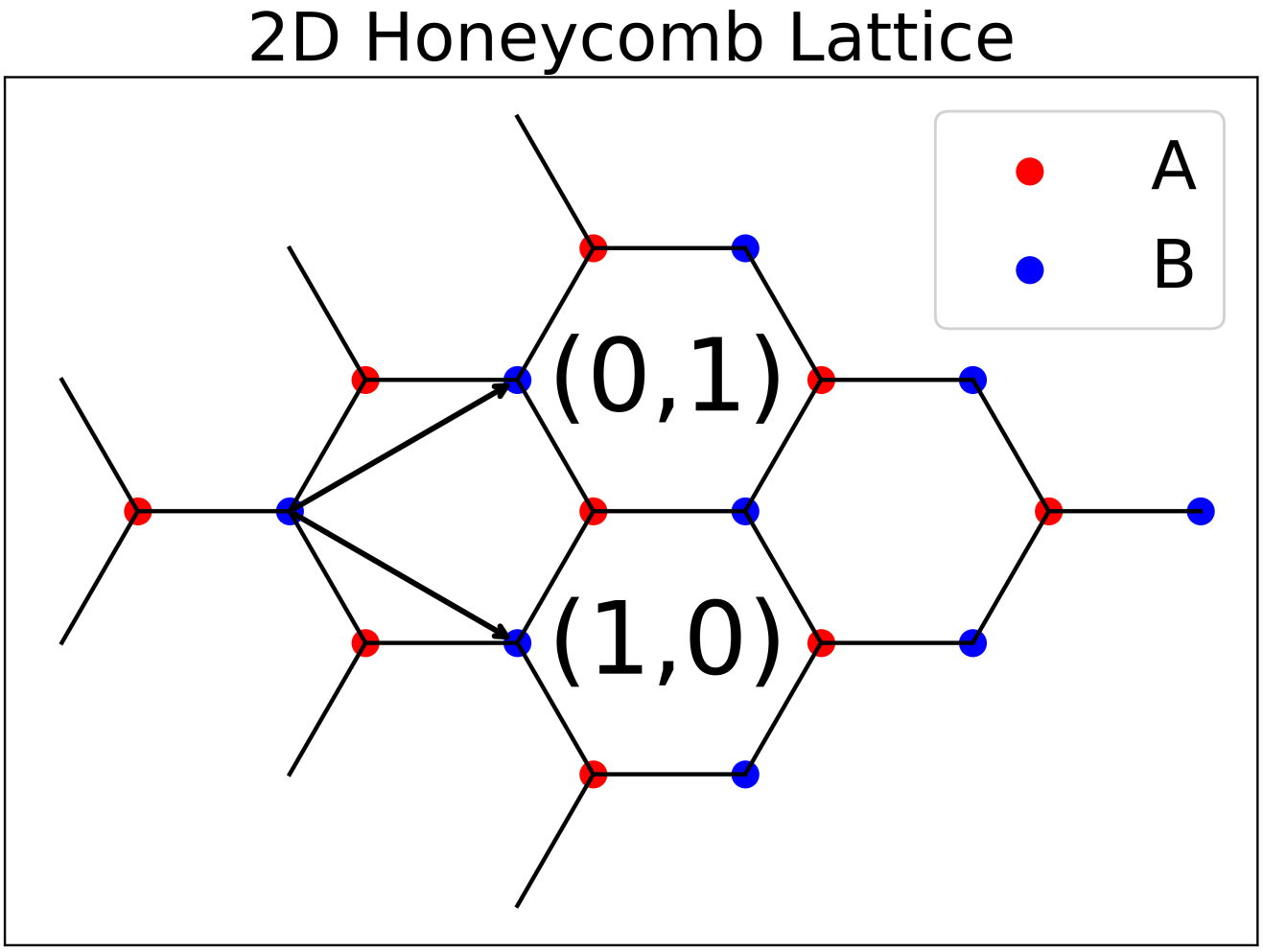
