School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

Mike Johnston, "Spaceman with Floating Pizza"

**fnrs**

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Hands-on Wed.4

# Carrier transport - Hands-on

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# Linearized Boltzmann transport equation

$$\mu_{\alpha\beta}^{\mathrm{d}} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v_{n\mathbf{k}}^\alpha \, \partial_{E_\beta} f_{n\mathbf{k}}$$

```
scattering = .true.
iterative_bte = .true.
restart = .true.
```

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

$$\times \left[ (n_{\mathbf{q}\nu} + 1 - f_{n\mathbf{k}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \right.$$

$$\left. + (n_{\mathbf{q}\nu} + f_{n\mathbf{k}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \right] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$$

where

$$\tau_{n\mathbf{k}}^{-1} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \left[ (n_{\mathbf{q}\nu} + 1 - f_{m\mathbf{k}+\mathbf{q}}^0) \right.$$

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

# Linearized Boltzmann transport equation

$$\mu_{\alpha\beta}^{\mathrm{d}} = \frac{-1}{V_{\mathrm{uc}}n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v_{n\mathbf{k}}^{\alpha}\ \partial_{E_{\beta}} f_{n\mathbf{k}}$$

```
scattering = .true.
iterative_bte = .true.
restart = .true.
```

**Note**: remove the `restart.fmt` file if you change any input parameters.

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

where

$$\tau_{n\mathbf{k}}^{-1} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[ (n_{\mathbf{q}\nu} + 1 - f_{m\mathbf{k}+\mathbf{q}}^0)$$
$$\times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f_{m\mathbf{k}+\mathbf{q}}^0)\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \big]$$

# Linearized Boltzmann transport equation

$$\mu_{\alpha\beta}^{\mathrm{d}} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v_{n\mathbf{k}}^{\alpha}\ \boxed{\partial_{E_\beta} f_{n\mathbf{k}}}$$

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

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

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

where

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

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

```
scattering  = .true.
iterative_bte = .true.
restart     = .true.
```

**Note**: remove the `restart.fmt` file if you change any input parameters.

```
epmatkqread  = .false.
mob_maxiter  = 300
broyden_beta = 1.0
```

# Linearized Boltzmann transport equation

$$\mu_{\alpha\beta}^{\mathrm{d}} = \frac{-1}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v_{n\mathbf{k}}^{\alpha} \boxed{\partial_{E_\beta} f_{n\mathbf{k}}}$$

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

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

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

where

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

$$\times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \big]$$
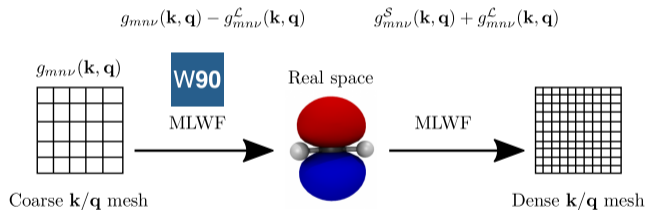
```
scattering = .true.
iterative_bte = .true.
restart = .true.
```

**Note**: remove the restart.fmt file if you change any input parameters.

```
epmatkqread   = .false.
mob_maxiter   = 300
broyden_beta  = 1.0
```

```
int_mob = .false.
carrier = .true.
ncarrier = -1E13  ! cm^-3
```
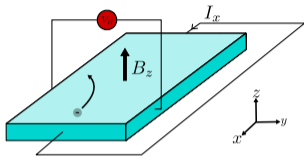
$$g_{mn\nu}(\mathbf{k}, \mathbf{q}) - g_{mn\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q}) \qquad g_{mn\nu}^{\mathcal{S}}(\mathbf{k}, \mathbf{q}) + g_{mn\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q})$$

$g_{mn\nu}(\mathbf{k}, \mathbf{q})$

**W90**

MLWF

Real space

MLWF

Coarse $\mathbf{k}/\mathbf{q}$ mesh

Dense $\mathbf{k}/\mathbf{q}$ mesh

```
polar = .true.
```

```
If quadrupole.fmt file
    present in running
    folder
```

