2022 Summer School on Electron-Phonon Physics

From First Principles

Austin Texas

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UCLouvain
Institute of Condensed Matter and Nanosciences

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Hands-on Wed.4

Carrier transport - Hands-on

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Linearized Boltzmann transport equation

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

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

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

where

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

Linearized Boltzmann transport equation

$$\mu^{\rm d}_{\alpha\beta} = \frac{-1}{V_{\rm uc} n_{\rm c}} \sum_n \int \frac{{\rm d}^3 k}{\Omega_{\rm BZ}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}$$

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where

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

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

Linearized Boltzmann transport equation

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

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where

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

```
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

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

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where

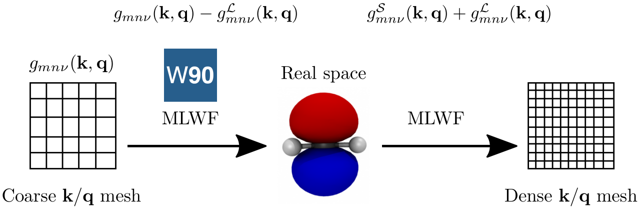
$$\tau^{-1}_{n\mathbf{k}} \equiv \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d^3 q}{\Omega_{\mathrm{BZ}}} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \big[(n_{\mathbf{q}\nu} + 1 - f^0_{m\mathbf{k}+\mathbf{q}}) \times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu})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

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

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

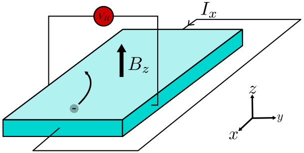
```
epmatkqread   = .false.
mob_maxiter   = 300
broyden_beta  = 1.0
```

```
int_mob = .false.
carrier = .true.
ncarrier = -1E13 ! cm^-3
```




```
polar = .true.
```

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



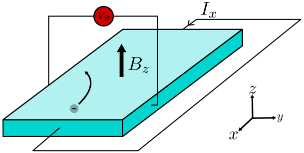

```
bfieldx = 0.0d0
bfieldy = 0.0d0
bfieldz = 1.0d-10 ! Tesla
```

$$\mu^{\mathrm{Hall}}_{\alpha\beta}(\hat{\mathbf{B}}) = \sum_{\gamma} \mu^{\mathrm{drift}}_{\alpha\gamma} \, r_{\gamma\beta}(\hat{\mathbf{B}})$$

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

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

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




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

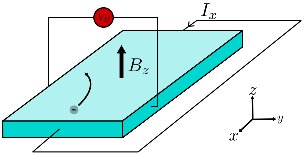
$$\mu^{\mathrm{Hall}}_{\alpha\beta}(\hat{\mathbf{B}}) = \sum_{\gamma} \mu^{\mathrm{drift}}_{\alpha\gamma} \, r_{\gamma\beta}(\hat{\mathbf{B}})$$

```
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
```

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

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

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




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

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

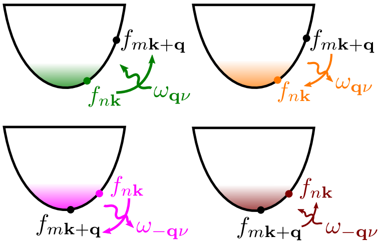
```
Mobility tensor without magnetic field       | with magnetic field [cm^2/Vs]
  0.65309E+03  -0.73478E-15   0.47461E-15   | -0.13733E-07   0.11856E-01   0.92830E-15
 -0.92617E-15   0.65309E+03  -0.47410E-15   | -0.11856E-01  -0.13733E-07   0.47576E-14
  0.27579E-15   0.80047E-16   0.65309E+03   |  0.16409E-14  -0.19264E-15   0.27114E-06
```

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

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

```
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
```

$$\mu^{\text{drift}}_{\alpha\beta} = \frac{-1}{S_{\text{uc}} n_{\text{c}}} \sum_n \int \frac{d^3k}{S_{\text{BZ}}} v_{n\mathbf{k}\alpha}\ \partial_{E_\beta} f_{n\mathbf{k}}$$



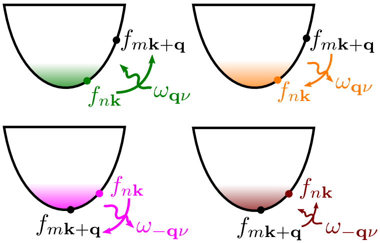

```
fsthick = 0.4 ! 0.3 eV
efermi_read = .true.
fermi_energy = 11.24
```

```
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
```

$$
\begin{aligned}
-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial \mathbf{k}} = \frac{2\pi}{\hbar}\sum_{m,\nu}\int\frac{\mathrm{d}^3q}{\Omega_{\mathrm{BZ}}}\,|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \\
\times\big[f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \\
+ f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1) \\
-(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \\
-(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)\big]
\end{aligned}
$$



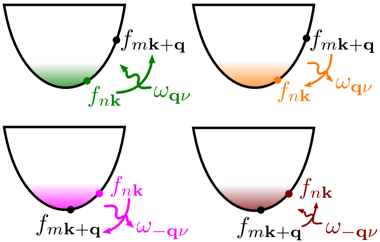
$$-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial\mathbf{k}} = \frac{2\pi}{\hbar}\sum_{m,\nu}\int\frac{\mathrm{d}^3q}{\Omega_{\mathrm{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$
$$\times\Big[f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\m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

