# 2021 Virtual School on Electron-Phonon Physics and the EPW code

June 14-18 2021

Hands-on Wed.3

# Transport module of EPW

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# Exercise 1

Compute the electric resistivity of fcc Pb using the Ziman formula and Boltzmann transport equation

Ziman formula rests on the lowest-order variational approximation (LOVA):

- the energy-resolved decay function is approximated $\gamma(\omega) \approx \gamma(\varepsilon = \varepsilon_{\mathrm{F}}, \varepsilon = \varepsilon'_{\mathrm{F}}, \omega)$
- $-\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \approx \delta(\varepsilon_{\mathrm{F}} - \varepsilon_{n\mathbf{k}})$
- use of an isotropic scattering rate $\langle \tau^{-1} \rangle$
- Derivation connecting SERTA with Ziman can be found in S. Poncé, *et al.* Rep. Prog. Phys. **83**, 036501 (2020).

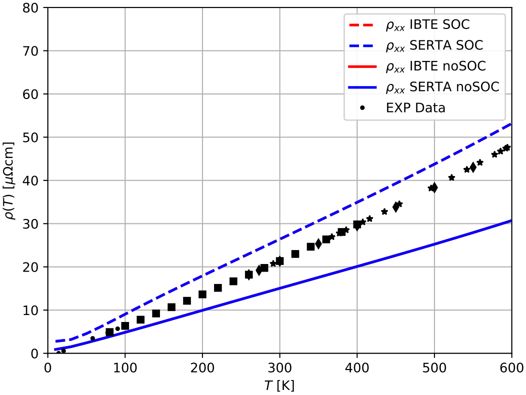


Figure courtesy of Félix Goudreault

# Exercise 1: Zimann resistivity formula

$$\rho(T) = \frac{4\pi m_e}{ne^2 k_B T}\int_0^\infty d\omega\, \hbar\omega\, \alpha^2_{\text{tr}}F(\omega)\, n(\omega,T)\big[1+n(\omega,T)\big],$$

where $n$ is the number of electrons per unit volume and $n(\omega, T)$ is the Bose-Einstein distribution.

The isotropic Eliashberg transport spectral function (see Thu.1, Thu.5 and Thu.6):

$$\alpha^2_{\text{tr}}F(\omega) = \frac{1}{2}\sum_{\nu}\int_{\text{BZ}}\frac{d\mathbf{q}}{\Omega_{\text{BZ}}}\omega_{\mathbf{q}\nu}\lambda_{\text{tr},\mathbf{q}\nu}\delta(\omega-\omega_{\mathbf{q}\nu}),$$

where the mode-resolved transport coupling strength is defined by:

$$\lambda_{\text{tr},\mathbf{q}\nu} = \frac{1}{N(\varepsilon_F)\omega_{\mathbf{q}\nu}}\sum_{nm}\int_{\text{BZ}}\frac{d\mathbf{k}}{\Omega_{\text{BZ}}}|g_{mn,\nu}(\mathbf{k},\mathbf{q})|^2\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{\text{F}})\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{\text{F}})\left(1-\frac{v_{n\mathbf{k}}\cdot v_{m\mathbf{k}+\mathbf{q}}}{|v_{n\mathbf{k}}|^2}\right).$$

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$n$ is the number of electrons that contribute to the mobility $\rightarrow$ `nc = 4.0d0`

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$n$ is the number of electrons that contribute to the mobility $\rightarrow$ `nc = 4.0d0`

$\alpha^2_{\mathrm{tr}} F(\omega)$ $\rightarrow$ `phonselfen = .true.` and `a2f = .true.`

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$$\approx \frac{1}{N(\varepsilon_F)\omega_{\mathbf{q}\nu}}\sum_{nm}\int_{\text{BZ}}\frac{d\mathbf{k}}{\Omega_{\text{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{\text{F}})\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{\text{F}})\left(1-\frac{v_{n\mathbf{k}}\cdot v_{m\mathbf{k}+\mathbf{q}}}{|v_{n\mathbf{k}}|^2}\right)$$

$\approx \rightarrow$ `delta_approx = .true.`

Note: $|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ should be $g^{\text{b},*}_{mn\nu}(\mathbf{k},\mathbf{q})g_{mn\nu}(\mathbf{k},\mathbf{q})$ for the phonon self-energy

# Exercise 1: Zimann resistivity formula

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$\approx \rightarrow$ `delta_approx = .true.`

