Symmetry in PWSCF and in Phonon

Crystal Symmetry

Crystal symmetry operations are in general (im)proper rotations with possibly a fractional Translation.

$$\mathcal{S} : r \longrightarrow r' = S(r + f)$$

Crystal symmetry operations form a Group.

$$\mathcal{S}, \mathcal{R} \in \mathcal{G} \Longrightarrow \mathcal{S}\mathcal{R} \in \mathcal{G}$$

Crystal Symmetry

$$\mathcal{S} : r \longrightarrow r' = S(r + f)$$

The Hamiltonian in invariant under symm.op.

$$\mathcal{S}\mathcal{H}\mathcal{S}^{\dagger} = \mathcal{H}$$

$$\mathcal{H}(r,p;R) = \mathcal{H}(r',p',R')$$
$$\mathcal{H}(r,p;R) = \mathcal{H}(S^{-1}r - f, S^{-1}p, S^{-1}R - f)$$

effect on a wfc:

if $\Psi(r)$ is an eigenfuntcion [eig.val ε]

so is $\Psi'(r) = \mathcal{S}\Psi(r) = \Psi(S^{-1}r - f)$ [eig.val ε]

Symmetry and Bloch states

$$\mathcal{S} : r \longrightarrow r' = S(r + f)$$

Effect on Block states:

if $\Psi_k(r) = \mathbf{exp}[ikr] \; u(r)$ [eig.val. ε_k]

then $\mathcal{S}\Psi_k(r) = \Psi_k(S^{-1}r - f)$

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if $\Psi_k(r) = \mathbf{exp}[ikr]\ \ u(r)$ [eig.val. ε_k]

then
$$\mathcal{S}\Psi_k(r) = \Psi_k(S^{-1}r - f)$$
$$= \mathbf{exp}[ikS^{-1}r - ikf]\ \ u(S^{-1}r - f)$$
$$= \mathbf{exp}[ikS^T r]\ \ u'(r)$$
$$= \mathbf{exp}[i(Sk)r]\ \ u'(r) = \Psi'_{Sk}(r)$$

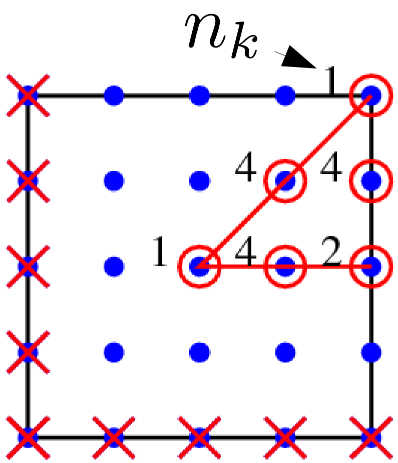
[eig.val. $\varepsilon_{Sk} = \varepsilon_k$]

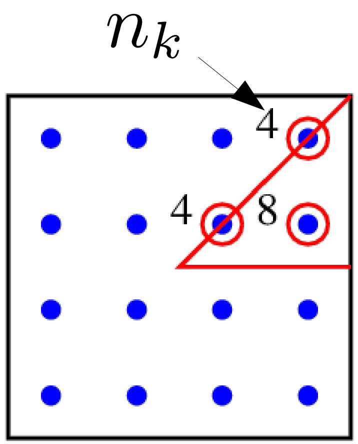
Symmetry and Charge Density

$$\mathcal{S} : r \longrightarrow r' = S(r + f)$$

$$\rho(r) = \frac{1}{N} \sum_{k \in BZ} |\Psi_k(r)|^2$$

$$\rho(r) = \frac{1}{N} \sum_{k \in IW} \sum_{\mathcal{S} \in \mathcal{G}} \frac{n_k}{N_s} |\Psi_{Sk}(r)|^2$$





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$$\rho(r) = \frac{1}{N_s} \sum_{\mathcal{S} \in \mathcal{G}} \tilde{\rho}(S^{-1}r - f)$$

Where $\tilde{\rho}(r) = \sum_{k \in IW} w_k |\Psi_k(r)|^2$ with $\sum_{k \in IW} w_k = 1$