```
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
```



$$
\begin{aligned}
-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial \mathbf{k}} = \frac{2\pi}{\hbar}\sum_{m,\nu}\int\frac{\mathrm{d}^3q}{\Omega_{\mathrm{BZ}}}\,|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \\
\times\Big[f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \\
+f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1) \\
-(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \\
-(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}-\hbar\omega_{\mathbf{q}\nu})(n_{\mathbf{q}\nu}+1)\Big]
\end{aligned}
$$

```
etf_mem  =  3
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```

```
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```
...
     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.
```

```
degaussw = 0.0
```

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

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

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

```
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:

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

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 $\hat{V}_{\mathrm{NL}}$):

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

```
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:

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

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

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

```
vme = 'wannier'
```

```
vmedata.fmt
```

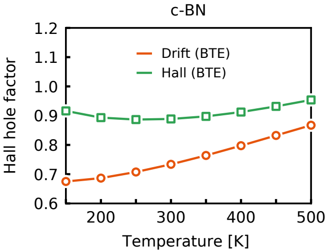
$\mathbf{b}$ are the vectors connecting $\mathbf{k}$ to its nearest neighbor and overlap matrices are:

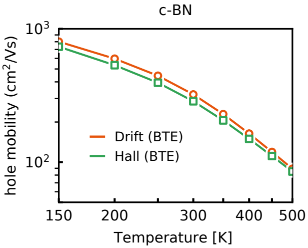
$$\langle u^{(\mathrm{W})}_{n\mathbf{k}} | u^{(\mathrm{W})}_{m\mathbf{k}+\mathbf{b}} \rangle = \sum_{n'm'} U^{\dagger}_{mm'\mathbf{k}} M_{mn\mathbf{k}} U_{nn'\mathbf{k}+\mathbf{b}},$$

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

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)





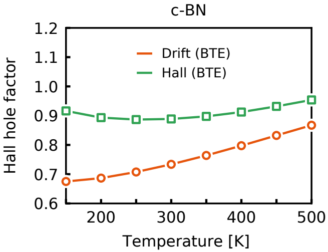

```
nstemp  =  10
temps   =  100  500
```

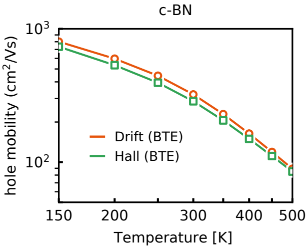
```
=============================================================================
BTE in the self-energy relaxation time approximation (SERTA)
=============================================================================

=============================================================================
  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
```

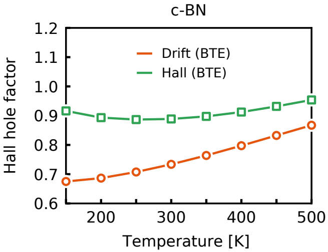
```
      Iteration number:         14

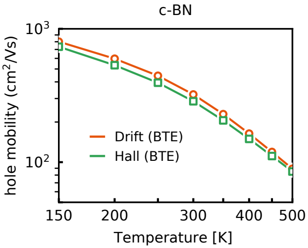
      =============================================================================================
        Temp      Fermi    Hole density  Population SR                  Hole mobility
         [K]       [eV]       [cm^-3]       [h per cell]                   [cm^2/Vs]
      =============================================================================================

       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






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

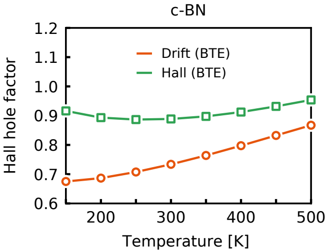
```
     Iteration number:          29

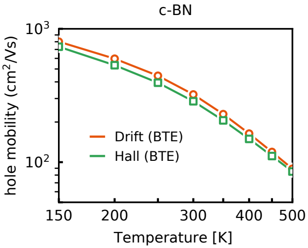
     ===========================================================================================
       Temp       Fermi    Hole density  Population SR                  Hole mobility
        [K]        [eV]      [cm^-3]      [h per cell]                    [cm^2/Vs]
     ===========================================================================================

      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



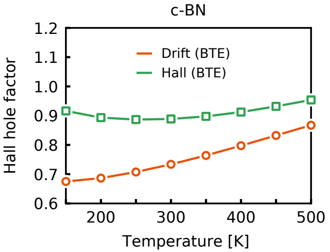


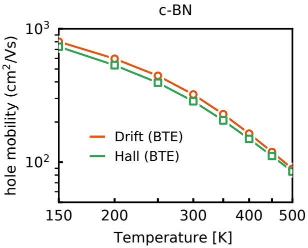

```
nstemp  =  10
temps   =  100  500
```

```
==========================================================================================
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
```

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

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

```
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