Density functional perturbation theory for lattice dynamics

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Outline

Description of a solid

Let's consider a periodic solid. We indicate with

$$\mathbf{R}_I = \mathbf{R}_\mu + \mathbf{d}_s$$

the equilibrium positions of the atoms. $\mathbf{R}_\mu$ indicate the Bravais lattice vectors and $\mathbf{d}_s$ the positions of the atoms in one unit cell ($s = 1, \ldots, N_{at}$).
We take N unit cells with Born-von Karman periodic boundary conditions. Ω is the volume of one cell and $V = N\Omega$ the volume of the solid.
At time t, each atom is displaced from its equilibrium position. $\mathbf{u}_I(t)$ is the displacement of the atom I.

Within the *Born-Oppenheimer adiabatic approximation* the nuclei move in a potential energy given by the total energy of the electron system calculated (for instance within DFT) at fixed nuclei. We call

$$E_{tot}(\mathbf{R}_I + \mathbf{u}_I)$$

this energy. The electrons are assumed to be in the ground state for each nuclear configuration.
If $|\mathbf{u}_I|$ is small, we can expand E_{tot} in a Taylor series with respect to $\mathbf{u}_I$. Within the *harmonic approximation*:

$$E_{tot}(\mathbf{R}_I+\mathbf{u}_I) = E_{tot}(\mathbf{R}_I)+\sum_{I\alpha} \frac{\partial E_{tot}}{\partial \mathbf{u}_{I\alpha}}\mathbf{u}_{I\alpha}+\frac{1}{2}\sum_{I\alpha,J\beta} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{I\alpha}\partial \mathbf{u}_{J\beta}}\mathbf{u}_{I\alpha}\mathbf{u}_{J\beta}+\ldots$$

where the derivatives are calculated at $\mathbf{u}_I = 0$ and α and β indicate the three Cartesian coordinates.

Equations of motion

At equilibrium $\frac{\partial E_{tot}}{\partial \mathbf{u}_{I\alpha}} = 0$, so the Hamiltonian of the ions becomes:

$$H = \sum_{I\alpha} \frac{\mathbf{P}_{I\alpha}^2}{2M_I} + \frac{1}{2} \sum_{I\alpha,J\beta} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{I\alpha} \partial \mathbf{u}_{J\beta}} \mathbf{u}_{I\alpha} \mathbf{u}_{J\beta}$$

where $\mathbf{P}_I$ are the momenta of the nuclei and M_I their masses. The classical motion of the nuclei is given by the $N \times 3 \times N_{at}$ functions $\mathbf{u}_{I\alpha}(t)$. These functions are the solutions of the Hamilton equations:

$$\begin{aligned} \dot{\mathbf{u}}_{I\alpha} &= \frac{\partial H}{\partial \mathbf{P}_{I\alpha}} \\ \dot{\mathbf{P}}_{I\alpha} &= -\frac{\partial H}{\partial \mathbf{u}_{I\alpha}} \end{aligned}$$

Equations of motion-II

With our Hamiltonian:

$$\begin{aligned} \dot{\mathbf{u}}_{I\alpha} &= \frac{\mathbf{P}_{I\alpha}}{M_I} \\ \dot{\mathbf{P}}_{I\alpha} &= -\sum_{J\beta} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{I\alpha} \partial \mathbf{u}_{J\beta}} \mathbf{u}_{J\beta} \end{aligned}$$

or:

$$M_I \ddot{\mathbf{u}}_{I\alpha} = -\sum_{J\beta} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{I\alpha} \partial \mathbf{u}_{J\beta}} \mathbf{u}_{J\beta}$$

The phonon solution

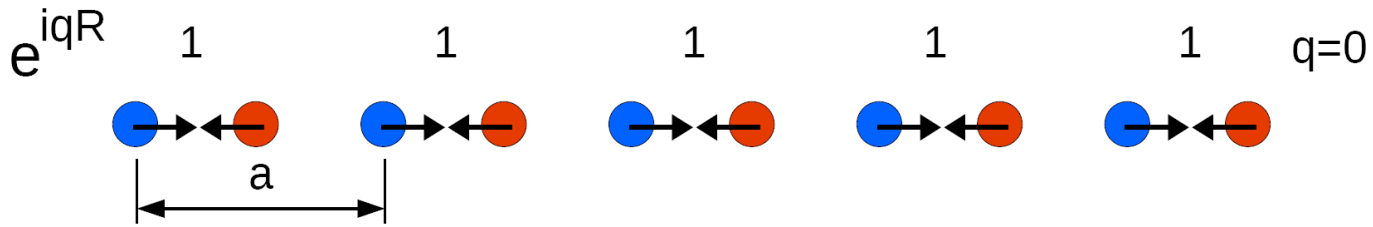
We can search the solution in the form of a phonon. Let's introduce a vector **q** in the first Brillouin zone. For each **q** we can write:

$$\mathbf{u}_{\mu s\alpha}(t) = \frac{1}{\sqrt{M_s}} \mathrm{Re}\left[\mathbf{u}_{s\alpha}(\mathbf{q}) e^{i(\mathbf{q}\mathbf{R}_\mu - \omega_{\mathbf{q}} t)}\right]$$

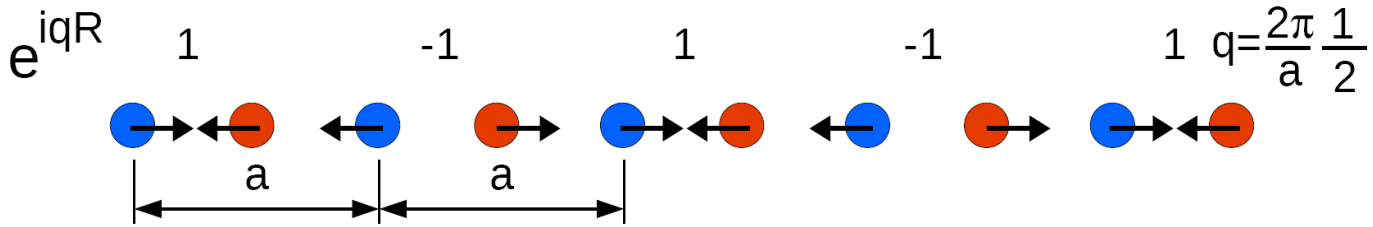
where the time dependence is given by simple phase factors $e^{\pm i\omega_{\mathbf{q}} t}$ and the displacement of the atoms in each cell identified by the Bravais lattice $\mathbf{R}_\mu$ can be obtained from the displacements of the atoms in one unit cell, for instance the one that corresponds to $\mathbf{R}_\mu = 0$: $\frac{1}{\sqrt{M_s}}\mathbf{u}_{s\alpha}(\mathbf{q})$.