$\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{\text{F}}) \rightarrow$ Gaussian of width: `degaussw = 0.1`

Note: $|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ should be $g^{\text{b},*}_{mn\nu}(\mathbf{k},\mathbf{q})g_{mn\nu}(\mathbf{k},\mathbf{q})$ for the phonon self-energy

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$\approx$ $\rightarrow$ `delta_approx = .true.`

$\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{\text{F}})$ $\rightarrow$ Gaussian of width: `degaussw = 0.1`

$\delta(\omega-\omega_{\mathbf{q}\nu})$ $\rightarrow$ Gaussian of width: `degaussq = 0.05`

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$\approx \rightarrow$ `delta_approx = .true.`

$\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{\text{F}}) \rightarrow$ Gaussian of width: `degaussw = 0.1`

$\delta(\omega-\omega_{\mathbf{q}\nu}) \rightarrow$ Gaussian of width: `degaussq = 0.05`

$N(\varepsilon_F) \rightarrow$ FD dist. for DOS and $\varepsilon_{\text{F}}$: `assume_metal = .true.` with `ngaussw = -99` with `temps=1`

Note: $|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ should be $g^{\text{b},*}_{mn\nu}(\mathbf{k},\mathbf{q})g_{mn\nu}(\mathbf{k},\mathbf{q})$ for the phonon self-energy

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$N(\varepsilon_F) \rightarrow$ FD dist. for DOS and $\varepsilon_{\text{F}}$: `assume_metal = .true.` with `ngaussw = -99` with `temps=1`

$v_{n\mathbf{k}} \rightarrow$ `vme = 'wannier'`

Note: $|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ should be $g^{\text{b},*}_{mn\nu}(\mathbf{k},\mathbf{q})g_{mn\nu}(\mathbf{k},\mathbf{q})$ for the phonon self-energy

# Linearized Boltzmann transport equation

Macroscopic average of the current density is

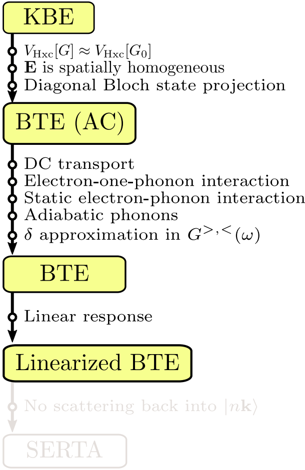
$$\mathbf{J}_{\mathrm{M}}(\mathbf{E}) = \frac{-e\hbar^2}{2m}\frac{1}{V}\int \mathrm{d}^3r \lim_{\mathbf{r}_2\to\mathbf{r}_1}(\nabla_2 - \nabla_1)G^{<}(\mathbf{r}_1,\mathbf{r}_2;t,t;\mathbf{E})$$
$$= \frac{-e}{V_{\mathrm{uc}}}\sum_n \int \frac{\mathrm{d}^3k}{\Omega_{\mathrm{BZ}}}\,\mathbf{v}_{n\mathbf{k}} f_{n\mathbf{k}}(\mathbf{E})$$

For weak $\mathbf{E}$, we can use the *linear response* of the current density to define the *conductivity*:

$$\sigma_{\alpha\beta} \equiv \frac{\partial J_{\mathrm{M},\alpha}}{\partial E_\beta}\bigg|_{\mathbf{E}=\mathbf{0}} = \frac{-e}{V_{\mathrm{uc}}}\sum_n\int\frac{\mathrm{d}^3k}{\Omega_{\mathrm{BZ}}}\, v^{\alpha}_{n\mathbf{k}}\partial_{E_\beta} f_{n\mathbf{k}}$$

where $\partial_{E_\beta} f_{n\mathbf{k}} = (\partial f_{n\mathbf{k}}/\partial E_\beta)|_{\mathbf{E}=\mathbf{0}}$.