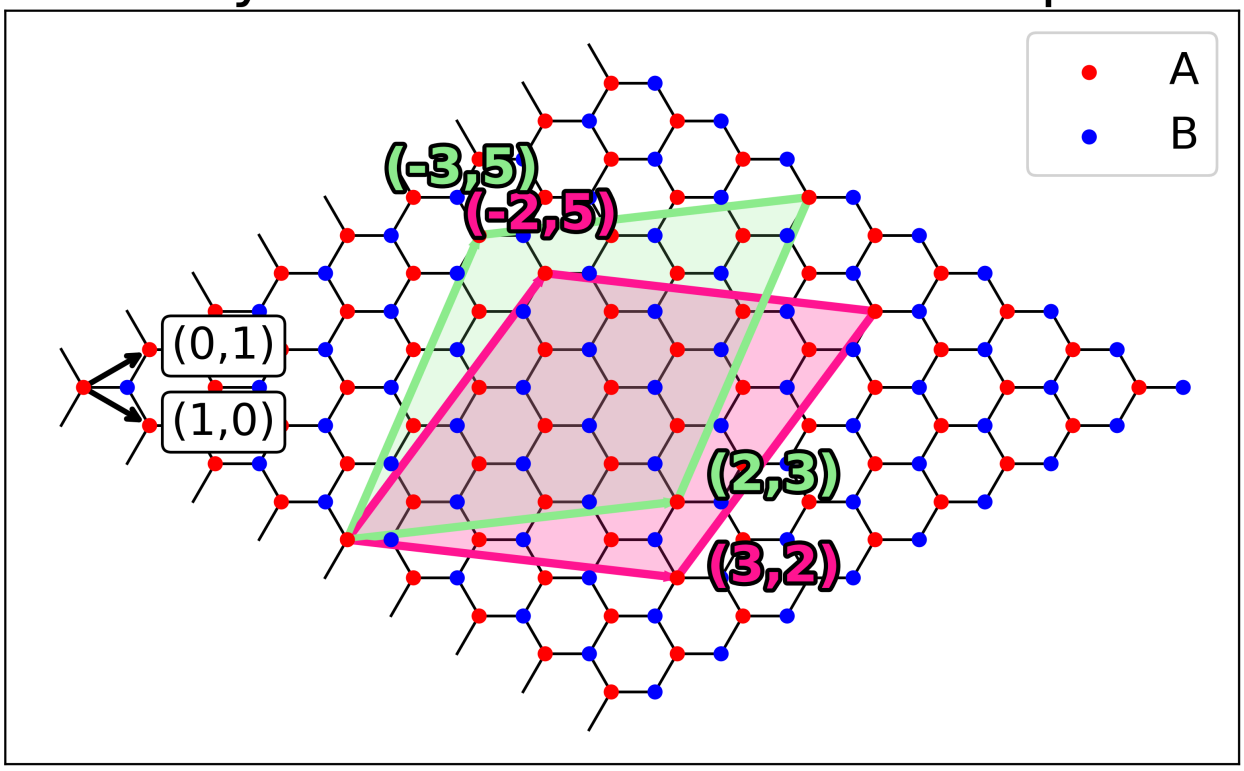
Reference:

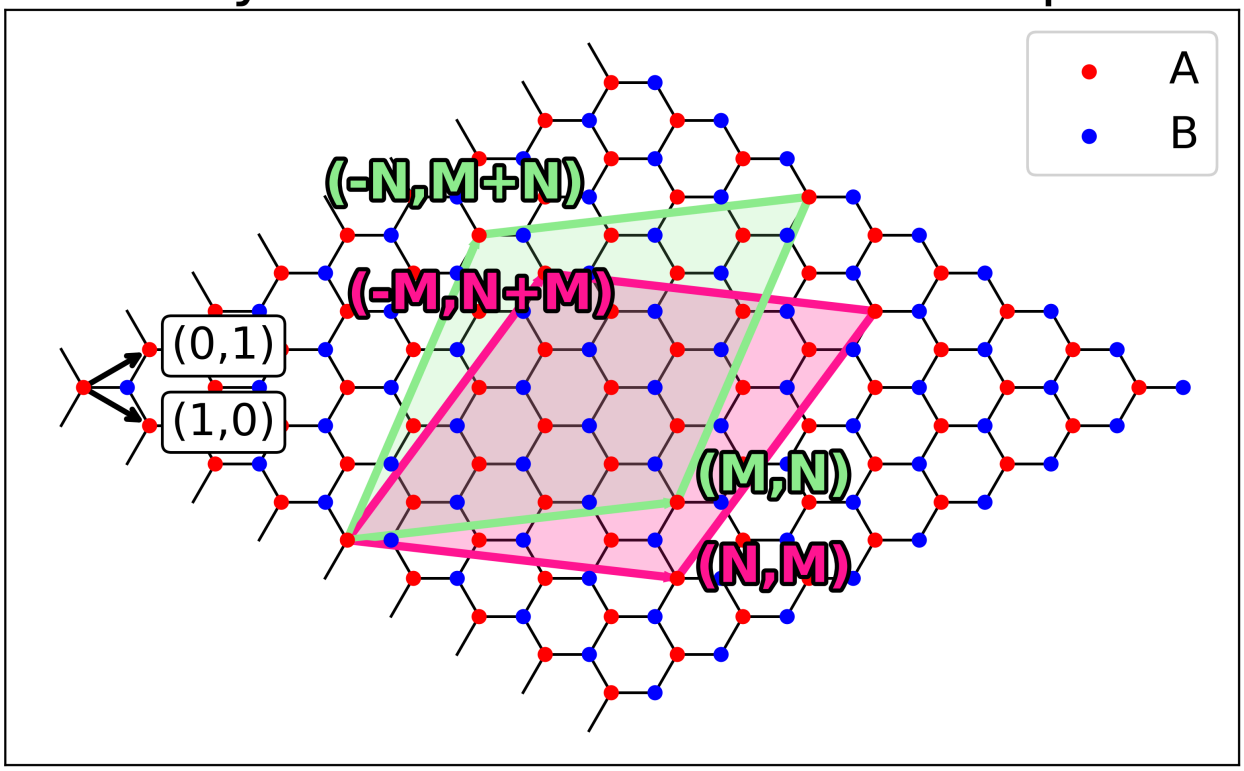
PHYSICAL REVIEW B 90, 155451 (2014)
Atomic corrugation and electron localization due to Moir´e patterns in twisted bilayer graphenes
Kazuyuki Uchida, Shinnosuke Furuya, Jun-Ichi Iwata, and Atsushi Oshiyama