Characteristic of a phonon - I

A Γ-*point* phonon has the same displacements in all unit cells ($\mathbf{q} = 0$):

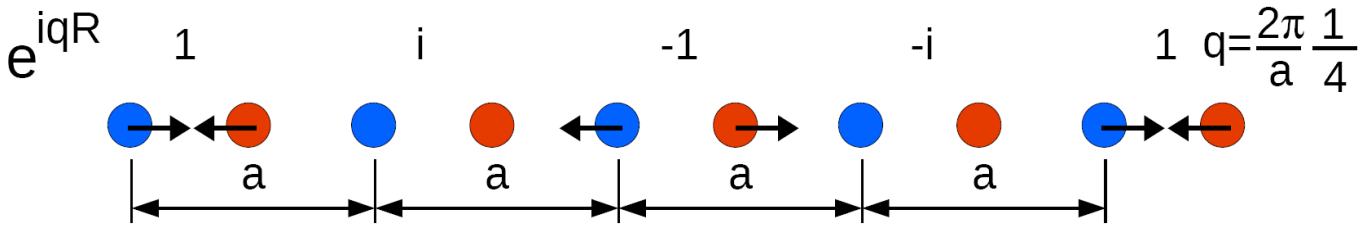


A zone border phonon with $\mathbf{q}_{ZB} = \mathbf{G}/2$, where $\mathbf{G}$ is a reciprocal lattice vector, has displacements which repeat periodically every two unit cells:

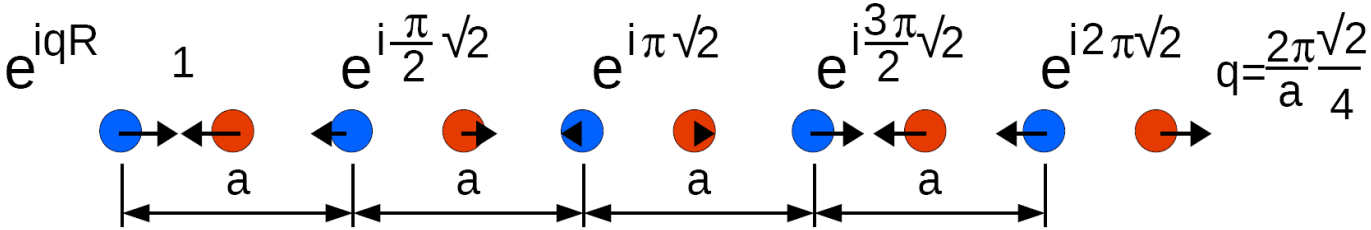


Characteristic of a phonon - II

A phonon with $\mathbf{q} = \mathbf{q}_{ZB}/2$ has displacements which repeat every four unit cells:



A phonon at a general wavevector **q** could be incommensurate with the underlying lattice:



The phonon solution-II

Inserting this solution in the equations of motion and writing $I = (\mu, s)$, $J = (\nu, s')$ we obtain an eigenvalue problem for the $3 \times N_{at}$ variables $\mathbf{u}_{s\alpha}(\mathbf{q})$:

$$\omega^2_{\mathbf{q}} \mathbf{u}_{s\alpha}(\mathbf{q}) = \sum_{s'\beta} D_{s\alpha s'\beta}(\mathbf{q}) \mathbf{u}_{s'\beta}(\mathbf{q})$$

where:

$$D_{s\alpha s'\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\nu} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}(\mathbf{R}_\nu - \mathbf{R}_\mu)}$$

is the dynamical matrix of the solid.

Within DFT the ground state total energy of the solid, calculated at fixed nuclei, is:

$$E_{tot} = \sum_i \langle \psi_i | -\frac{1}{2}\nabla^2 | \psi_i \rangle + \int V_{loc}(\mathbf{r})\rho(\mathbf{r})d^3r + E_H[\rho] + E_{xc}[\rho] + U_{II}$$

where $\rho(\mathbf{r})$ is the density of the electron gas:

$$\rho(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$$

and $|\psi_i\rangle$ are the solution of the Kohn and Sham equations. E_H is the Hartree energy, E_{xc} is the exchange and correlation energy and U_{II} is the ion-ion interaction. According to the Hellmann-Feynman theorem, the first order derivative of the ground state energy with respect to an external parameter is:

$$\frac{\partial E_{tot}}{\partial \lambda} = \int \frac{\partial V_{loc}(\mathbf{r})}{\partial \lambda}\rho(\mathbf{r})d^3r + \frac{\partial U_{II}}{\partial \lambda}$$

Deriving with respect to a second parameter μ:

$$\begin{aligned}\frac{\partial^2 E_{tot}}{\partial\mu\partial\lambda} &= \int \frac{\partial^2 V_{loc}(\mathbf{r})}{\partial\mu\partial\lambda}\rho(\mathbf{r})d^3r + \frac{\partial^2 U_{II}}{\partial\mu\partial\lambda} \\ &+ \int \frac{\partial V_{loc}(\mathbf{r})}{\partial\lambda}\frac{\partial\rho(\mathbf{r})}{\partial\mu}d^3r\end{aligned}$$

So the new quantity that we need to calculate is the charge density induced, at first order, by the perturbation:

$$\frac{\partial\rho(\mathbf{r})}{\partial\mu} = \sum_i \frac{\partial\psi_i^*(\mathbf{r})}{\partial\mu}\psi_i(\mathbf{r}) + \psi_i^*(\mathbf{r})\frac{\partial\psi_i(\mathbf{r})}{\partial\mu}$$