Symmetry and Forces

$$\mathcal{S} : r \longrightarrow r' = S(r + f)$$

$$F_{I\alpha} = \frac{1}{N} \sum_{k \in BZ} \langle \Psi_k | - \frac{\partial V}{\partial R_{I\alpha}} | \Psi_k \rangle$$

$$F_{I\alpha} = \frac{1}{N_s} \sum_{\mathcal{S} \in \mathcal{G}} \sum_{\beta} S_{\alpha\beta} \, \tilde{F}_{s(I)\beta}$$

where $$\tilde{F}_{I\alpha} = \sum_{k \in IW} w_k \langle \Psi_k | - \frac{\partial V}{\partial R_{I\alpha}} | \Psi_k \rangle$$

with $$\sum_{k \in IW} w_k = 1$$

Symmetry and Stress

$$\mathcal{S} : r \longrightarrow r' = S(r + f)$$

$$\sigma_{\alpha\beta} = \frac{1}{N} \sum_{k \in BZ} \langle \Psi_k | - \frac{1}{\Omega} \frac{\partial H}{\partial \epsilon_\alpha \beta} | \Psi_k \rangle$$

$$\sigma_{\alpha\beta} = \frac{1}{N_s} \sum_{\mathcal{S} \in \mathcal{G}} \sum_{\alpha', \beta'} S_{\alpha\alpha'} S_{\beta\beta'} \, \tilde{\sigma}_{\alpha'\beta'}$$

where

$$\tilde{\sigma}_{\alpha\beta} = \sum_{k \in BZ} w_k \langle \Psi_k | - \frac{1}{\Omega} \frac{\partial H}{\partial \epsilon_\alpha \beta} | \Psi_k \rangle$$

with

$$\sum_{k \in IW} w_k = 1$$

Symmetry and Dynamical Matrix

$$\mathcal{S}: r \longrightarrow r' = S(r+f)$$

$$D^q_{I\alpha,J\beta} = \frac{1}{N}\sum_{k\in BZ}\langle\Psi_k|" - \frac{\partial^2 H(q)}{\partial R_{I\alpha}\partial R_{J\beta}}"|\Psi_k\rangle$$

$$D^q_{I\alpha,J\beta} = \frac{1}{N_s}\sum_{\mathcal{S}\in\mathcal{G}}\sum_{I\alpha',J\beta'} S_{\alpha\alpha'} S_{\beta\beta'}\ \tilde{D}^{Sq}_{s(I)\alpha',s(J)\beta'}$$

where $\tilde{D}^q_{I\alpha,J\beta} = \sum_{k\in IW} w_k\langle\Psi_k|" - \frac{\partial^2 H(q)}{\partial R_{I\alpha}\partial R_{J\beta}}"|\Psi_k\rangle$

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Displacements for all q in the star,
                  all atoms in the cell,
                  all Cartesian directions
    would be needed to advance scf dfpt


    this is most often too much
       (except for bulk semiconductors...)
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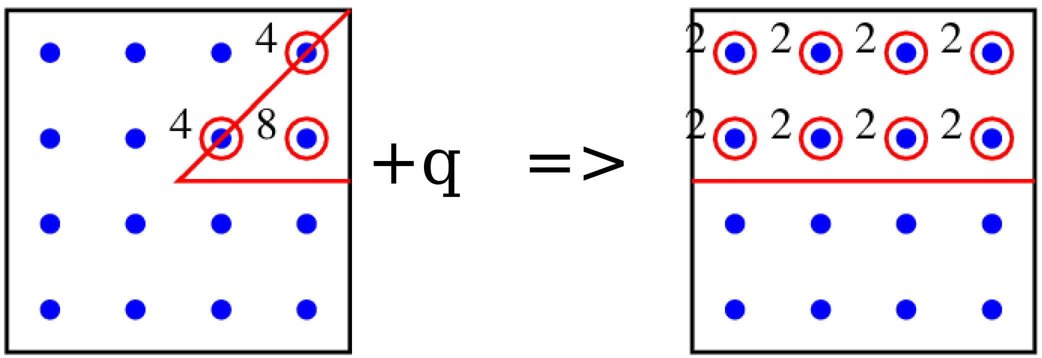
Symmetry and Dynamical Matrix

