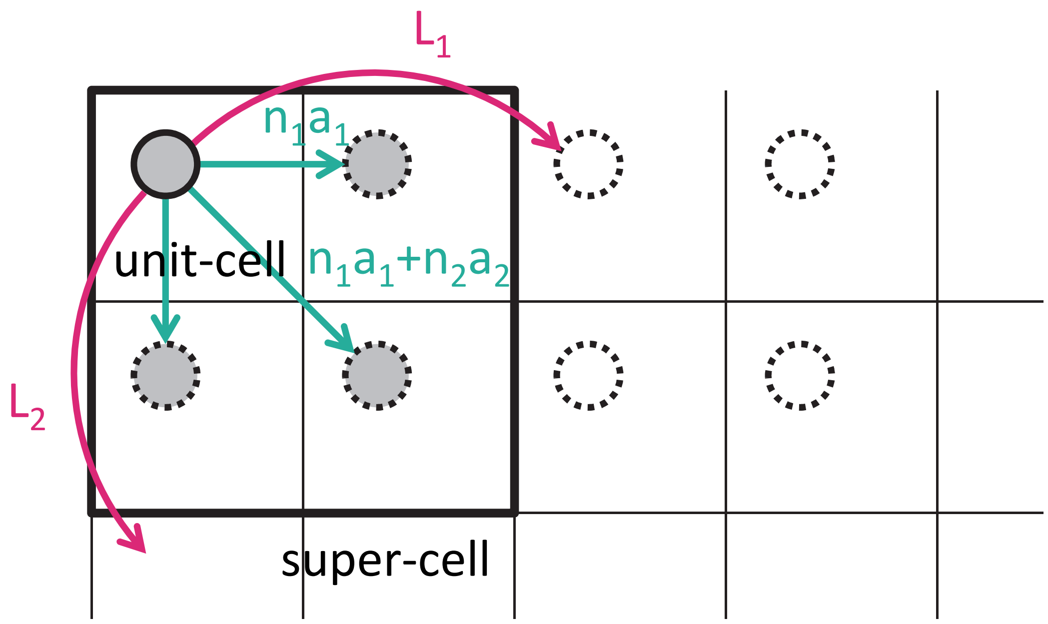
Translational Symmetry

Input:

- Primitive unit cell {nAtoms; coordinates, basis info}
- Lattice vector (real-space) {a_1, a_2, a_3}
- Repetition vector {n_1, n_2, n_3}

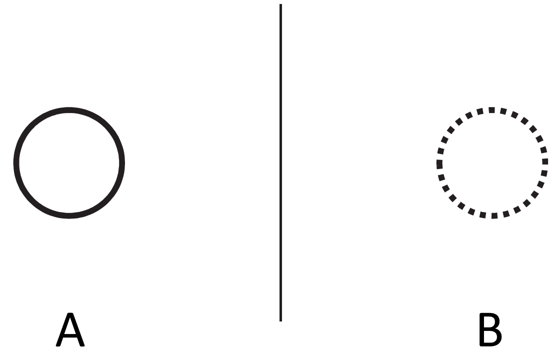
Output:

- Atoms in super-cell {nSpaceSymAtoms; coordinates, basis info, **weight**}
- Lattice vector (reciprocal-space) {b_1, b_2, b_3}
- Super-cell vector (real-space) {L_1, L_2, L_3}
- Volume



They might be reduced by space-group symmetry (not to be considered)