To fix the ideas we can think that $\lambda = \mathbf{u}_{\mu s\alpha}$ and $\mu = \mathbf{u}_{\nu s'\beta}$

The wavefunctions obey the following equation:

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

where $V_{KS} = V_{loc}(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r})$. $V_{KS}(\mathbf{r},\mu)$ depends on μ so that also $\psi_i(\mathbf{r},\mu)$, and $\varepsilon_i(\mu)$ depend on μ. We can expand these quantities in a Taylor series:

$$\begin{aligned}
V_{KS}(\mathbf{r},\mu) &= V_{KS}(\mathbf{r},\mu=0) + \mu\frac{\partial V_{KS}(\mathbf{r})}{\partial\mu} + \dots \\
\psi_i(\mathbf{r},\mu) &= \psi_i(\mathbf{r},\mu=0) + \mu\frac{\partial\psi_i(\mathbf{r})}{\partial\mu} + \dots \\
\varepsilon_i(\mu) &= \varepsilon_i(\mu=0) + \mu\frac{\partial\varepsilon_i}{\partial\mu} + \dots
\end{aligned}$$

Inserting these equations and keeping only the first order in μ we obtain:

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r}) - \varepsilon_i\right]\frac{\partial\psi_i(\mathbf{r})}{\partial\mu} = -\frac{\partial V_{KS}}{\partial\mu}\psi_i(\mathbf{r}) + \frac{\partial\varepsilon_i}{\partial\mu}\psi_i(\mathbf{r})$$

where: $\frac{\partial V_{KS}}{\partial\mu} = \frac{\partial V_{loc}}{\partial\mu} + \frac{\partial V_H}{\partial\mu} + \frac{\partial V_{xc}}{\partial\mu}$ and

$$\begin{aligned}\frac{\partial V_H}{\partial\mu} &= \int \frac{1}{|\mathbf{r}-\mathbf{r}'|}\frac{\partial\rho(\mathbf{r}')}{\partial\mu}d^3r' \\ \frac{\partial V_{xc}}{\partial\mu} &= \frac{dV_{xc}}{d\rho}\frac{\partial\rho(\mathbf{r})}{\partial\mu}\end{aligned}$$

depend self-consistently on the charge density induced by the perturbation.

The induced charge density depends only on $P_c \frac{\partial \psi_i}{\partial \mu}$ where $P_c = 1 - P_v$ is the projector on the conduction bands and $P_v = \sum_i |\psi_i\rangle\langle\psi_i|$ is the projector on the valence bands. In fact:

$$\begin{aligned}\frac{\partial \rho(\mathbf{r})}{\partial \mu} &= \sum_i P_c \frac{\partial \psi_i^*(\mathbf{r})}{\partial \mu}\psi_i(\mathbf{r}) + \psi_i^*(\mathbf{r}) P_c \frac{\partial \psi_i(\mathbf{r})}{\partial \mu} \\ &+ \sum_i P_v \frac{\partial \psi_i^*(\mathbf{r})}{\partial \mu}\psi_i(\mathbf{r}) + \psi_i^*(\mathbf{r}) P_v \frac{\partial \psi_i(\mathbf{r})}{\partial \mu}\end{aligned}$$

$$\begin{aligned}\frac{\partial \rho(\mathbf{r})}{\partial \mu} &= \sum_i P_c \frac{\partial \psi_i^*(\mathbf{r})}{\partial \mu}\psi_i(\mathbf{r}) + \psi_i^*(\mathbf{r}) P_c \frac{\partial \psi_i(\mathbf{r})}{\partial \mu} \\ &+ \sum_{ij} \psi_j^*(\mathbf{r})\psi_i(\mathbf{r}) \left(\langle \frac{\partial \psi_i}{\partial \mu} | \psi_j \rangle + \langle \psi_i | \frac{\partial \psi_j}{\partial \mu} \rangle \right)\end{aligned}$$

DFPT

Therefore we can solve the self-consistent linear system:

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r}) - \varepsilon_i\right] P_c \frac{\partial \psi_i(\mathbf{r})}{\partial \mu} = -P_c \frac{\partial V_{KS}}{\partial \mu} \psi_i(\mathbf{r})$$

where

$$\frac{\partial V_{KS}}{\partial \mu} = \frac{\partial V_{loc}}{\partial \mu} + \frac{\partial V_H}{\partial \mu} + \frac{\partial V_{xc}}{\partial \mu}$$

and

$$\frac{\partial \rho(\mathbf{r})}{\partial \mu} = \sum_i P_c \frac{\partial \psi_i^*(\mathbf{r})}{\partial \mu} \psi_i(\mathbf{r}) + \psi_i^*(\mathbf{r}) P_c \frac{\partial \psi_i(\mathbf{r})}{\partial \mu}$$

Dynamical matrix at finite **q** - I

The dynamical matrix is:

$$D_{s\alpha s'\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\nu} e^{-i\mathbf{q}\mathbf{R}_\mu} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}} \bigg|_{\mathbf{u}=0} e^{i\mathbf{q}\mathbf{R}_\nu}.$$

Inserting the expression of the second derivative of the total energy we have (neglecting the ion-ion term):

$$\begin{aligned} D_{s\alpha s'\beta}(\mathbf{q}) &= \frac{1}{\sqrt{M_s M_{s'}}} \left[\frac{1}{N} \int_V d^3 r \sum_{\mu\nu} \left(e^{-i\mathbf{q}\mathbf{R}_\mu} \frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} \right) \rho(\mathbf{r}) \right. \\ &+ \left. \frac{1}{N} \int_V d^3 r \left(\sum_{\mu} e^{-i\mathbf{q}\mathbf{R}_\mu} \frac{\partial V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\mu s\alpha}} \right) \left(\sum_{\nu} \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} \right) \right]. \end{aligned}$$

We now show that these integrals can be done over Ω.

