Symmetry in PWSCF and other QE codes (PHonon in particular)

Gamma point

When dealing with large systems Gamma point sampling is often used.

CP is written with Gamma point sampling only.

This is due to special properties that can be exploited for Gamma that make the calculation faster than for a generic k

Special properties of Gamma point

If Gamma point is used

the wave functions can be assumed to be
real in real space !

$$\psi_{v\Gamma}(r) = \psi^*_{v\Gamma}(r) = u(r)$$

This imposes **constraints** in its
reciprocal space representation

$$u(-G) = u^*(G)$$

hence only **half of the PW component** are independent and need to be stored/processed.

Special properties of Gamma point

Operators in Reciprocal Space require simple adjustments to cut in half the cost

Normalization:

$$\langle\psi|\psi\rangle = \sum_{G}^{G_{max}} |\psi(G)|^2 = \; 2 \sum_{G\in\{G_>\}}^{G_{max}} |\psi(G)|^2 - |\psi(0)|^2$$

Where $G_>$ are the G vectors whose first cartesian component is positive

Kinetic energy:

$$\langle\psi|T|\psi\rangle = \sum_{G}^{G_{max}} \frac{\hbar^2}{2m}|G|^2|\psi(G)|^2 = \; 2 \sum_{G\in\{G_>\}}^{G_{max}} \frac{\hbar^2}{2m}|G|^2|\psi(G)|^2$$

Special properties of Gamma point

Operators in Real Space can exploit REAL Arithmetics

Potential times wavefunction:

```
do ir=1, nrr
   vpsi(ir) = v(ir) * psi(ir)
end do
```

one COMPLEX multiplication takes 4 REAL ones

calls to REAL blas and lapack routines are similarly more efficients and use less memory.

Special properties of Gamma point

FFT operations are a big part of the calculation

```
 ig  = FFT index of a G
 aux(ig )= psi(ig,ibnd)        + (0.0,1.0) * psi(ig,ibnd+1)
 img = FFT index of -G
 aux(img)= CONJG(psi(ig,ibnd))+ (0.0,1.0) * CONJG(psi(ig,ibnd+1)
 call invfft (aux)
 psir(ir, ibnd)   = REAL ( aux(ir) )
 psir(ir, ibnd+1) = DIMAG( aux(ir) )
```

the FFT of two wfcs at Gamma can be performed at the same time! Similarly for the fwfft

```
 aux(ir) = CMPLX( psir(ir, ibnd),psir(ir, ibnd+1))
 call fwfft (aux)
 psi(ig, ibnd)   = 0.5 *( aux(ig) + CONJG(aux(img)) )
 psi(ig, ibnd+1) = 0.5 *( aux(ig) - CONJG(aux(img)) )/(0.0,1.0)
```

Exploiting these properties the gamma_only calculations are at least twice faster and use less memory !

Crystal Symmetry

In calculations involving generic k-points crystal symmetry is exploited to reduce the amount of work needed for a given desired k-point sampling

Time Reversal Symmetry

A symmetry that is always present is the one due to time reversal (reality of the hamiltonian)

This implies $\Psi_{-k}(r) = \Psi_k^*(r)$ [eig.val. $\varepsilon_{-k} = \varepsilon_k$]

So we can always use only half of the k-points.

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 is invariant under sym.ops.

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

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

effect on a wfc:

if $\Psi(r)$ is an eigenfunction [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 $\Psi_k(r) = \exp[ikr]\ u(r)$ [eig.val. ε_k]

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

Symmetry and Bloch states

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

Effect on Block states:

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

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

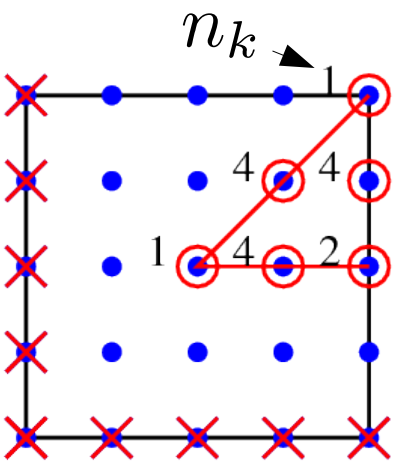
[eig.val. $\varepsilon_{Sk} = \varepsilon_k$]

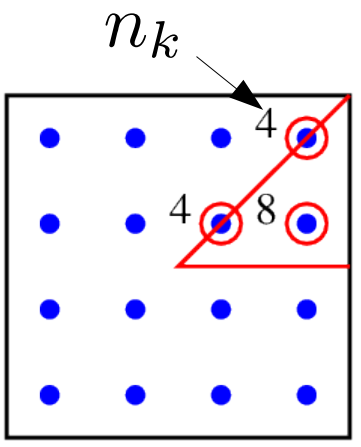
Symmetry and Charge Density

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

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

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





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

w_k

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

Symmetry and Charge Density

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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

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

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

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

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

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

Symmetry and Dynamical Matrix

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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...)

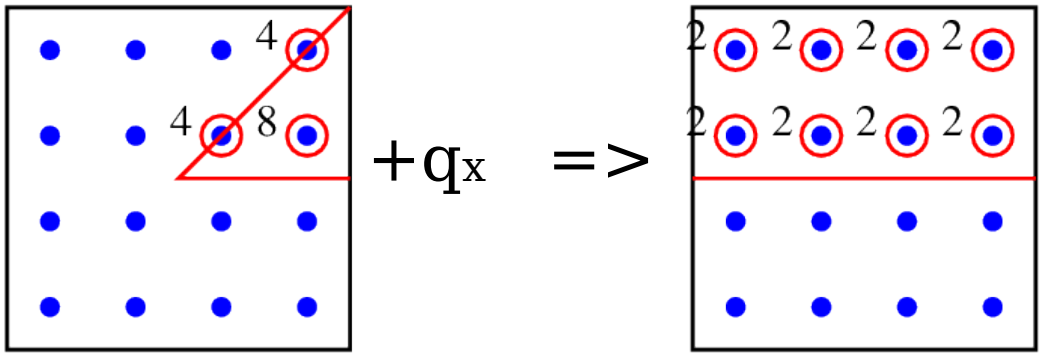
Symmetry and Dynamical Matrix

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

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

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

this can be reduced to
displacements for all atoms in the cell,
all Cartesian directions
The price 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

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

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

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

$$\Delta\tilde{\rho}_{q,I\alpha}(r) = 2 \sum_{k \in IW'} w_k\ \Psi^*_k(r)\ \ \Delta\Psi_{k+q,I\alpha}(r)$$

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. reps.

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

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

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

$$\Delta\tilde{\rho}_{q,\mu}(r) = 2 \sum_{k \in IW'} w_k \; \Psi^*_k(r) \;\; \Delta\Psi_{k+q,\mu}(r)$$

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. reps. ?

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

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.