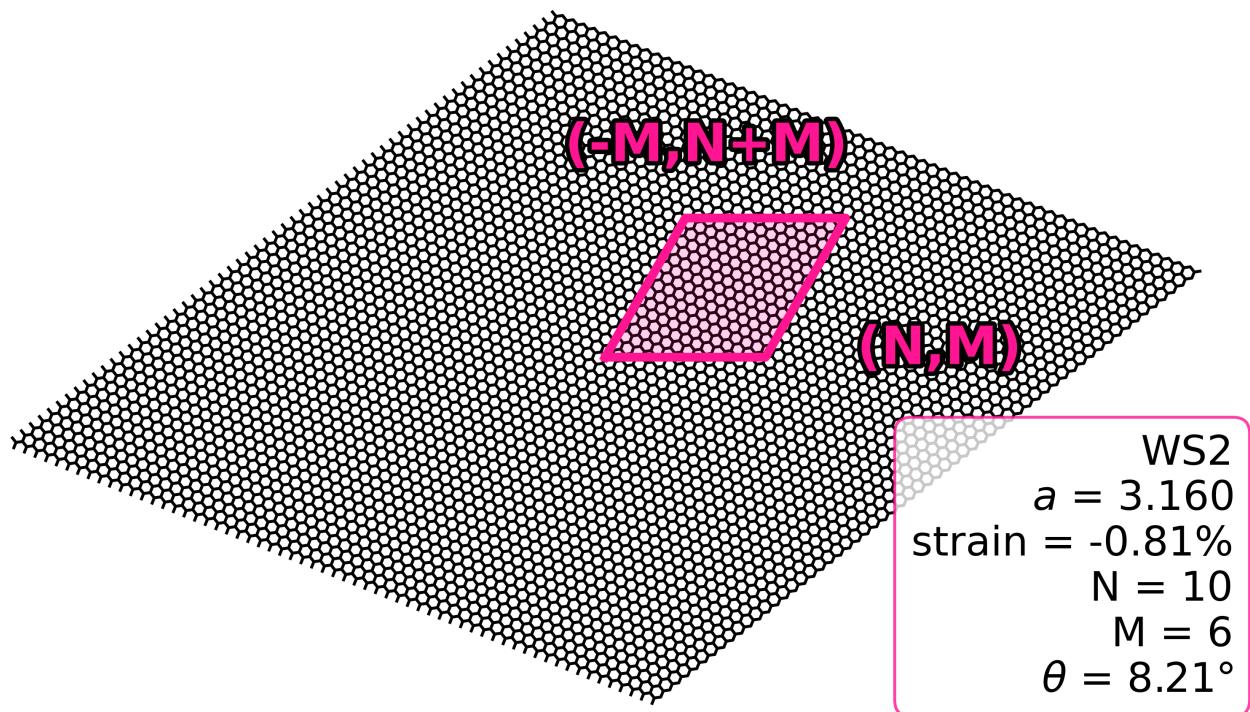
2D Honeycomb Lattice with Two Supercells