Dynamical matrix at finite **q** - II

Defining:

$$\frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}^*_{s\alpha}(\mathbf{q}) \partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\mu\nu} e^{-i\mathbf{q}\mathbf{R}_\mu} \frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu}$$

we can show (see below) that $\frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}^*_{s\alpha}(\mathbf{q}) \partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ is a lattice-periodic function. Then we can define

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu}$$

and show that $\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = e^{i\mathbf{q}\mathbf{r}} \frac{\tilde{\partial} \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$, where $\frac{\tilde{\partial} \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ is a lattice-periodic function.

Dynamical matrix at finite **q** - III

In the same manner, by defining

$$\left(\frac{\partial V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s\alpha}(\mathbf{q})}\right)^* = \frac{1}{\sqrt{M_s}} \sum_{\mu} e^{-i\mathbf{q}\mathbf{R}_\mu} \frac{\partial V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\mu s\alpha}}$$

and showing that $\frac{\partial V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s\alpha}(\mathbf{q})} = e^{i\mathbf{q}\mathbf{r}} \frac{\partial \tilde{V}_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s\alpha}(\mathbf{q})}$, where $\frac{\partial \tilde{V}_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s\alpha}(\mathbf{q})}$ is a lattice-periodic function, we can write the dynamical matrix at finite **q** as:

$$\begin{aligned} D_{s\alpha s'\beta}(\mathbf{q}) &= \int_\Omega d^3r \frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}^*_{s\alpha}(\mathbf{q}) \partial \mathbf{u}_{s'\beta}(\mathbf{q})} \rho(\mathbf{r}) \\ &+ \int_\Omega d^3r \left(\frac{\partial \tilde{V}_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s\alpha}(\mathbf{q})}\right)^* \left(\frac{\partial \tilde{\rho}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}\right). \end{aligned}$$

Dynamical matrix at finite **q** - IV

$$\frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}^*_{s\alpha}(\mathbf{q}) \partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\mu\nu} e^{-i\mathbf{q}\mathbf{R}_\mu} \frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}}\bigg|_{\mathbf{u}=0} e^{i\mathbf{q}\mathbf{R}_\nu}$$

is a lattice-periodic function because the local potential can be written as $V_{loc}(\mathbf{r}) = \sum_\mu \sum_s v^s_{loc}(\mathbf{r} - \mathbf{R}_\mu - \mathbf{d}_s - \mathbf{u}_{\mu s})$, and $\frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}}$ vanishes if $\mu \neq \nu$ or $s \neq s'$. Since $\mu = \nu$ the two phase factors cancel, and we remain with a lattice-periodic function:

$$\frac{\partial^2 V_{loc}(\mathbf{r})}{\partial \mathbf{u}^*_{s\alpha}(\mathbf{q}) \partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{\delta_{s,s'}}{M_s} \sum_{\mu} \frac{\partial^2 v^s_{loc}(\mathbf{r} - \mathbf{R}_\mu - \mathbf{d}_s - \mathbf{u}_{\mu s})}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\mu s\beta}}\bigg|_{\mathbf{u}=0}.$$

Dynamical matrix at finite **q** - V

In order to show that:

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} = e^{i\mathbf{q}\mathbf{r}} \frac{\partial \tilde{\rho}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$$

where $\frac{\partial \tilde{\rho}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ is a lattice-periodic function, we can calculate the Fourier transform of $\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ and show that it is different from zero only at vectors $\mathbf{q} + \mathbf{G}$, where $\mathbf{G}$ is a reciprocal lattice vector. We have

$$\frac{\partial \rho}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}(\mathbf{k}) = \frac{1}{V} \int_V d^3r \; e^{-i\mathbf{k}\mathbf{r}} \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu}.$$

Dynamical matrix at finite **q** - VI

Due to the translational invariance of the solid, if we displace the atom s' in the direction β in the cell $\nu = 0$ and probe the charge at the point $\mathbf{r}$, or we displace in the same direction the atom s' in the cell ν and probe the charge at the point $\mathbf{r} + \mathbf{R}_\nu$, we should find the same value. Therefore

$$\frac{\partial \rho(\mathbf{r} + \mathbf{R}_\nu)}{\partial \mathbf{u}_{\nu s' \beta}} = \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{0 s' \beta}}$$

or, taking $\mathbf{r} = \mathbf{r}' - \mathbf{R}_\nu$, we have $\frac{\partial \rho(\mathbf{r}')}{\partial \mathbf{u}_{\nu s' \beta}} = \frac{\partial \rho(\mathbf{r}' - \mathbf{R}_\nu)}{\partial \mathbf{u}_{0 s' \beta}}$ which can be inserted in the expression of the Fourier transform to give:

$$\frac{\partial \rho}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})}(\mathbf{k}) = \frac{1}{V} \int_V d^3 r \; e^{-i\mathbf{k}\mathbf{r}} \frac{1}{\sqrt{M_{s'}}} \sum_\nu \frac{\partial \rho(\mathbf{r} - \mathbf{R}_\nu)}{\partial \mathbf{u}_{0 s' \beta}} e^{i\mathbf{q}\mathbf{R}_\nu}.$$

Dynamical matrix at finite **q** - VII

Changing variable in the integral and setting $\mathbf{r}' = \mathbf{r} - \mathbf{R}_\nu$, we have

$$\frac{\partial \rho}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}(\mathbf{k}) = \frac{1}{V}\int_V d^3r' e^{-i\mathbf{k}\mathbf{r}'} \frac{1}{\sqrt{M_{s'}}} \sum_\nu \frac{\partial \rho(\mathbf{r}')}{\partial \mathbf{u}_{0s'\beta}} e^{i(\mathbf{q}-\mathbf{k})\mathbf{R}_\nu}.$$

The sum over ν: $\sum_\nu e^{i(\mathbf{q}-\mathbf{k})\mathbf{R}_\nu}$ gives N if $\mathbf{k} = \mathbf{q} + \mathbf{G}$ and 0 otherwise. Hence $\frac{\partial \rho}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}(\mathbf{k})$ is non-vanishing only at $\mathbf{k} = \mathbf{q} + \mathbf{G}$. It follows that:

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = e^{i\mathbf{q}\mathbf{r}} \sum_{\mathbf{G}} \frac{\partial \rho}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}(\mathbf{q}+\mathbf{G}) e^{i\mathbf{G}\mathbf{r}}$$

and the sum over **G** gives a lattice-periodic function.