Unitcell plot

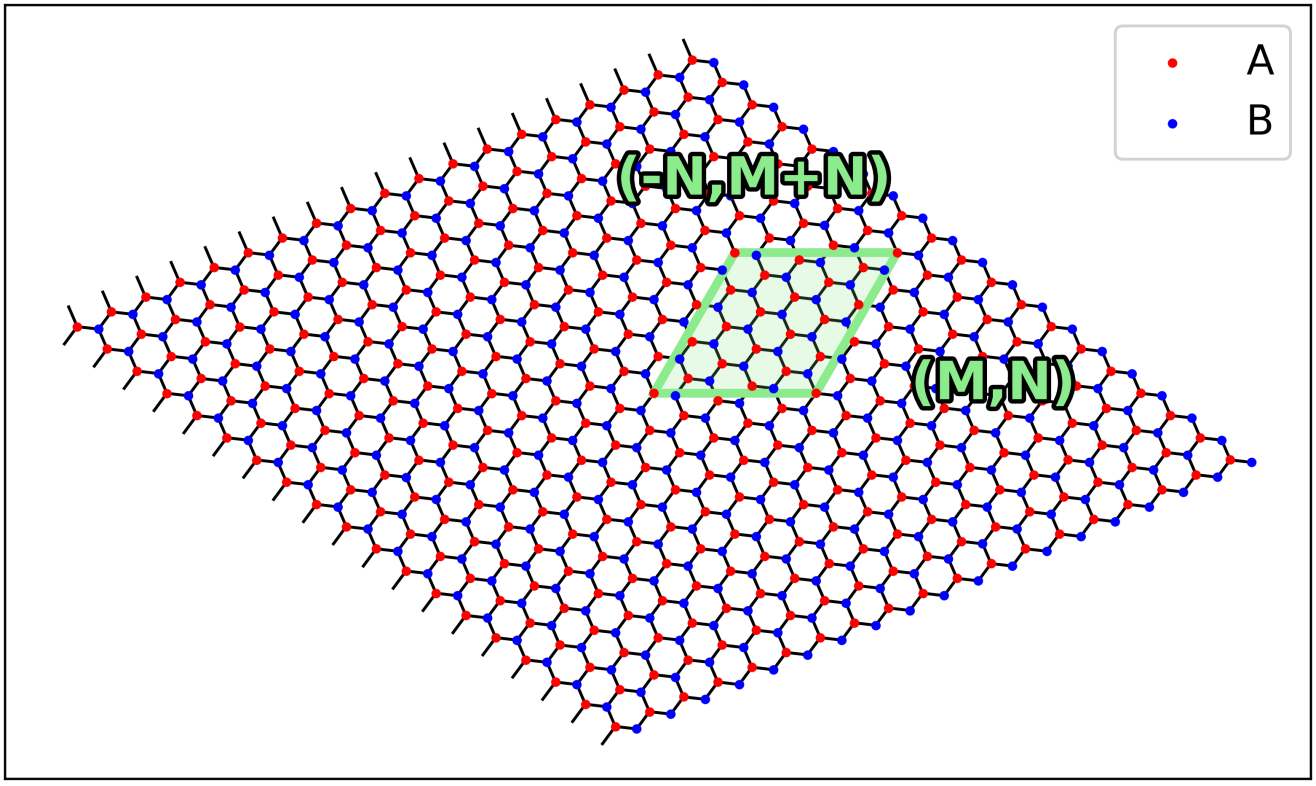


Supercell plot

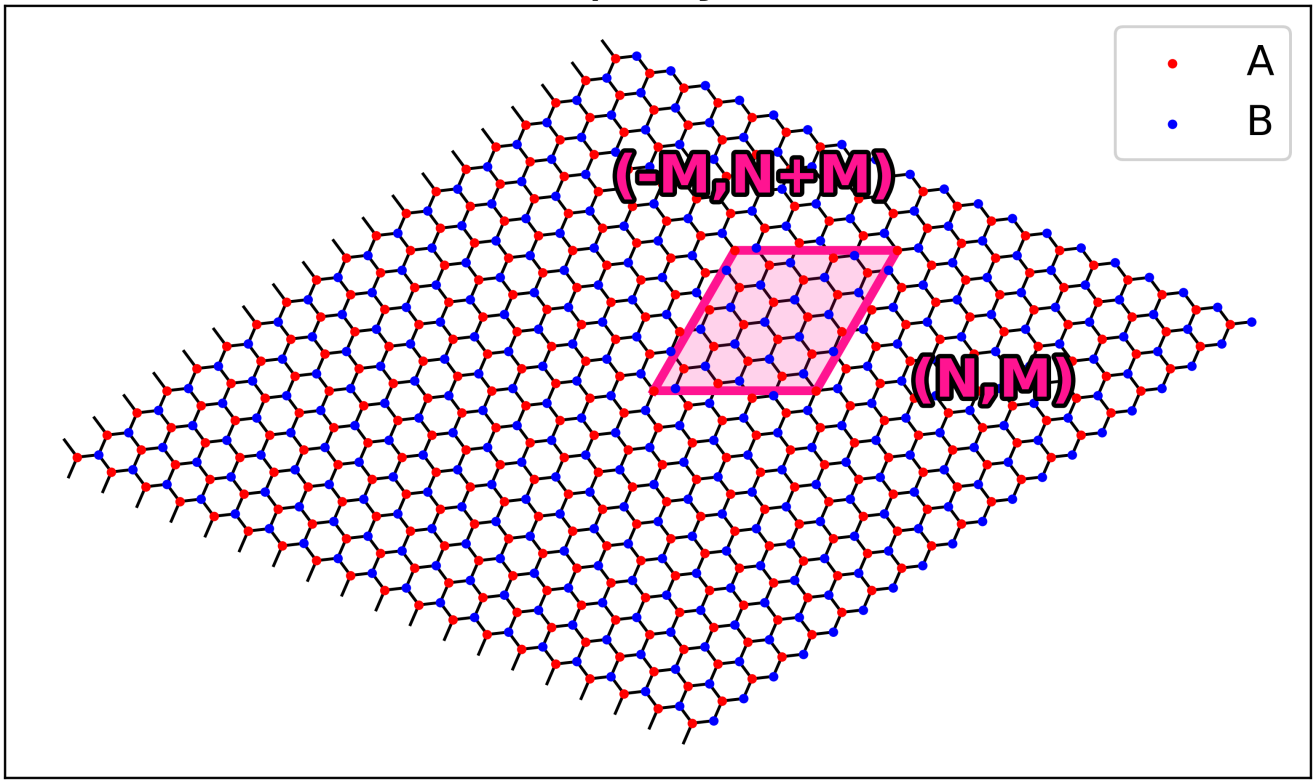

2D Honeycomb Lattice with Two Supercells
A
B
(-3,5)
(-2,5)
(0,1)
(1,0)
(2,3)
(3,2)


2D Honeycomb Lattice with Two Supercells
A
B
(-N,M+N)
(-M,N+M)
(0,1)
(1,0)
(M,N)
(N,M)