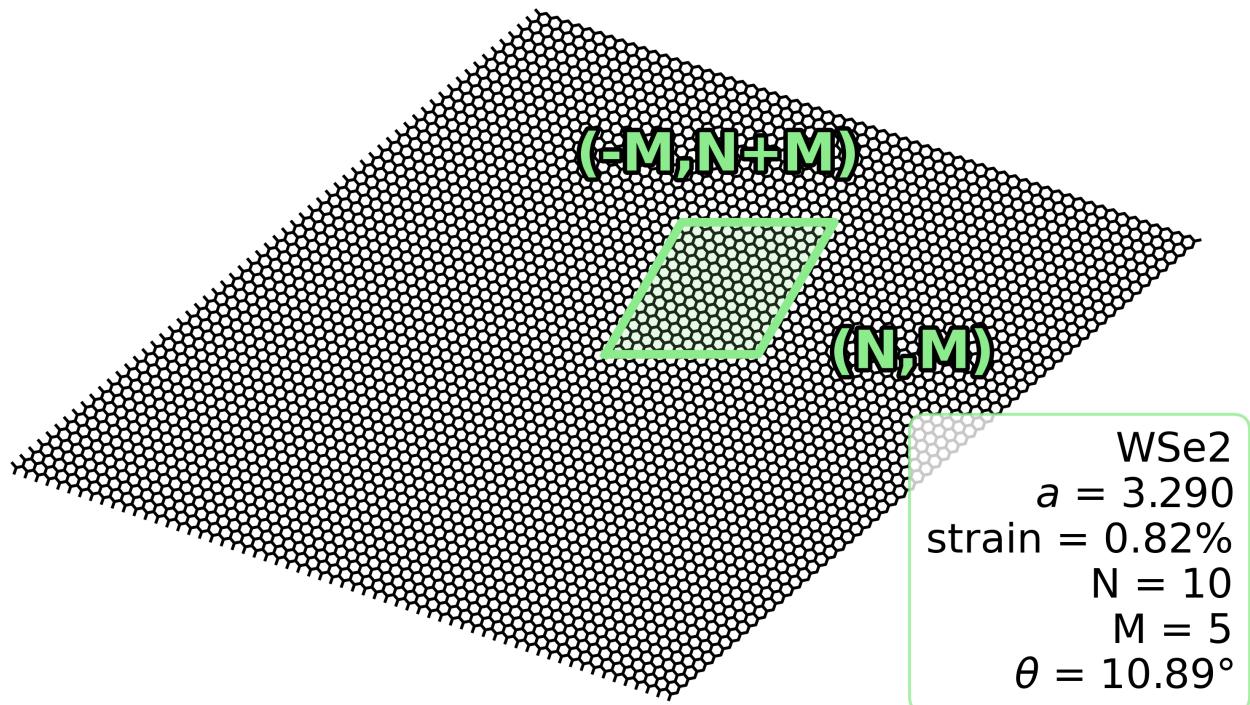
2D Honeycomb Lattice with Two Supercells