The *carrier drift mobility* is $\mu^{\mathrm{d}}_{\alpha\beta} \equiv \dfrac{\sigma_{\alpha\beta}}{e n_{\mathrm{c}}}$




S. Poncé *et al.*,
Rep. Prog. Phys. **83**, 036501 (2020)

# Drift mobility

$$\mu^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

where

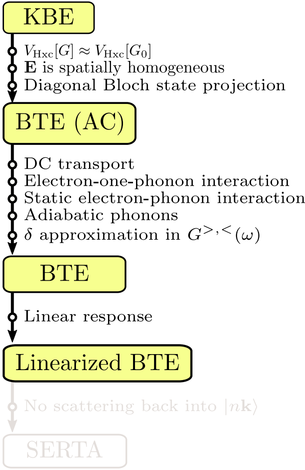
$$\partial_{E_\beta} f_{n\mathbf{k}} = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$

$$\times \Big[(n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})\Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

where the scattering rate is:

$$\tau^{-1}_{n\mathbf{k}} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[(n_{\mathbf{q}\nu} + 1 - f^0_{m\mathbf{k}+\mathbf{q}})$$

$$\times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})\big]$$

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`assume_metal = .true.`

$$\sigma_{\alpha\beta} = \frac{-e}{V_{\rm uc}} \sum_n \int \frac{{\rm d}^3 k}{\Omega_{\rm BZ}} v_{n\mathbf{k}}^{\alpha} \partial_{E_\beta} f_{n\mathbf{k}}$$

$$\rho_{\alpha\beta} = \frac{1}{\sigma_{\alpha\beta}}$$

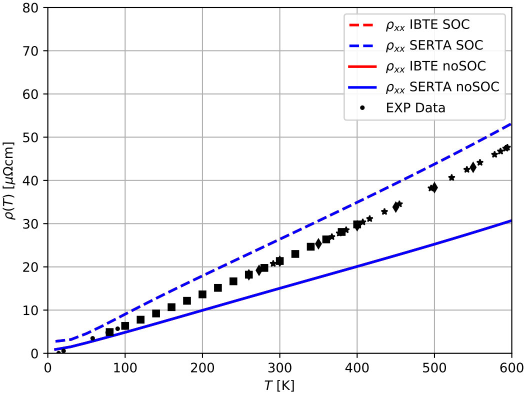


Figure courtesy of Félix Goudreault

# Drift conductivity

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

where

$$\partial_{E_\beta} f_{n\mathbf{k}} = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi\tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \times \Big[(n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})\Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

`int_mob = .true.` $\rightarrow$ computes drift mobility (also conductivity)

# Drift conductivity

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

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`int_mob = .true.` → computes drift mobility (also conductivity)
`iterative_bte = .true.` → computes the mobility iteratively (BTE+SERTA) with a `broyden_beta = 0.7` Broyden linear mixing and stops after `mob_maxiter = 200` if convergence is not reached.

# Drift conductivity

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$\int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} \rightarrow$ use crystal symmetries on fine $\mathbf{k}$ grid: `mp_mesh_k = .true.`

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$\int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}}$ → use crystal symmetries on fine $\mathbf{k}$ grid: `mp_mesh_k = .true.`

$\int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}}$ and $\int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}}$ → consider states within an `fsthick = 0.4` eV energy around $\varepsilon_{\mathrm{F}}$.

# Drift conductivity

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

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`int_mob = .true.` $\rightarrow$ computes drift mobility (also conductivity)
`iterative_bte = .true.` $\rightarrow$ computes the mobility iteratively (BTE+SERTA) with a `broyden_beta = 0.7` Broyden linear mixing and stops after `mob_maxiter = 200` if convergence is not reached.

$\int \frac{\mathrm{d}^3k}{\Omega_{\mathrm{BZ}}}$ $\rightarrow$ use crystal symmetries on fine $\mathbf{k}$ grid: `mp_mesh_k = .true.`

$\int \frac{\mathrm{d}^3k}{\Omega_{\mathrm{BZ}}}$ and $\int \frac{\mathrm{d}^3q}{\Omega_{\mathrm{BZ}}}$ $\rightarrow$ consider states within an `fsthick = 0.4` eV energy around $\varepsilon_{\mathrm{F}}$.

`carrier = .false.` $\rightarrow$ metal $\rightarrow$ no carrier concentration can be imposed.

# Drift conductivity

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

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$$\times \Big[ (n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

`restart = .true.` → activate restart where restart point are written to file every `restart_step = 50` **q**-points.
`selecqread = .false.` → produce a `selecq.fmt` file which contains the list of **q**-points within the **fsthick**.
If `selecqread = .true.` then read the `selecq.fmt` file (the code will exit if the file is not found).

