Phonon unfolding: real space and reciprocal space methods

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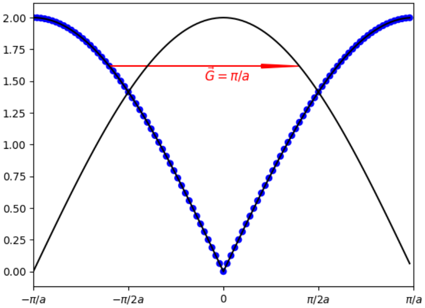
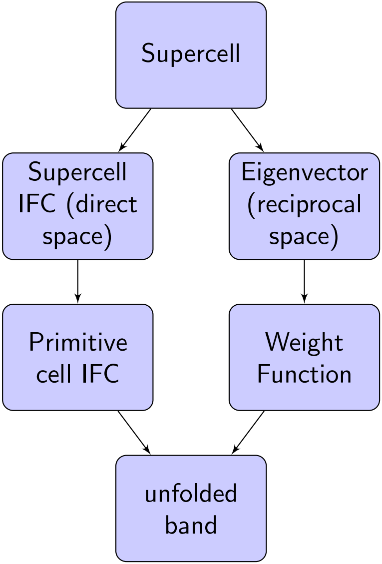
Phonon unfolding

- What is phonon unfolding? Get the phonon band structure in the primitive cell from that in a supercell.
- Why do we need it?.
  - Magnetic structure.
  - structure with defects.





Real space method (1)

- Calculation of phonon band structure.

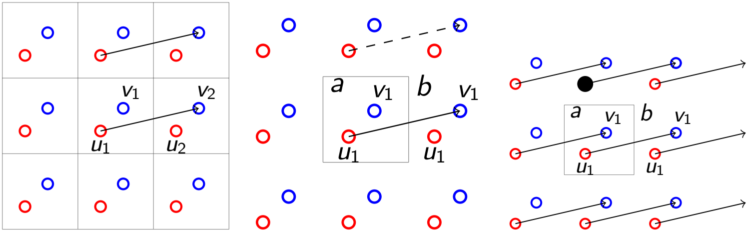
$$D^{SR}_{u\alpha,v\beta}(\vec{q}) = \frac{1}{\sqrt{M_u M_v}} \sum_R C^{SR}_{u\alpha,v\beta}(\vec{r}_{u,v} + \vec{R}) e^{-i\vec{q}\cdot(\vec{r}_{u,v}+\vec{R})}$$

$$D_{u\alpha,v\beta}(\vec{q}) = D^{SR}_{u\alpha,v\beta}(\vec{q}) + D^{DD}_{u\alpha,v\beta}(\vec{q})$$

- D^{DD}: Ewald summation method

$$D(\vec{q})|\Psi_{\vec{q}J}\rangle = \omega^2_{\vec{q}J}|\Psi_{\vec{q}J}\rangle$$

Real Space Method (2)



(a) Supercell (b) Primitive cell (c) With defect

The short range part of IFC's

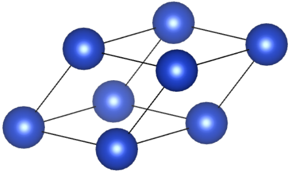
$$C^{PC}_{u_1\alpha,v_1\beta}(\vec{r}_{u_1,v_1}+\vec{R}_{ab}) = C^{SC}_{u_i\alpha,v_j\beta}(\vec{r}_{u_1,v_2}+0)$$

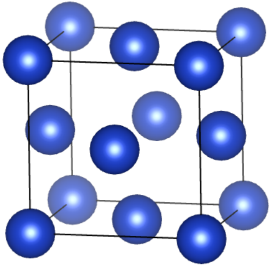
$$C^{PC}_{u_1\alpha,v_1\beta}(\vec{r}_{u_1,v_1}+\vec{R}_{ab}) = Average[C^{PC}_{u_1\alpha,v_1\beta}(\vec{r}_{u_1,v_1}+\vec{R}_{mn})]$$

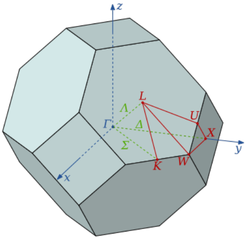
, where $\vec{R}_{mn} = \vec{R}_{ab}$

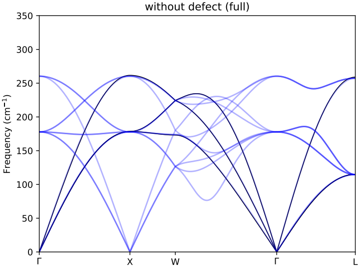
$$D^{PC}_{u_1\alpha,v_1\beta}(\vec{q}) = \frac{1}{\sqrt{M_u M_v}} \sum_R C^{PC}_{u_1\alpha,v_1\beta}(\vec{r}_{u_1,v_1}+\vec{R}) e^{-i\vec{q}\cdot(\vec{r}_{u_1,v_1}+\vec{R})}$$