# Hall mobility

```
bfieldx = 0.0d0
bfieldy = 0.0d0
bfieldz = 1.0d-10 ! Tesla
```
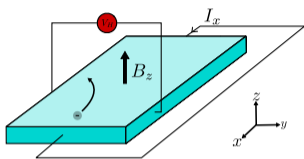
$$\mu_{\alpha\beta}^{\mathrm{Hall}}(\hat{\mathbf{B}}) = \sum_{\gamma} \mu_{\alpha\gamma}^{\mathrm{drift}} \, r_{\gamma\beta}(\hat{\mathbf{B}})$$

$$r_{\alpha\beta}(\hat{\mathbf{B}}) \equiv \lim_{\mathbf{B}\to 0} \sum_{\delta\epsilon} \frac{[\, \mu_{\alpha\delta}^{\mathrm{drift}} \,]^{-1} \, \mu_{\delta\epsilon}(\mathbf{B}) \, [\, \mu_{\epsilon\beta}^{\mathrm{drift}} \,]^{-1}}{|\mathbf{B}|}$$

$$\mu_{\alpha\beta}(B_\gamma) = \frac{-1}{S_{\mathrm{uc}} n_{\mathrm{c}}} \sum_{n} \int \frac{\mathrm{d}^3 k}{S_{\mathrm{BZ}}} v_{n\mathbf{k}\alpha} \big[\, \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma) - \partial_{E_\beta} f_{n\mathbf{k}} \,\big]$$

$$\mu_{\alpha\beta}^{\mathrm{drift}} = \frac{-1}{S_{\mathrm{uc}} n_{\mathrm{c}}} \sum_{n} \int \frac{\mathrm{d}^3 k}{S_{\mathrm{BZ}}} v_{n\mathbf{k}\alpha} \, \partial_{E_\beta} f_{n\mathbf{k}}$$

# Hall mobility



```
bfieldx = 0.0d0
bfieldy = 0.0d0
bfieldz = 1.0d-10 ! Tesla
```

$$\mu_{\alpha\beta}^{\mathrm{Hall}}(\hat{\mathbf{B}}) = \sum_{\gamma} \mu_{\alpha\gamma}^{\mathrm{drift}} \; r_{\gamma\beta}(\hat{\mathbf{B}})$$

```
Mobility tensor without magnetic field    | with magnetic field [cm^2/Vs]
  0.65309E+03   -0.73478E-15    0.47461E-15 |  -0.13733E-07    0.11856E-01    0.92830E-15
 -0.92617E-15    0.65309E+03   -0.47410E-15 |  -0.11856E-01   -0.13733E-07    0.47576E-14
  0.27579E-15    0.80047E-16    0.65309E+03 |   0.16409E-14   -0.19264E-15    0.27114E-06
```
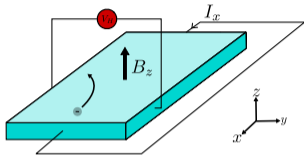
$$r_{\alpha\beta}(\hat{\mathbf{B}}) \equiv \lim_{\mathbf{B}\to 0} \sum_{\delta\epsilon} \frac{[\; \mu_{\alpha\delta}^{\mathrm{drift}} \;]^{-1} \; \mu_{\delta\epsilon}}{|\mathbf{B}|}$$

$$\mu_{\alpha\beta}(B_{\gamma}) = \frac{-1}{S_{\mathrm{uc}} n_{\mathrm{c}}} \sum_{n} \int \frac{\mathrm{d}^3 k}{S_{\mathrm{BZ}}} v_{n\mathbf{k}\alpha} [\; \partial_{E_{\beta}} f_{n\mathbf{k}}(B_{\gamma}) \; - \; \partial_{E_{\beta}} f_{n\mathbf{k}} \;]$$

$$\mu_{\alpha\beta}^{\mathrm{drift}} = \frac{-1}{S_{\mathrm{uc}} n_{\mathrm{c}}} \sum_{n} \int \frac{\mathrm{d}^3 k}{S_{\mathrm{BZ}}} v_{n\mathbf{k}\alpha} \; \partial_{E_{\beta}} f_{n\mathbf{k}}$$