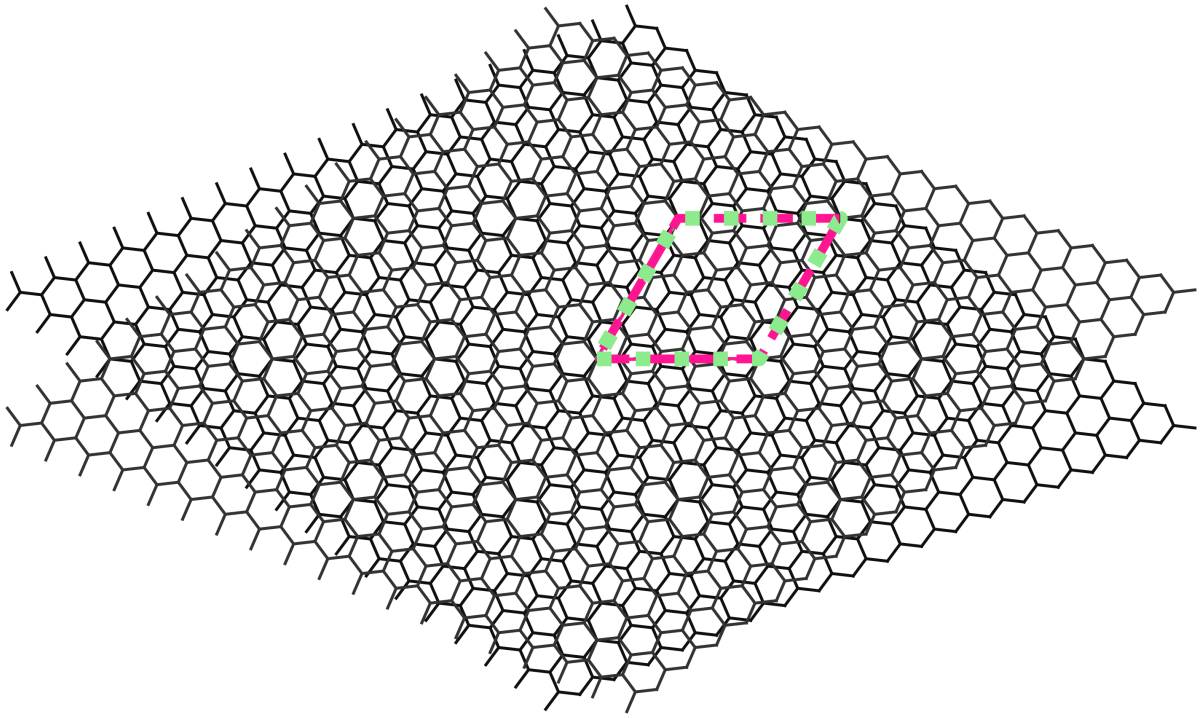
Bottom layer



Top layer



moire supercell



moire 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}:

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

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

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, $\vec{b}_2'$.

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.

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

Explicit calculation of R_{basis}:

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

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

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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, $\vec{b}_2'$.

Supercell basis vector 1:

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

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

Formula for the second supercell basis vector after rotation:

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

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 (homobilayer)

For homobilayer, θ is determined by the angle between (N, M) and (M, N):

$$\vec{u} = \begin{pmatrix} N \\ M \end{pmatrix}, \quad \vec{v} = \begin{pmatrix} M \\ N \end{pmatrix}$$

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

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

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

Generalized inner product using the lattice Gram matrix:

$$\vec{u} \cdot \vec{v} = \vec{u}^{\,T} G \vec{v} = \begin{pmatrix} N & M \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} M \\ N \end{pmatrix}$$

$$= \begin{pmatrix} N & M \end{pmatrix} \begin{pmatrix} \frac{1}{2}N + M \\ N + \frac{1}{2}M \end{pmatrix}$$

$$= \frac{1}{2}(N^2 + 4NM + M^2)$$

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:

$$|\vec{u}|^2 = |\vec{v}|^2 = \vec{u}\cdot\vec{u} = \vec{u}^{\,T} G \vec{u} = (N, M) \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} N \\ M \end{pmatrix}$$

$$= (N, M) \begin{pmatrix} N + \frac{1}{2}M \\ \frac{1}{2}N + M \end{pmatrix} = N^2 + NM + M^2$$

Final formula for the twist angle cosine:

$$\Rightarrow \quad \cos\theta = \frac{N^2 + 4NM + M^2}{2(N^2 + NM + M^2)}$$

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 homobilayer moiré superlattice.

moire supercell lattice constant & number of atoms

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

$$L_{\text{cell}} = a\sqrt{N^2 + NM + M^2}$$

Therefore, this supercell has $N^2 + NM + M^2$ unit cells.

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