# Drift conductivity

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

where

$$\partial_{E_\beta} f_{n\mathbf{k}} = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$
$$\times \Big[ (n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

`restart = .true.` → activate restart where restart point are written to file every `restart_step = 50` **q**-points.
`selecqread = .false.` → produce a `selecq.fmt` file which contains the list of **q**-points within the **fsthick**.
If `selecqread = .true.` then read the `selecq.fmt` file (the code will exit if the file is not found).

$n, f, \tau$ → dependent on the temperature given by `temps = 100 500` and `nstemp = 9`.

# Drift conductivity

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \frac{-e}{V_{\mathrm{uc}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

where

$$\partial_{E_\beta} f_{n\mathbf{k}} = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$
$$\times \Big[ (n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

`restart = .true.` → activate restart where restart point are written to file every `restart_step = 50` **q**-points.
`selecqread = .false.` → produce a `selecq.fmt` file which contains the list of **q**-points within the **fsthick**.
If `selecqread = .true.` then read the `selecq.fmt` file (the code will exit if the file is not found).

$n, f, \tau$ → dependent on the temperature given by `temps = 100 500` and `nstemp = 9`.

$\delta$ → adaptative broadening `degaussw = 0.0` degaussw = 0.0

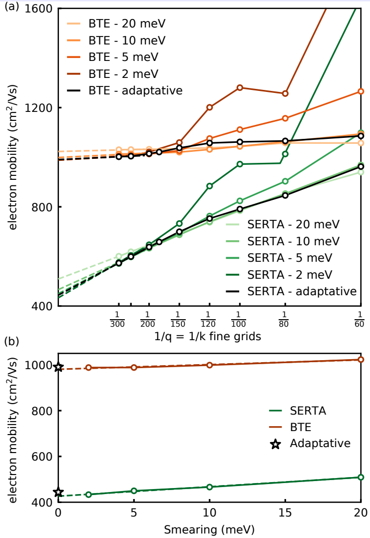
$$\tau_{n\mathbf{k}}^{-1} = \frac{2\pi}{\hbar}\sum_{m\nu}\int \frac{d^3q}{\Omega_{\text{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \times\Big[(n_{\mathbf{q}\nu}+1-f^0_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu}) +(n_{\mathbf{q}\nu}+f^0_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})\Big].$$

Adaptative broadening:

$$\eta_{n\mathbf{k}}(\mathbf{q}\nu) = \frac{\hbar}{\sqrt{12}}\sqrt{\sum_{\alpha}\left[\left(\mathbf{v}_{\mathbf{q}\nu\nu}-\mathbf{v}_{nn\mathbf{k}+\mathbf{q}}\right)\cdot\frac{\mathbf{G}_\alpha}{N_\alpha}\right]^2},$$

where the phonon velocity is:

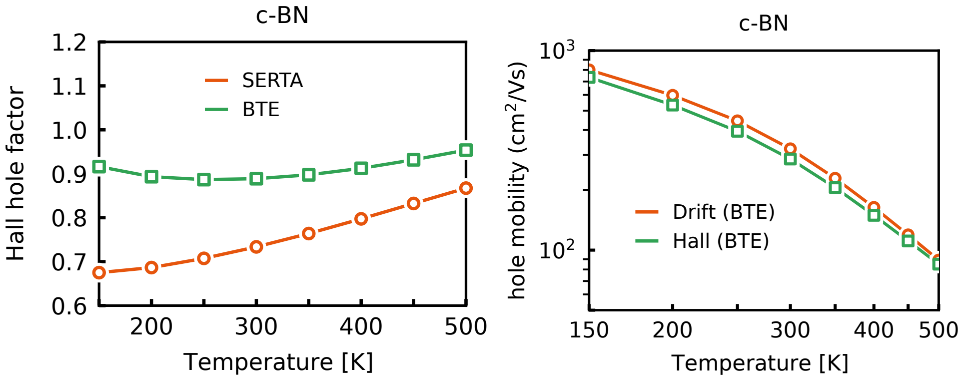
$$v_{\mathbf{q}\mu\nu\beta} = \frac{1}{2\omega_{\mathbf{q}\nu}}\frac{\partial D_{\mu\nu}(\mathbf{q})}{\partial q_\beta} = \frac{1}{2\omega_{\mathbf{q}\nu}}\sum_{\mathbf{R}} iR_\beta e^{i\mathbf{q}\cdot\mathbf{R}}D_{\mu\nu}(\mathbf{R}).$$




W. Li *et al.*, Comput. Phys. Commun. **185**, 1747 (2014)

S. Poncé *et al.*, arXiv:2105.04192 (2021)

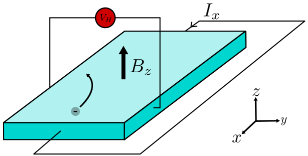
Compute the drift and Hall hole mobility of c-BN as well as Hall factor.