Properties of the wavefunctions: Bloch theorem

According to the Bloch theorem, the solution of the Kohn and Sham equations in a periodic potential $V_{KS}(\mathbf{r}+\mathbf{R}_\mu) = V_{KS}(\mathbf{r})$:

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r})\right]\psi_{\mathbf{k}v}(\mathbf{r}) = \epsilon_{\mathbf{k}v}\psi_{\mathbf{k}v}(\mathbf{r})$$

can be indexed by a **k**-vector in the first Brillouin zone and by a band index v, and:

$$\psi_{\mathbf{k}v}(\mathbf{r}+\mathbf{R}_\mu) = e^{i\mathbf{k}\mathbf{R}_\mu}\psi_{\mathbf{k}v}(\mathbf{r}),$$

$$\psi_{\mathbf{k}v}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}v}(\mathbf{r}),$$

where $u_{\mathbf{k}v}(\mathbf{r})$ is a lattice-periodic function. By time reversal symmetry, we also have:

$$\psi^*_{-\mathbf{k}v}(\mathbf{r}) = \psi_{\mathbf{k}v}(\mathbf{r}).$$

Charge density response at finite **q** - I

The lattice-periodic part of the induced charge density at finite **q** can be calculated as follows. We have:

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_{s'}}} \sum_{\mathbf{k}v} \left[P_c \left(\sum_{\nu} \frac{\partial \psi^*_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} \right) \psi_{\mathbf{k}v}(\mathbf{r}) + \psi^*_{\mathbf{k}v}(\mathbf{r}) P_c \left(\sum_{\nu} \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} \right) \right].$$

Changing **k** with $-\mathbf{k}$ in the first term, using time reversal symmetry $\psi_{-\mathbf{k}v}(\mathbf{r}) = \psi^*_{\mathbf{k}v}(\mathbf{r})$, and defining:

$$\frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu},$$

Charge density response at finite **q** - II

we have:

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = 2 \sum_{\mathbf{k}v} \psi^*_{\mathbf{k}v}(\mathbf{r}) P_c \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}.$$

We can now use the following identities to extract the periodic part of the induced charge density:

$$\begin{aligned} \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} &= e^{i\mathbf{k}\mathbf{r}} \frac{\partial u_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = e^{i\mathbf{k}\mathbf{r}} \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial u_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} \\ &= e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}} \frac{\partial \tilde{u}_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}, \end{aligned}$$

where $\frac{\partial \tilde{u}_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ is a lattice-periodic function.

Charge density response at finite **q** - III

The projector in the conduction band $P_c = 1 - P_v$ is:

$$\begin{aligned} P_c &= \sum_{\mathbf{k}'c} \psi_{\mathbf{k}'c}(\mathbf{r})\psi^*_{\mathbf{k}'c}(\mathbf{r}') \\ &= \sum_{\mathbf{k}'c} e^{i\mathbf{k}'\mathbf{r}} u_{\mathbf{k}'c}(\mathbf{r}) u^*_{\mathbf{k}'c}(\mathbf{r}') e^{-i\mathbf{k}'\mathbf{r}'} \\ &= \sum_{\mathbf{k}'} e^{i\mathbf{k}'\mathbf{r}} P_c^{\mathbf{k}'} e^{-i\mathbf{k}'\mathbf{r}'}, \end{aligned}$$

but only the term $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ gives a non zero contribution when applied to $\frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$. We have therefore:

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = e^{i\mathbf{q}\mathbf{r}} 2 \sum_{\mathbf{k}v} u^*_{\mathbf{k}v}(\mathbf{r}) P_c^{\mathbf{k}+\mathbf{q}} \frac{\partial \tilde{u}_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})},$$

Charge density response at finite **q** - IV

so the lattice-periodic part of the induced charge density, written in terms of lattice-periodic functions is:

$$\frac{\tilde{\partial}\rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = 2\sum_{\mathbf{k}v} u^*_{\mathbf{k}v}(\mathbf{r}) P_c^{\mathbf{k}+\mathbf{q}} \frac{\tilde{\partial} u_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}.$$

First-order derivative of the wavefunctions - I

$\frac{\partial \tilde{u}_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ is a lattice-periodic function which can be calculated with the following considerations. From first order perturbation theory we get, for each displacement $\mathbf{u}_{\nu s'\beta}$, the equation:

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r}) - \epsilon_{\mathbf{k}v}\right] P_c \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} = -P_c \frac{\partial V_{KS}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} \psi_{\mathbf{k}v}(\mathbf{r}).$$

Multiplying every equation by $\frac{1}{\sqrt{M_{s'}}} e^{i\mathbf{q}\mathbf{R}_\nu}$ and summing on ν, we get:

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r}) - \epsilon_{\mathbf{k}v}\right] \quad P_c \quad \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$$
$$= \quad -P_c \frac{\partial V_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} \psi_{\mathbf{k}v}(\mathbf{r}).$$

First-order derivative of the wavefunctions - II

Using the translational invariance of the solid we can write

$$\frac{\partial V_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial V_{KS}(\mathbf{r})}{\partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}\mathbf{R}_\nu} = e^{i\mathbf{q}\mathbf{r}} \frac{\partial \tilde{V}_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})},$$

where $\frac{\partial \tilde{V}_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ is a lattice-periodic function. The right-hand side of the linear system becomes:

$$-e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}} P_c^{\mathbf{k}+\mathbf{q}} \frac{\partial \tilde{V}_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} u_{\mathbf{k}v}(\mathbf{r}).$$