Top layer



Bottom layer



WS₂ / WSe₂ Moiré Supercells

WS₂

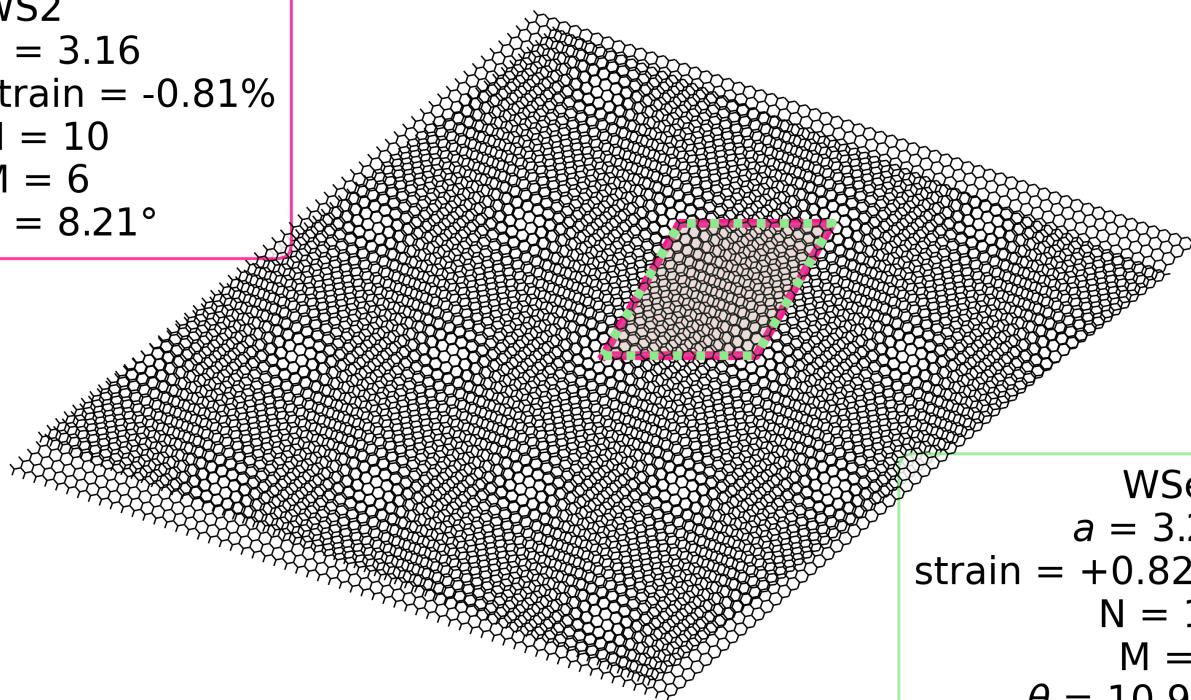
$a = 3.16$

strain = -0.81%

$N = 10$

$M = 6$

$\theta = 8.21^\circ$



Hetero-moiré Supercell Example

Layer	N	M	Lattice Constant (Å)	Strain (%)	Twisted Angle (deg)
Top (WS ₂)	10	6	3.16	-0.81	8.21
Bottom (WSe ₂)	10	5	3.29	+0.82	10.90

- Moiré rotation angle: 2.68°

- Total atoms: 1113

moiré supercell lattice vector derivation

Primitive lattice vectors of the honeycomb lattice:

$$\vec{b}_1 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2} \right)$$

$$\vec{b}_2 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

Here, \vec{b}_1 and \vec{b}_2 are the primitive lattice vectors in Cartesian coordinates, describing the repeating structure of the 2D honeycomb lattice.

Lattice matrix constructed from the primitive vectors:

$$B = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Matrix B uses \vec{b}_1 and \vec{b}_2 as its columns. This matrix is useful for transforming between lattice and Cartesian coordinates.

General formula for the inverse of a 2×2 matrix:

$$B^{-1} = \frac{1}{\det(B)} \begin{pmatrix} b_{22} & -b_{12} \\ -b_{21} & b_{11} \end{pmatrix}$$

B^{-1} is the inverse of matrix B , written in terms of the matrix elements b_{ij} . This formula applies to any 2×2 matrix.

Explicit calculation of B^{-1} for the honeycomb lattice:

$$B^{-1} = \frac{2}{\sqrt{3}} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & 1 \end{pmatrix}$$

By substituting the specific entries of B and its determinant, we get this explicit inverse for the honeycomb lattice.

Definition of the Gram matrix (metric tensor):

$$G = B^T B = \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}$$

The Gram matrix G encodes the inner products of the lattice vectors, capturing geometric properties such as lengths and angles in the lattice.

Supercell basis vector 1:

$$\vec{b}'_1 = (N, M)$$

Here, \vec{b}'_1 defines the first supercell lattice vector as an integer linear combination of the original basis vectors.

Supercell basis vector 2 via 60° rotation:

$$\vec{b}'_2 = R_{\text{basis}}(60^\circ) \vec{b}'_1$$

The second supercell vector \vec{b}'_2 is obtained by rotating \vec{b}'_1 by 60° in the basis coordinate system.

60° rotation matrix in Cartesian coordinates:

$$R_{\text{cart}}(60^\circ) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

This matrix rotates a vector by 60° counterclockwise in Cartesian space.

60° rotation matrix in lattice basis:

$$R_{\text{basis}} = B^{-1} R_{\text{cart}} B$$

To rotate in lattice coordinates, sandwich the Cartesian rotation matrix between B^{-1} and B .

Explicit calculation of R_{basis} :

$$\begin{aligned} R_{\text{basis}} &= \begin{pmatrix} \frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & 1 \end{pmatrix} \begin{pmatrix} \frac{\sqrt{3}}{2} & 0 \\ \frac{1}{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} \end{aligned}$$

Step-by-step calculation of the rotation matrix in the lattice basis, starting from its definition in terms of B , B^{-1} , and $R_{\text{cart}}(60^\circ)$.