# Hall mobility



```
bfieldx = 0.0d0
bfieldy = 0.0d0
bfieldz = 1.0d-10 ! Tesla
```

$$\mu_{\alpha\beta}^{\text{Hall}}(\hat{\mathbf{B}}) = \sum_{\gamma} \mu_{\alpha\gamma}^{\text{drift}} \; r_{\gamma\beta}(\hat{\mathbf{B}})$$

```
Mobility tensor without magnetic field   | with magnetic field [cm^2/Vs]
   0.65309E+03   -0.73478E-15   0.47461E-15 |  -0.13733E-07   0.11856E-01   0.92830E-15
  -0.92617E-15    0.65309E+03  -0.47410E-15 |  -0.11856E-01  -0.13733E-07   0.47576E-14
   0.27579E-15    0.80047E-16   0.65309E+03 |   0.16409E-14  -0.19264E-15   0.27114E-06
```
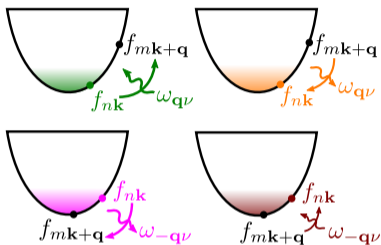
$$r_{\alpha\beta}(\hat{\mathbf{B}}) \equiv \lim_{\mathbf{B}\to 0} \sum_{\delta\epsilon} \frac{[\; \mu_{\alpha\delta}^{\text{drift}} \;]^{-1} \; \mu_{\delta\epsilon}}{|\mathbf{B}|}$$

```
Hall factor
  -0.854978E-06   0.738128E+00   0.577927E-13
  -0.738128E+00  -0.854971E-06   0.296192E-12
   0.102159E-12  -0.119933E-13   0.168802E-04
```

$$\mu_{\alpha\beta}(B_\gamma) = \frac{-1}{S_{\text{uc}} n_{\text{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{S_{\text{BZ}}} v_{n\mathbf{k}\alpha} \big[\; \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma) \; - \; \partial_{E_\beta} f_{n\mathbf{k}} \;\big]$$

$$\mu_{\alpha\beta}^{\text{drift}} = \frac{-1}{S_{\text{uc}} n_{\text{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{S_{\text{BZ}}} v_{n\mathbf{k}\alpha} \; \partial_{E_\beta} f_{n\mathbf{k}}$$
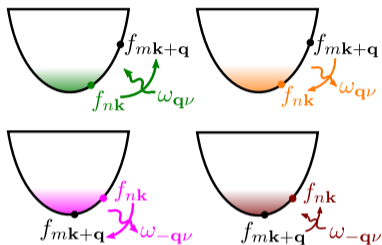
# Energy window



```
fsthick = 0.4 ! 0.3 eV
efermi_read = .true.
fermi_energy = 11.24
```

```
Valence band maximum     =  11.14 eV

Temperature   300.000 K
Mobility VB Fermi level =  11.687812 eV
```

```
Fermi Surface thickness =   0.400000 eV
This is computed with respect to the fine Fermi level 11.24 eV
Only states between  10.84 eV and  11.64 eV will be included
```

$$-e\mathbf{E} \cdot \frac{1}{\hbar} \frac{\partial f_{n\mathbf{k}}}{\partial \mathbf{k}} = \frac{2\pi}{\hbar} \sum_{m,\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2$$

$$\times \left[ f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \right.$$

$$+ f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)$$

$$- (1 - f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}$$

$$\left. - (1 - f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1) \right]$$
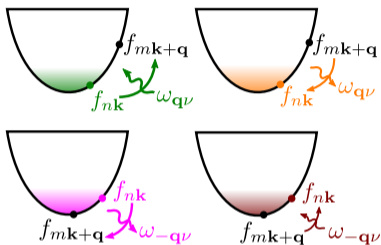
# Energy window + k-point symmetry



```
etf_mem = 3
mp_mesh_k = .true.
```

```
Number of k-points inside fsthick * 1.2 in the full BZ: 4667
Size of k point mesh for interpolation:        544
Max number of k points per pool:                 2

Fermi energy coarse grid =  11.281268 eV
```

```
...
    Number selected, total          13000        197752
    Number selected, total          14000        201663
    Number selected, total          15000        205560
    Number selected, total          16000        209529
    Number selected, total          17000        215227
    We only need to compute   17412 q-points
```

$$-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial\mathbf{k}}=\frac{2\pi}{\hbar}\sum_{m,\nu}\int\frac{\mathrm{d}^3q}{\Omega_{\mathrm{BZ}}}\left|g_{mn\nu}(\mathbf{k},\mathbf{q})\right|^2$$

$$\times\left[f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}\right.$$

$$+\,f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)$$

$$-\,(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}$$

$$\left.-\,(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)\right]$$

# Energy window + k-point symmetry



```
etf_mem = 3
mp_mesh_k = .true.
```

```
Number of k-points inside fsthick * 1.2 in the full BZ: 4667
Size of k point mesh for interpolation:          544
Max number of k points per pool:                   2

Fermi energy coarse grid =  11.281268 eV
```

```
...
    Number selected, total          13000          197752
    Number selected, total          14000          201663
    Number selected, total          15000          205560
    Number selected, total          16000          209529
    Number selected, total          17000          215227
    We only need to compute    17412 q-points
```

```
selecqread = .true.
```