S. Poncé *et al.*, arXiv:2105.04192 (2021)

# Hall mobility

`bfieldz = 1.0d-10`




$$\mu^{\mathrm{H}}_{\alpha\beta\gamma} = \frac{-e}{V_{\mathrm{uc}} n_{\mathbf{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma)$$

BTE:

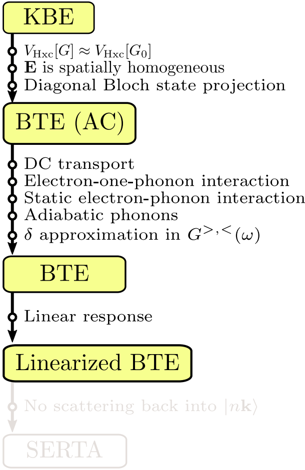
$$\Big[1 - \frac{e}{\hbar}\tau_{n\mathbf{k}}(\mathbf{v}_{n\mathbf{k}} \times \mathbf{B}) \cdot \nabla_{\mathbf{k}}\Big] \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma) = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}} + \frac{2\pi \tau_{n\mathbf{k}}}{\hbar} \sum_{m\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$

$$\times \Big[(n_{\mathbf{q}\nu} + 1 - f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f^0_{n\mathbf{k}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})\Big] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}(B_\gamma)$$

Hall factor:

$$\mu^{\mathrm{H}}_{\alpha\beta\gamma} = r^{\mathrm{H}}_{\alpha\beta\gamma} \mu^{\mathrm{d}}_{\alpha\beta}$$

$$r^{\mathrm{H}}_{\alpha\beta\gamma} \equiv \sum_{\delta\epsilon} \frac{(\mu^{\mathrm{d}}_{\alpha\delta})^{-1}\, \mu^{\mathrm{H}}_{\delta\epsilon\gamma}\, (\mu^{\mathrm{d}}_{\epsilon\beta})^{-1}}{B_\gamma},$$




F. Macheda *et al.*,
Phys. Rev. B **98**, 201201 (2018)

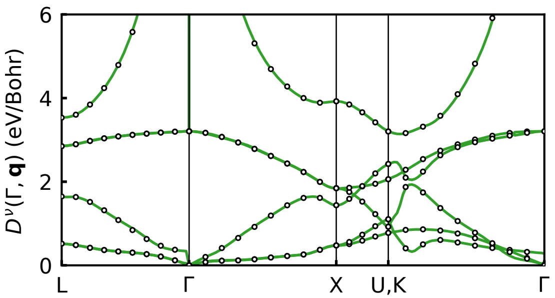
# Long-range interaction: Fröhlich dipole

`lpolar = .true.`

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}_{mn\nu}(\mathbf{k},\mathbf{q}) + g^{\mathcal{L}}_{mn\nu}(\mathbf{k},\mathbf{q})$$

$$g^{\mathcal{L}}_{mn\nu}(\mathbf{k},\mathbf{q}) \approx g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) + \cdots$$

$$g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) = i\frac{4\pi}{V_{\mathrm{uc}}}\frac{e^2}{4\pi\varepsilon^0}\sum_{\kappa}\left[\frac{\hbar}{2N_{p'}M_\kappa\omega_{\mathbf{q}\nu}}\right]^{\frac{1}{2}}\sum_{\mathbf{G}\neq-\mathbf{q}} \times \frac{(\mathbf{G}+\mathbf{q})\cdot\mathbf{Z}^*_\kappa\cdot\mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\varepsilon}^\infty\cdot(\mathbf{G}+\mathbf{q})}e^{-i(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\tau}_\kappa} \times \langle\Psi_{m\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\Psi_{n\mathbf{k}}\rangle,$$