Reducing the symmetry to only those sym.ops. that do not rotate the q vector

$$\mathcal{S} : r \longrightarrow r' = S(r+f) \qquad\qquad Sq = q$$

$$D^q_{I\alpha,J\beta} = \frac{1}{N_s} \sum_{\mathcal{S}\in\mathcal{G}'} \sum_{I\alpha',J\beta'} S_{\alpha\alpha'} S_{\beta\beta'} \, \tilde{D}^q_{s(I)\alpha',s(J)\beta'}$$

this can be reduced to
displacements for all atoms in the cell,
all Cartesian directions
The prize is an increased number of k-points



This is most often still too much

Symmetry and Delta rho

If we reduce the symmetry to only those sym.ops. that do not rotate the q vector

$$\mathcal{S} : r \longrightarrow r' = S(r+f) \qquad\qquad Sq = q$$

$$\Delta\rho_{q,I\alpha}(r) = \frac{2}{N} \sum_{k\in BZ} \Psi_k^*(r) \;\; \Delta\Psi_{k+q,I\alpha}(r)$$

$$\Delta\rho_{q,I\alpha}(r) = \frac{1}{N_s} \sum_{\mathcal{S}\in\mathcal{G}'} \sum_{\beta} S_{\alpha\beta} \;\; \Delta\tilde{\rho}_{q,s(I)\beta}(S^{-1}r - f)\mathtt{exp}[i\phi_s^q]$$

$$\Delta\tilde{\rho}_{q,I\alpha}(r) = \sum_{k\in IW'} w_k \Psi_k^*(r) \;\; \Delta\Psi_{k+q,I\alpha}(r)$$

We can perform DFPT calculations on small groups of patterns that transform among themselves

→ irreducible representations

Symmetry and Delta rho

Let's have

$$\mathcal{S} : r \longrightarrow r' = S(r + f) \qquad\qquad Sq = q$$

Let's assume we have irr. rep.

$$\mathcal{S} : u_\mu \longrightarrow u'_\mu = \sum_\nu \mathcal{D}_{\mu\nu} u_\nu$$

$$\Delta\rho_{q,\mu}(r) = \frac{2}{N} \sum_{k \in BZ} \Psi^*_k(r) \; \Delta\Psi_{k+q,\mu}(r)$$

$$\Delta\rho_{q,\mu}(r) = \frac{1}{N_s} \sum_{\mathcal{S} \in \mathcal{G}'} \sum_\nu \mathcal{D}_{\mu\nu} \; \Delta\tilde{\rho}_{q,\nu}(S^{-1}r - f) \mathtt{exp}[i\phi^q_s]$$

$$\Delta\tilde{\rho}_{q,\mu}(r) = \sum_{k \in IW'} w_k \Psi^*_k(r) \; \Delta\Psi_{k+q,\mu}(r)$$

Symmetry and Delta rho

Let's have

$$\mathcal{S} : r \longrightarrow r' = S(r+f) \qquad\qquad Sq = q$$

How do we get the irr. Rep. ?

$$\mathcal{S} : u_\mu \longrightarrow u'_\mu = \sum_\nu \mathcal{D}_{\mu\nu} u_\nu$$

1) Generate a Random Matrix RM

$$RM^q_{I\alpha,J\beta} = (rand, rand)$$

2) Symmetrize it

$$D^q_{I\alpha,J\beta} = \frac{1}{N_s} \sum_{\mathcal{S}\in\mathcal{G}} \sum_{I\alpha',J\beta'} S_{\alpha\alpha'} S_{\beta\beta'} \, RM^q_{s(I)\alpha',s(J)\beta'}$$

3) Diagonalize it

$$\sum_{J\beta} D^q_{I\alpha,J\beta} u^\mu_{J,\beta} = M\omega^2_\mu u^\mu_{I\alpha}$$

4) each degenerate level identifies an irr.rep.