$$-e\mathbf{E} \cdot \frac{1}{\hbar} \frac{\partial f_{n\mathbf{k}}}{\partial \mathbf{k}} = \frac{2\pi}{\hbar} \sum_{m,\nu} \int \frac{\mathrm{d}^3 q}{\Omega_{\mathrm{BZ}}} \left| g_{mn\nu}(\mathbf{k}, \mathbf{q}) \right|^2$$

$$\times \left[ f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \right.$$

$$+ f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)$$

$$- (1 - f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}$$

$$\left. - (1 - f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1) \right]$$

# Adaptive 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 $\mathbf{G}_\alpha$ are the reciprocal lattice vectors, $N_\alpha$ the q-point grid density. The phonon velocity $\mathbf{v}_{\mathbf{q}\nu\nu}$ is obtained from

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

```
degaussw = 0.0
```

```
Progression iq (fine) =       1000/    17412
 Adaptative smearing = Min:      4.453489 meV
                       Max:    103.289944 meV
Progression iq (fine) =       2000/    17412
 Adaptative smearing = Min:      3.204561 meV
                       Max:    102.790189 meV
```

W. Li, J. Carrete, N. A. Katcho, and N. Mingo, Comput. Phys. Commun. **185**, 1747 (2014)

X. Wang, J. R. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B **74**, 195118 (2006)

## Electronic velocity

Obtained from the commutator:

$$\hat{\mathbf{v}} = (i/\hbar)[\hat{H}, \hat{\mathbf{r}}]$$

$$\mathbf{v}_{nm\mathbf{k}} = \langle \psi_{m\mathbf{k}} | \hat{\mathbf{p}}/m_e + (i/\hbar)[\hat{V}_{NL}, \hat{\mathbf{r}}] | \psi_{n\mathbf{k}} \rangle,$$

where $\hat{\mathbf{p}} = -i\hbar \partial/\partial \mathbf{r}$ is the momentum operator.
$P_c r_\alpha | \psi_{n\mathbf{k}} \rangle$ are the solution of the linear system:

$$[H - \varepsilon_{n\mathbf{k}} S] P_c r_\alpha | \psi_{n\mathbf{k}} \rangle = P_c^\dagger [H - \varepsilon_{n\mathbf{k}} S, r_\alpha] | \psi_{n\mathbf{k}} \rangle,$$

where $S$ is the overlap matrix and $P_c$ the projector over the empty states.

In the local approximation (neglecting $\hat{V}_{NL}$):

$$v_{mn\mathbf{k}\mathbf{k}'\alpha} \approx \langle \psi_{m\mathbf{k}'} | \hat{p}_\alpha | \psi_{n\mathbf{k}} \rangle = \delta(\mathbf{k} - \mathbf{k}') \left( k_\alpha \delta_{mn} - i \int d\mathbf{r} u_{m\mathbf{k}'}^*(\mathbf{r}) \nabla_\alpha u_{n\mathbf{k}}(\mathbf{r}) \right)$$

```
vme = 'dipole'
```

```
dmedata.fmt
```

J. Tóbik and A. D. Corso, J. Chem. Phys. **120**, 9934 (2004)

X. Wang, J. R. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B **74**, 195118 (2006)

# Electronic velocity

Wannier interpolated velocities:

$$v_{nm\mathbf{k}',\alpha} = \frac{1}{\hbar} H_{nm\mathbf{k}',\alpha} - \frac{i}{\hbar}(\varepsilon_{m\mathbf{k}'} - \varepsilon_{n\mathbf{k}'}) A_{mn\mathbf{k}',\alpha}$$

$$A_{mn\mathbf{k}',\alpha} = \sum_{m'n'} U^{\dagger}_{mm'\mathbf{k}'} A^{(W)}_{m'n'\mathbf{k}',\alpha} U_{n'n\mathbf{k}'}$$

$$A^{(W)}_{nm\mathbf{k},\alpha} = i \sum_{\mathbf{b}} w_b b_\alpha (\langle u^{(W)}_{n\mathbf{k}} | u^{(W)}_{m\mathbf{k}+\mathbf{b}} \rangle - \delta_{nm}),$$