C. Verdi *et al.*, Phys. Rev. Lett. **115**, 176401 (2015)
J. Sjakste *et al.*, Phys. Rev. B **92**, 054307 (2015)

S. Poncé *et al.*, arXiv:2105.04192 (2021)

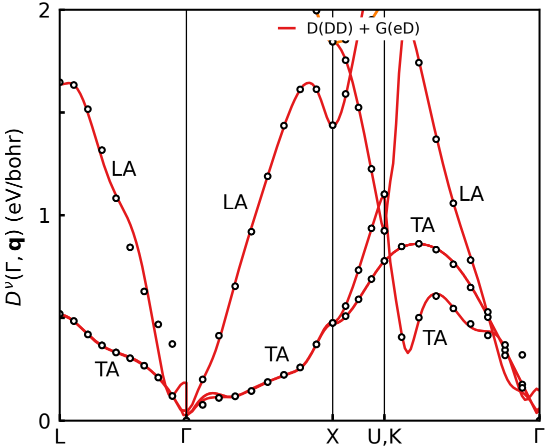
 `lpolar = .true.`

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}_{mn\nu}(\mathbf{k},\mathbf{q}) + g^{\mathcal{L}}_{mn\nu}(\mathbf{k},\mathbf{q})$$

$$g^{\mathcal{L}}_{mn\nu}(\mathbf{k},\mathbf{q}) \approx g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) + \cdots$$

$$g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) = i\frac{4\pi}{V_{\mathrm{uc}}}\frac{e^2}{4\pi\varepsilon^0}\sum_{\kappa}\left[\frac{\hbar}{2N_{p'}M_\kappa\omega_{\mathbf{q}\nu}}\right]^{\frac{1}{2}}\sum_{\mathbf{G}\neq-\mathbf{q}} \times \frac{(\mathbf{G}+\mathbf{q})\cdot\mathbf{Z}^*_\kappa\cdot\mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\varepsilon}^\infty\cdot(\mathbf{G}+\mathbf{q})}e^{-i(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\tau}_\kappa} \times \langle\Psi_{m\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\Psi_{n\mathbf{k}}\rangle,$$

C. Verdi *et al.*, Phys. Rev. Lett. **115**, 176401 (2015)
J. Sjakste *et al.*, Phys. Rev. B **92**, 054307 (2015)




S. Poncé *et al.*, arXiv:2105.04192 (2021)

# Long-range interaction: dynamic quadrupole

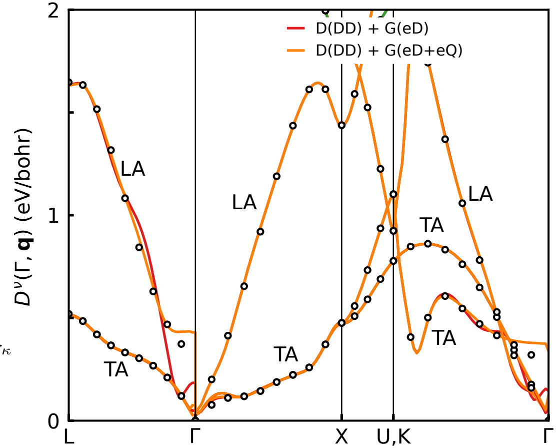
`quadrupole.fmt`

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}_{mn\nu}(\mathbf{k},\mathbf{q}) + g^{\mathcal{L}}_{mn\nu}(\mathbf{k},\mathbf{q})$$

$$g^{\mathcal{L}}_{mn\nu}(\mathbf{k},\mathbf{q}) \approx g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) + g^{\mathcal{L},\mathrm{Q}}_{mn\nu}(\mathbf{k},\mathbf{q}) + \cdots$$

$$g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) = i\frac{4\pi}{V_{\mathrm{uc}}}\frac{e^2}{4\pi\varepsilon^0}\sum_{\kappa}\left[\frac{\hbar}{2N_{p'}M_\kappa\omega_{\mathbf{q}\nu}}\right]^{\frac{1}{2}}\sum_{\mathbf{G}\neq-\mathbf{q}} \times\frac{(\mathbf{G}+\mathbf{q})\cdot\mathbf{Z}^*_\kappa\cdot\mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\varepsilon}^\infty\cdot(\mathbf{G}+\mathbf{q})}e^{-i(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\tau}_\kappa} \times\langle\Psi_{m\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\Psi_{n\mathbf{k}}\rangle,$$