First-order derivative of the wavefunctions - III

In the left-hand side we have

$$P_c \frac{1}{\sqrt{M_{s'}}} \sum_{\nu} \frac{\partial \psi_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{\nu s' \beta}} e^{i\mathbf{q}\mathbf{R}_\nu} = e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}} P_c^{\mathbf{k}+\mathbf{q}} \frac{\partial \tilde{u}_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})},$$

and defining

$$H^{\mathbf{k}+\mathbf{q}} = e^{-i(\mathbf{k}+\mathbf{q})\mathbf{r}} \left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r}) \right] e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}},$$

we obtain the linear system:

$$\left[H^{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}v} \right] P_c^{\mathbf{k}+\mathbf{q}} \frac{\partial \tilde{u}_{\mathbf{k}v}(\mathbf{r})}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})} = -P_c^{\mathbf{k}+\mathbf{q}} \frac{\partial \tilde{V}_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})} u_{\mathbf{k}v}(\mathbf{r}).$$

Linear response: the self-consistent potential - I

The lattice-periodic component of the self-consistent potential can be obtained with the same techniques seen above. We have:

$$\frac{\partial V_{KS}(\mathbf{r})}{\partial \mathbf{u}_{\nu s' \beta}} = \frac{\partial V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{\nu s' \beta}} + \int d^3 r' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \frac{\partial \rho(\mathbf{r}')}{\partial \mathbf{u}_{\nu s' \beta}} + \frac{\partial V_{xc}}{\partial \rho} \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{\nu s' \beta}}.$$

Multiplying by $\frac{1}{\sqrt{M_{s'}}} e^{i\mathbf{q}\mathbf{R}_\nu}$ and adding, we obtain:

$$\frac{\partial V_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})} = \frac{\partial V_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})} + \int d^3 r' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \frac{\partial \rho(\mathbf{r}')}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})} + \frac{\partial V_{xc}}{\partial \rho} \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s' \beta}(\mathbf{q})}.$$

Linear response: the self-consistent potential - II

Keeping only the lattice periodic parts gives:

$$e^{i\mathbf{qr}}\frac{\partial \tilde{V}_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = e^{i\mathbf{qr}}\frac{\partial \tilde{V}_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} + \int d^3r' \frac{1}{|\mathbf{r}-\mathbf{r}'|} e^{i\mathbf{qr}'}\frac{\partial \tilde{\rho}(\mathbf{r}')}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} + \frac{\partial V_{xc}}{\partial \rho} e^{i\mathbf{qr}}\frac{\partial \tilde{\rho}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})},$$

or equivalently:

$$\frac{\partial \tilde{V}_{KS}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} = \frac{\partial \tilde{V}_{loc}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} + \int d^3r' \frac{1}{|\mathbf{r}-\mathbf{r}'|} e^{i\mathbf{q}(\mathbf{r}'-\mathbf{r})}\frac{\partial \tilde{\rho}(\mathbf{r}')}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})} + \frac{\partial V_{xc}(\mathbf{r})}{\partial \rho}\frac{\partial \tilde{\rho}(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}.$$

ph.x

The program `ph.x` solves this self-consistent linear system for $3 \times N_{at}$ perturbations at a fixed vector $\mathbf{q}$. With $\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{u}_{s'\beta}(\mathbf{q})}$ for all perturbations, it calculates the dynamical matrix

$$D_{s\alpha s'\beta}(\mathbf{q})$$

at the given $\mathbf{q}$ as discussed above. Diagonalizing this matrix we obtain $3 \times N_{at}$ frequencies $\omega_{\mathbf{q}}$. By repeating this procedure for several $\mathbf{q}$ we could plot $\omega_{\mathbf{q}}$ as a function of $\mathbf{q}$ and display the phonon dispersions. However, it is more convenient to adopt a different approach that requires the calculation of the dynamical matrix in a small set of vectors $\mathbf{q}$.

Phonon dispersions

The dynamical matrix of the solid:

$$D_{s\alpha s'\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\nu} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}} e^{i\mathbf{q}(\mathbf{R}_\nu - \mathbf{R}_\mu)} \tag{1}$$

is a periodic function of $\mathbf{q}$ with $D_{s\alpha s'\beta}(\mathbf{q}+\mathbf{G}) = D_{s\alpha s'\beta}(\mathbf{q})$ for any reciprocal lattice vector $\mathbf{G}$. Furthermore, due to the translational invariance of the solid, it does not depend on μ. Eq.1 is a Fourier expansion of a three dimensional periodic function. We have Fourier components only at the discrete values $\mathbf{R}_\nu$ of the Bravais lattice and we can write:

$$\frac{1}{\sqrt{M_s M_{s'}}} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}} = \frac{\Omega}{(2\pi)^3} \int d^3\mathbf{q} D_{s\alpha s'\beta}(\mathbf{q}) e^{-i\mathbf{q}(\mathbf{R}_\nu - \mathbf{R}_\mu)}. \tag{2}$$

Discrete Fourier transform

We can use the properties of the discrete Fourier transform and sample the integral in a uniform mesh of **q** vectors. This will give the inter-atomic force constants only for a certain range of values of $\mathbf{R}_\nu$ neighbors of $\mathbf{R}_\mu$.
In order to recall the main properties of the discrete Fourier transform, let us consider a one dimensional periodic function $f(x+a) = f(x)$ with period a. This function can be expanded in a Fourier series and will have a discrete set of Fourier components at $k_n = \frac{2\pi}{a} n$, where n is an integer (positive, negative or zero).

$$f(x) = \sum_n c_n e^{ik_n x}$$

where the coefficients of the expansion are:

Discrete Fourier transform - II

$$c_n = \frac{1}{a}\int_0^a f(x)e^{-ik_n x}dx.$$

In general, if $f(x)$ is a sufficiently smooth function, $c_n \to 0$ at large n. Now suppose that we discretize $f(x)$ in a uniform set of N points $x_j = j\Delta x$ where $\Delta x = a/N$ and $j = 0, \ldots, N-1$, then we can calculate:

$$\tilde{c}_n = \frac{1}{N}\sum_{j=0}^{N-1} f(x_j)e^{-i\frac{2\pi}{N}nj},$$

$\tilde{c}_n$ is a periodic function of n and $\tilde{c}_{n+N} = \tilde{c}_n$. So, if N is sufficiently large that $c_n = 0$ when $|n| \geq N/2$, $\tilde{c}_n$ is a good approximation of c_n for $|n| < N/2$ and the function