Real Space Method (Example: without defect)

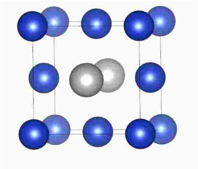


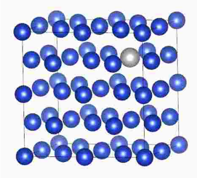


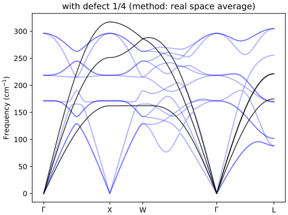


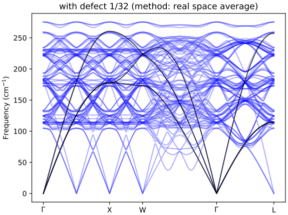


Real Space Method (Example: with defect)



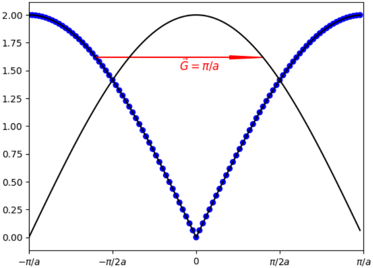


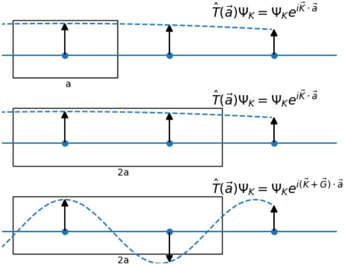




Reciprocal Space Method (1)

- Reciprocal method: find the phonon modes which has the translation symmetry of the primitive cell. (Ref: P. B. Allen *et al.* Phys Rev B 87, 085322 (2013))





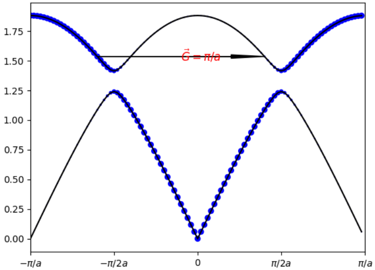
$$\vec{R} = \sum_i m_i \vec{A}_i \qquad \vec{r} = \sum_i n_i \vec{a}_i$$
$$\vec{A}_i \cdot \vec{B}_j = 2\pi\delta_{ij} \qquad \vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$
$$\vec{G} = \sum_i m_i \vec{B}_i \qquad \vec{g} = \sum_i n_i \vec{b}_i$$

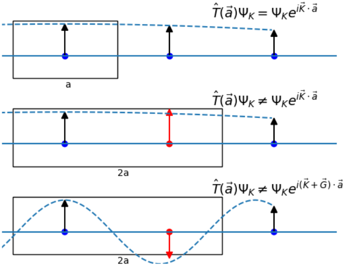
$$\hat{T}(\vec{r}_i)\psi_{\vec{K}+\vec{G}} = \psi_{\vec{K}+\vec{G}} e^{i(\vec{K}+\vec{G})\cdot\vec{r}_i}$$

Reciprocal Space Method (2)

- Reciprocal method:

  Weight Function. $W_{\vec{K}}(\vec{G}) = \frac{\langle \psi_{\vec{K}+\vec{G}} | \psi_{\vec{K}+\vec{G}} \rangle}{\langle \Psi_{\vec{K}} | \Psi_{\vec{K}} \rangle} = \frac{\langle \Psi_{\vec{K}} | \hat{P}(\vec{K} \to \vec{K}+\vec{G}) | \Psi_{\vec{K}} \rangle}{\langle \Psi_{\vec{K}} | \Psi_{\vec{K}} \rangle}$





$$\Psi_{\vec{K}} = \sum_{G} \psi_{\vec{K}+\vec{G}}$$

$$\hat{P}(\vec{K} \to \vec{K} + \vec{G}) = \frac{1}{N} \sum_{i=1}^{N} \hat{T}(\vec{r_i}) e^{-i(\vec{K}+\vec{G})\cdot\vec{r_i}}$$

Reciprocal Space Method (Example: with defect)