Final 60° rotation matrix in basis coordinates:

$$R_{\text{basis}} = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}$$

The final form of the rotation matrix in the lattice basis.

Formula for the second supercell basis vector after rotation:

$$\Rightarrow \vec{b}'_2 = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} N \\ M \end{pmatrix} = \begin{pmatrix} -M \\ N+M \end{pmatrix}$$

Applying the rotation to \vec{b}'_1 gives the explicit expression for the second supercell basis vector, \vec{b}'_2 .

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moire supercell twist angle derivation (heterobilayer)

For heterobilayer, θ is determined by the angle between (N_t, M_t) and (M_b, N_b) :

$$\vec{u}_t = \begin{pmatrix} N_t \\ M_t \end{pmatrix}, \quad \vec{u}_b = \begin{pmatrix} N_b \\ M_b \end{pmatrix}$$

The cosine of the angle between \vec{u} and \vec{v} :

$$\cos \theta = \frac{\vec{u}_t \cdot \vec{u}_b}{|\vec{u}_t| |\vec{u}_b|}$$

This is the standard definition of the angle between two vectors.

Generalized inner product using the lattice Gram matrix:

$$\begin{aligned} \vec{u}_t \cdot \vec{u}_b &= \vec{u}_t^T G \vec{u}_b = (N_t \quad M_t) \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} N_b \\ M_b \end{pmatrix} \\ &= (N_t \quad M_t) \begin{pmatrix} N_b + \frac{1}{2}M_b \\ \frac{1}{2}N_b + M_b \end{pmatrix} \\ &= N_t N_b + \frac{1}{2} N_t M_b + \frac{1}{2} N_b M_t + M_t M_b \end{aligned}$$

The Gram matrix G encodes the geometric information of the lattice. (This term is needed for non-orthogonal basis)

The squared norm of either vector:

$$\begin{aligned}
|\vec{u}_t|^2 &= \vec{u}_t \cdot \vec{u}_t = \vec{u}_t^T G \vec{u}_t = (N_t, M_t) \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} N_t \\ M_t \end{pmatrix} \\
&= (N_t, M_t) \begin{pmatrix} N_t + \frac{1}{2}M_t \\ \frac{1}{2}N_t + M_t \end{pmatrix} = N_t^2 + N_t M_t + M_t^2
\end{aligned}$$

Final formula for the twist angle cosine:

$$\Rightarrow \cos \theta = \frac{N_t N_b + \frac{1}{2} N_t M_b + \frac{1}{2} N_b M_t + M_t M_b}{\sqrt{N_t^2 + N_t M_t + M_t^2} \sqrt{N_b^2 + N_b M_b + M_b^2}}$$

This formula gives the cosine of the angle between the first supercell basis vectors \vec{b}'_1 of the top and bottom layers, which also corresponds to the twist angle of the heterobilayer moiré superlattice.

moiré supercell lattice constant & number of atoms

$$|\vec{u}|^2 = |\vec{v}|^2 = N^2 + NM + M^2$$

After applying unit cell lattice constant scaling

$$L_{\text{cell}} = a_t \sqrt{N_t^2 + N_t M_t + M_t^2} = a_b \sqrt{N_b^2 + N_b M_b + M_b^2}$$

The core of constructing a heterobilayer moiré supercell is to find pairs of supercell indices (N_t, M_t) and (N_b, M_b) that satisfy the equations above.

This supercell has $N^2 + NM + M^2$ unit cells for each layer.

Therefore, it has $3(N^2 + NM + M^2)$ atoms per layer.

The formula for calculating the total number of atoms is:

$$N_{\text{atoms}} = 3(N_t^2 + N_t M_t + M_t^2) + 3(N_b^2 + N_b M_b + M_b^2).$$