Discrete Fourier transform - III

$$f(x) = \sum_{n=-N/2}^{n=N/2} \tilde{c}_n e^{ik_n x}$$

is a good approximation of the function $f(x)$ also on the points x different from x_j. In three dimensions the discretization of Eq. 2 on a uniform mesh of $\mathbf{q}_i$ vectors is:

$$\frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s \alpha} \partial \mathbf{u}_{\nu s' \beta}} = \frac{1}{N_q} \sum_{i=1}^{N_q} C_{s\alpha s'\beta}(\mathbf{q}_i) e^{-i\mathbf{q}_i(\mathbf{R}_\nu - \mathbf{R}_\mu)},$$

where we defined $C_{s\alpha s'\beta}(\mathbf{q}) = \sqrt{M_s M_{s'}} D_{s\alpha s'\beta}(\mathbf{q})$. Since $\frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s \alpha} \partial \mathbf{u}_{\nu s' \beta}}$ depends only on the vector $\mathbf{R} = \mathbf{R}_\mu - \mathbf{R}_\nu$, we can call

q2r.x

$C_{s\alpha s'\beta}(\mathbf{R}) = \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{\mu s\alpha} \partial \mathbf{u}_{\nu s'\beta}}$ and write the relationship:

$$C_{s\alpha s'\beta}(\mathbf{R}) = \frac{1}{N_q} \sum_{i=1}^{N_q} C_{s\alpha s'\beta}(\mathbf{q}_i) e^{i\mathbf{q}_i \mathbf{R}}.$$

The code `q2r.x` reads a set of dynamical matrices obtained for a uniform mesh of $\mathbf{q}_i$ vectors and calculates, using this equation, the inter-atomic force constants for some neighbors of the point $\mathbf{R} = 0$.

matdyn.x

If the dynamical matrix is a sufficiently smooth function of **q**, the inter-atomic force constants decay sufficiently rapidly in real space and we can use Eq. 1 limiting the sum over ν to the few neighbors of $\mathbf{R}_\mu$ for which we have calculated the inter-atomic force constants. With the present notation Eq. 1 becomes:

$$C_{s\alpha s'\beta}(\mathbf{q}) = \sum_{\mathbf{R}} C_{s\alpha s'\beta}(\mathbf{R}) e^{-i\mathbf{qR}}, \tag{3}$$

a relationship that allows the interpolation of the dynamical matrix at arbitrary **q**, by a few inter-atomic force constants. The program `matdyn.x` reads the inter-atomic force constants calculated by `q2r.x` and calculates the dynamical matrices at an arbitrary **q** using this equation.

This procedure fails in two cases:

- In metals when there are Kohn anomalies. In this case $D_{s\alpha s'\beta}(\mathbf{q})$ is not a smooth function of $\mathbf{q}$ and the inter-atomic force constants are long range.
- In polar insulators where the atomic displacements generate long range electrostatic interactions and the dynamical matrix is non analytic for $\mathbf{q} \to 0$. This case, however, can be dealt with by calculating the Born effective charges and the dielectric constant of the material.

Use of symmetry

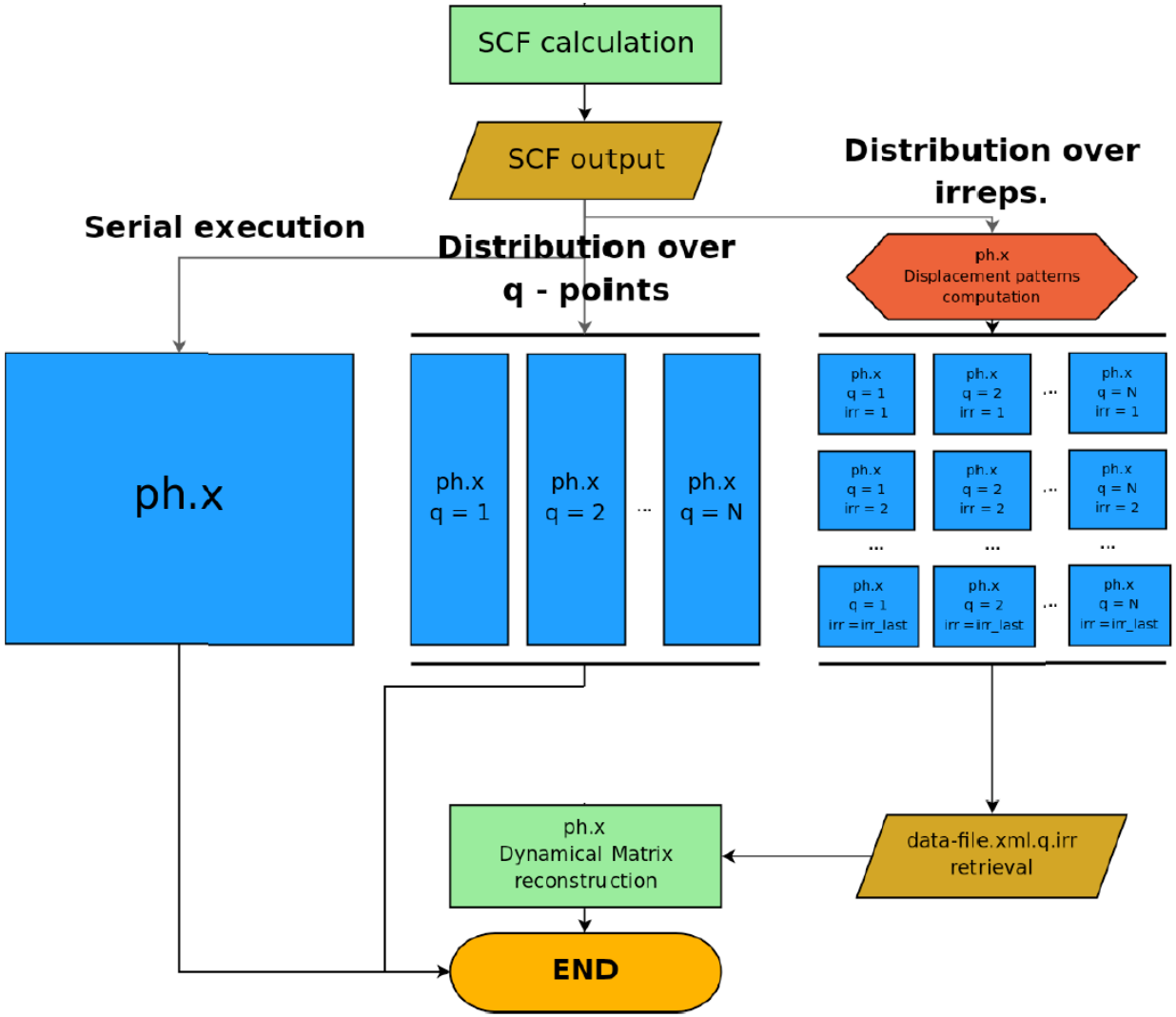
Phonon dispersions require the DFPT calculation on a uniform mesh $N_{q_1} \times N_{q_2} \times N_{q_3} = N_q$ of **q** vectors. The CPU time can be roughly estimated as