**b** are the vectors connecting **k** to its nearest neighbor and overlap matrices are:

$$\langle u^{(W)}_{n\mathbf{k}} | u^{(W)}_{m\mathbf{k}+\mathbf{b}} \rangle = \sum_{n'm'} U^{\dagger}_{mm'\mathbf{k}} M_{mn\mathbf{k}} U_{nn'\mathbf{k}+\mathbf{b}},$$

$M_{mn\mathbf{k}} = \langle u_{n\mathbf{k}} | u_{m\mathbf{k}+\mathbf{b}} \rangle$ is the phase relation between neighboring Bloch orbitals.
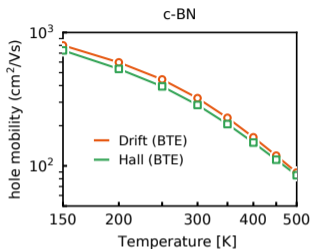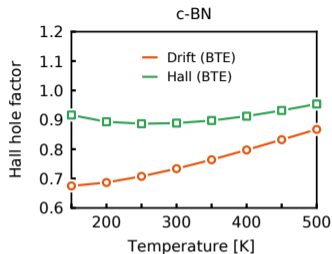
```
vme = 'wannier'
```

```
vmedata.fmt
```

J. Tóbik and A. D. Corso, J. Chem. Phys. **120**, 9934 (2004)

X. Wang, J. R. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B **74**, 195118 (2006)

# Temperature dependence



c-BN — Hall hole factor vs Temperature [K]; c-BN — hole mobility (cm²/Vs) vs Temperature [K]; Drift (BTE), Hall (BTE)

```
nstemp = 10
temps  = 100 500
```

```
=========================================================================
BTE in the self-energy relaxation time approximation (SERTA)
=========================================================================


=========================================================================
 Temp     Fermi    Hole density  Population SR                Hole mobility
  [K]      [eV]      [cm^-3]      [h per cell]                 [cm^2/Vs]
=========================================================================

 300.000  11.6878  0.99999E+13   0.33452E-22    0.575130E+03   0.118710E-15  -0.152676E-15
                                                0.267516E-15   0.575130E+03  -0.640294E-15
                                                0.134541E-14  -0.333160E-15   0.575130E+03
```
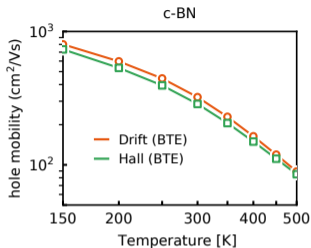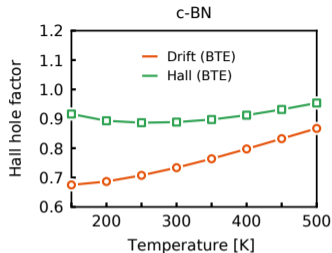
# Temperature dependence



```
nstemp = 10
temps  = 100 500
```

```
    Iteration number:      14

    ==================================================================================
     Temp    Fermi    Hole density  Population SR                 Hole mobility
     [K]     [eV]      [cm^-3]       [h per cell]                 [cm^2/Vs]
    ==================================================================================

    300.000  11.6878  0.99999E+13   0.11254E-21   0.653089E+03  -0.926165E-15   0.275785E-15
                                                  -0.734776E-15   0.653089E+03   0.800469E-16
                                                   0.474613E-15  -0.474100E-15   0.653089E+03

                                                   0.991642E-06   Max error
```
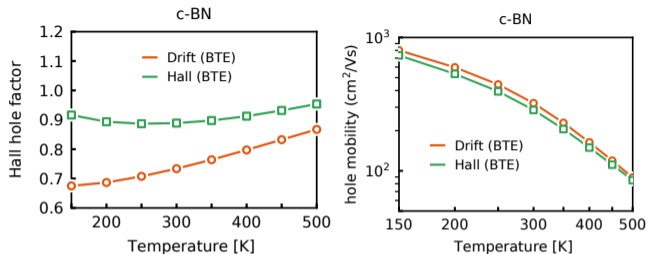
# Temperature dependence



c-BN — Hall hole factor vs Temperature [K]; c-BN — hole mobility (cm²/Vs) vs Temperature [K]; Drift (BTE), Hall (BTE)

```
nstemp = 10
temps  = 100 500
```

```
    Iteration number:       29

    =================================================================================
     Temp    Fermi    Hole density  Population SR                  Hole mobility
     [K]     [eV]      [cm^-3]       [h per cell]                  [cm^2/Vs]
    =================================================================================

    300.000  11.6878  0.99999E+13  -0.41913E-21    0.653089E+03  -0.118563E-01   0.191673E-14
                                                   0.118563E-01   0.653089E+03  -0.112593E-15
                                                   0.140291E-14   0.428354E-14   0.653089E+03

                                                   0.000000E+00   Max error
```