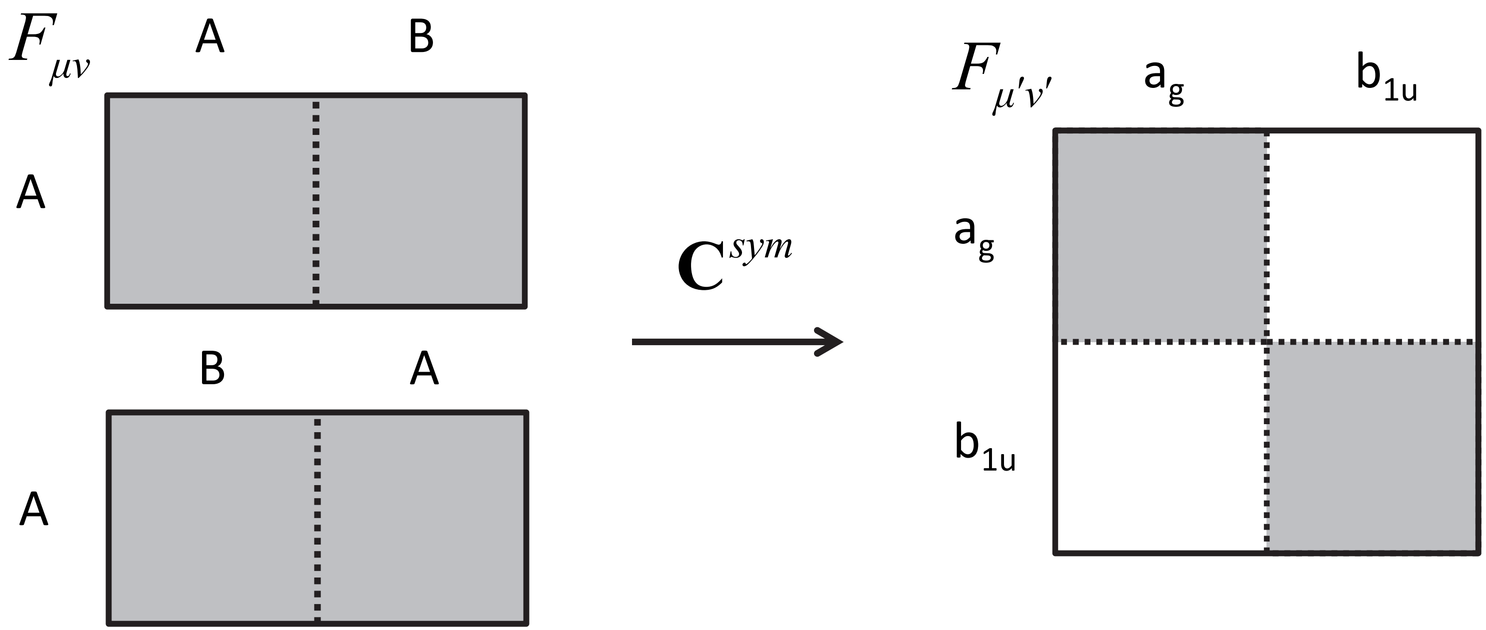
Point-Group Symmetry



symmetry-unique

$$\varphi_{\mu'}^{a_g} = \frac{1}{\sqrt{2}}(\varphi_A + \varphi_B)$$

$$\varphi_{\mu'}^{b_{1u}} = \frac{1}{\sqrt{2}}(\varphi_A - \varphi_B)$$



Point-Group Symmetry

Input:

- Primitive unit cell {nAtoms; coordinates, basis info}

Output:

- Symmetry-unique atoms in unit-cell {nSymAtoms; coordinates, basis info}
- Transformation matrix {real(nAO, nSO_iRep, nRep)}
- Symmetry object (C_1, C_S, C_i, C_2, C_{2v}, C_{2h}, D_2, D_{2h}) {nRep, nSO_iRep(*)}

Usage: lattice summation & Fock matrix construction

$$G_{\mu\nu} = \frac{1}{2}\sum_{\lambda\sigma}\sum_{\mathbf{T}}\sum_{\mathbf{Q}} P_{\lambda\sigma}^{\mathbf{Q}} \sum_{\mathbf{S}} [(\varphi_\mu^{\mathbf{0}}\varphi_\nu^{\mathbf{T}} \mid \varphi_\lambda^{\mathbf{S}}\varphi_\sigma^{\mathbf{S+Q}}) - \frac{1}{2}(\varphi_\mu^{\mathbf{0}}\varphi_\lambda^{\mathbf{S}} \mid \varphi_\nu^{\mathbf{T}}\varphi_\sigma^{\mathbf{S+Q}})]$$

$$F_{\mu'\nu'}^{irep} = \sum_{\mu\nu} C_{\mu'\mu}^{irep,\dagger} F_{\mu\nu} \widetilde{C}_{\nu\nu'}^{irep}$$

Indices in unit cell runs

μ: AOs in symmetry-unique atoms

ν $\lambda\sigma$: AOs in all atoms

$\mu'\nu'$: SA-AOs in irep symmetry group

Overall Structure

Called from main routine

- Primitive unit cell {nAtoms; coordinates, basis info}
- Lattice vector (real-space) {a_1, a_2, a_3}
- Repetition vector {n_1, n_2, n_3}

Interface to C/Fortran

or, C++ input class

Returns

- Atoms in super-cell {nAtoms x nUnitCells; coordinates, basis info, weight}
- Lattice vector (reciprocal-space) {b_1, b_2, b_3}
- Volume
- Super-cell vector (real-space) {L_1, L_2, L_3}