$$N_q \times 3 \times N_{\mathrm{at}} \times T_{\mathrm{scf}}$$

where T_{scf} is the CPU time of a single self-consistent calculation. Using symmetry the **q**-vector mesh is reduced to a set of $\bar{N}_q$ non equivalent **q** vectors. The calculation of the dynamical matrix at each **q** vector requires an amount of CPU time roughly proportional to the size of its star of **q** vectors. So low symmetry **q** vectors require much more CPU time than high symmetry **q** vectors mainly because `ph.x` uses only the symmetries of the small group of **q** to reduce the **k** points.

Use of symmetry - II

On the other hand, from the dynamical matrix at **q** we can obtain, for free, the dynamical matrices of the star of **q** that is larger for low symmetry **q**. Not all the $3 \times N_{\mathrm{at}}$ perturbations have to be calculated simultaneously at each **q**. Choosing displacement patterns that transform according to an irreducible representation (irrep) of the small group of **q**, the number of patterns that transform among themselves is equal to the dimension of the irreducible representation. For standard point groups the maximum dimension is 3, while for **q** at zone border and nonsymmorphic point groups the maximum dimension could be larger, up to 6.


SCF calculation
SCF output
Distribution over irreps.
Serial execution
Distribution over q - points
ph.x
Displacement patterns computation
ph.x
ph.x q = 1
ph.x q = 2
ph.x q = N
ph.x q = 1 irr = 1
ph.x q = 2 irr = 1
ph.x q = N irr = 1
ph.x q = 1 irr = 2
ph.x q = 2 irr = 2
ph.x q = N irr = 2
ph.x q = 1 irr = irr_last
ph.x q = 2 irr = irr_last
ph.x q = N irr = irr_last
ph.x Dynamical Matrix reconstruction
data-file.xml.q.irr retrieval
END

q-vectors parallelization

The phonon code is parallelized as the `pw.x` code: reciprocal lattice vectors **G** can be distributed among CPUs and/or **k** vectors used for the integration over the Brillouin zone can be distributed among pools of CPUs. In addition, it is possible to calculate in parallel the contribution to the dynamical matrix of each irrep for each **q** vector.
Different **q** vectors might require quite different CPU time so the dynamical matrix of each **q** vector is calculated independently. The two input parameters `start_q` and `last_q` allow the choice of the **q** vector in the list of $\bar{N}_q$ vectors. To parallelize only on **q** vectors it is convenient to send many runs on different CPUs with different `outdir` directories. Preliminarily, the `outdir` produced by `pw.x` has to be copied in all the `outdir` directories where `ph.x` will run.

q vectors and irreps parallelization

q vectors and irreps parallelization is slightly more complex because each run must use the same displacement patterns. Therefore, after running `pw.x`, a preliminary run of `ph.x` with the two flags `start_irr=0` and `last_irr=0` calculates and saves on disk the displacement patterns for all **q** vectors and irreps. Then `ph.x` can run separately on different machines or on different CPUs. Each run calculates one or more irrep as specified by the four variables `start_q`, `last_q`, `start_irr`, `last_irr`. The `outdir` produced by `pw.x` and by the preliminary run of `ph.x` has to be copied in all the `outdir` directories where `ph.x` will run.

Collecting the results

After running `ph.x` for all **q** vectors and all irreps the results are collected in a single `outdir` directory and `ph.x` is run again to produce the dynamical matrices. The files with the contributions of the irreps to the dynamical matrix are in the `outdir/_phprefix.phsave` directories and are called `data-file.xml.#iq.#irr`. All these files have to be copied in one `outdir/_phprefix.phsave` directory and `ph.x` must be run on this `outdir` without any flag. Note that if the file `data-file.xml.#iq.#irr` for some **q**-vector or for some irreps is missing `ph.x` will recalculate the missing contribution to the dynamical matrix.

Bibliography

1 S. Baroni, P. Giannozzi, and A. Testa, Phys. Rev. Lett. **58**, 1861 (1987); P. Giannozzi, S. de Gironcoli, P. Pavone, and S. Baroni, Phys. Rev. B **43**, 7231 (1991).

2 S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Rev. Mod. Phys. **73**, 515 (2001).

3 A. Dal Corso, Phys. Rev. B **64**, 235118 (2001).

4 X. Gonze and C. Lee, Phys. Rev. B **55**, 10355 (1997).

5 R. di Meo, A. Dal Corso, P. Giannozzi, and S. Cozzini, Calculation of phonon dispersions on the GRID using Quantum ESPRESSO, ICTP lecture notes **24**, 163 (2009).