# Temperature dependence



```
nstemp = 10
temps  = 100 500
```

```
==================================================================================
BTE in the self-energy relaxation time approximation (SERTA)
==================================================================================

Temperature:   300.0000 K
Conductivity tensor without magnetic field | with magnetic field [Siemens/m]
  0.92145E-01    0.42861E-19    0.21556E-18 |  -0.61929E-15    0.13909E-05   -0.20556E-18
  0.19019E-19    0.92145E-01   -0.53378E-19 |  -0.13909E-05   -0.63751E-15    0.27616E-18
 -0.24461E-19   -0.10259E-18    0.92145E-01 |  -0.26334E-18   -0.48242E-19    0.16393E-15
Mobility tensor without magnetic field     | with magnetic field [cm^2/Vs]
  0.57513E+03    0.26752E-15    0.13454E-14 |  -0.38654E-11    0.86813E-02   -0.12830E-14
  0.11871E-15    0.57513E+03   -0.33316E-15 |  -0.86813E-02   -0.39790E-11    0.17237E-14
 -0.15268E-15   -0.64029E-15    0.57513E+03 |  -0.16436E-14   -0.30111E-15    0.10232E-11
Hall factor
 -0.310301E-09    0.696911E+00   -0.102997E-12
 -0.696911E+00   -0.319427E-09    0.138373E-12
 -0.131947E-12   -0.241719E-13    0.821385E-10
```
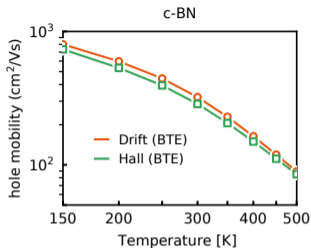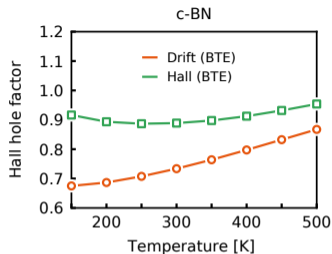
# Temperature dependence



```
nstemp = 10
temps  = 100 500
```

```
================================================================================
BTE
================================================================================

Temperature:   300.0000 K
Conductivity tensor without magnetic field | with magnetic field [Siemens/m]
  0.10464E+00  -0.11772E-18   0.76041E-19 |  -0.22003E-11   0.18996E-05   0.14873E-18
 -0.14839E-18   0.10464E+00  -0.75959E-19 |  -0.18996E-05  -0.22003E-11   0.76225E-18
  0.44185E-19   0.12825E-19   0.10464E+00 |   0.26291E-18  -0.30864E-19   0.43441E-10
Mobility tensor without magnetic field    | with magnetic field [cm^2/Vs]
  0.65309E+03  -0.73478E-15   0.47461E-15 |  -0.13733E-07   0.11856E-01   0.92830E-15
 -0.92617E-15   0.65309E+03  -0.47410E-15 |  -0.11856E-01  -0.13733E-07   0.47576E-14
  0.27579E-15   0.80047E-16   0.65309E+03 |   0.16409E-14  -0.19264E-15   0.27114E-06
Hall factor
 -0.854978E-06   0.738128E+00   0.577927E-13
 -0.738128E+00  -0.854971E-06   0.296192E-12
  0.102159E-12  -0.119933E-13   0.168802E-04
```

## Resistivity in metals - Ziman

Lowest-order variational approximation (LOVA) / Ziman formula:

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

```
phonselfen = .true.
a2f = .true.
nc = 4.0d0
degaussq = 0.05 ! meV
assume_metal = .true.
ngaussw = -99 ! FD
```

**Note**: A file pb.res.01.1.000 will be created.

# References

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- S. Poncé, W. Li, S. Reichardt, and F. Giustino, Rep. Prog. Phys. **83**, 036501 (2020) [link]

- F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B **76**, 165108 (2007) [link]

- F. Giustino, Rev. Mod. Phys. **89**, 015003 (2017) [link]

- G. Grimvall, *The electron-phonon interaction in metals*, 1981, (North-Holland, Amsterdam)

- N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Rev. Mod. Phys. **84**, 1419 (2012) [link]

# Supplemental Slides