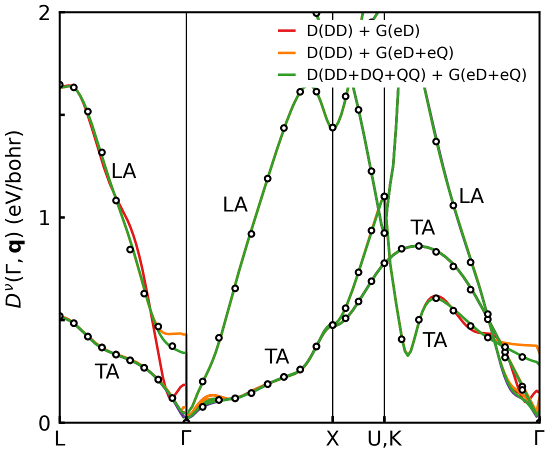
$$g^{\mathcal{L},\mathrm{Q}}_{mn\nu}(\mathbf{k},\mathbf{q}) = \frac{4\pi}{V_{\mathrm{uc}}}\frac{e^2}{4\pi\varepsilon^0}\sum_{\kappa}\left[\frac{\hbar}{2N_{p'}M_\kappa\omega_{\mathbf{q}\nu}}\right]^{\frac{1}{2}}\sum_{\mathbf{G}\neq-\mathbf{q}} \times\frac{(\mathbf{G}+\mathbf{q})\cdot(\mathbf{G}+\mathbf{q})\cdot\mathbf{e}_{\kappa\mathbf{q}\nu}\cdot\tilde{\mathbf{Q}}_{mn\kappa}(\mathbf{k},\mathbf{q})}{(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\varepsilon}^\infty\cdot(\mathbf{G}+\mathbf{q})}e^{-i(\mathbf{G}+\mathbf{q})\cdot\boldsymbol{\tau}_\kappa}$$




C. Verdi *et al.*, Phys. Rev. Lett. **115**, 176401 (2015)
J. Sjakste *et al.*, Phys. Rev. B **92**, 054307 (2015)
G. Brunin *et al.*, Phys. Rev. Lett. **125**, 136601 (2020)
V.A. Jhalani *et al.*, Phys. Rev. Lett. **125**, 136602 (2020)

S. Poncé *et al.*, arXiv:2105.04192 (2021)

$$D^{\mathcal{L},\mathrm{D+Q}}_{\kappa\alpha,\kappa'\beta}(\mathbf{q}) = \frac{e^{i\mathbf{q}\cdot(\boldsymbol{\tau}_{\kappa}-\boldsymbol{\tau}_{\kappa'})}e^{\frac{-\mathbf{q}\cdot\boldsymbol{\varepsilon}^{\infty}\cdot\mathbf{q}}{4\Lambda^2}}}{\mathbf{q}\cdot\boldsymbol{\varepsilon}^{\infty}\cdot\mathbf{q}}\Big[\mathbf{q}\cdot\mathbf{Z}^{*}_{\kappa\alpha}\cdot\mathbf{q}\cdot\mathbf{Z}^{*}_{\kappa'\beta} + \frac{1}{4}\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa\alpha}\cdot\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa'\beta} + \frac{i}{2}\mathbf{q}\cdot\mathbf{Z}^{*}_{\kappa\alpha}\cdot\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa'\beta} - \frac{i}{2}\mathbf{q}\cdot\mathbf{q}\cdot\mathbf{Q}_{\kappa\alpha}\cdot\mathbf{q}\cdot\mathbf{Z}^{*}_{\kappa'\beta}\Big]$$




M. Royo *et al.*, Phys. Rev. Lett. **125**, 217602 (2020)

S. Poncé *et al.*, arXiv:2105.04192 (2021)

# Additional notes

`efermi_read = .true` and `fermi_energy = 11.246840` eV need to be provided and the `fsthick` energy window is computed with respect to that level.

Suggestion: select the `fermi_energy` to be $+0.1$ eV above the VBM for hole mobility calculation and -0.1 eV below the CBM for electron mobility.

`ncarrier = -1E13` is the target carrier concentration in cm$^{-3}$. If negative it means hole mobility and positive electron mobility. An absolute value of `ncarrier` below 1E5 will result in an intrinsic mobility calculation and the Fermi level will be determined such that electron and hole have the same carrier density. For large bandgap and low temperature this will result in very low carrier concentration and thus be very unstable.

For reasonable carrier concentration (i.e. values between 1E10 and 1E16), the resulting mobility will be independent of carrier concentration. For large carrier concentration, ionized impurity scattering needs to be taken account (not cover in this hands-on).