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

June 14-18 2021

Lecture Wed.1

Transport module of EPW

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Theory and Simulation of Materials (THEOS)

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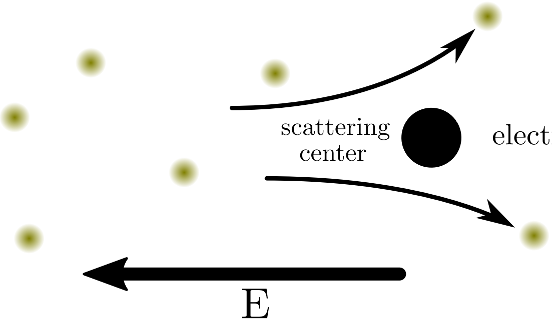
Lecture Summary

- Carrier transport
- Quantum theory of mobility
- Boltzmann transport equation
- Technical details
- Applications to semiconductors and metals
- Ionized impurity scattering

Carrier transport: experimental evidences

$$\text{Mobility } \mu \propto \frac{\partial}{\partial E} \int d\mathbf{k} f_{\mathbf{k}} v_{\mathbf{k}}$$



electron-phonon interaction

- **lattice (phonon) scattering**
- ionized impurity scattering
- alloy scattering
- defects scattering

Carrier transport: experimental evidences

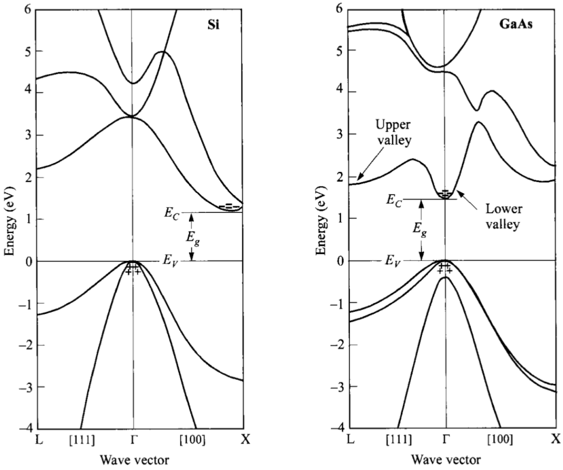
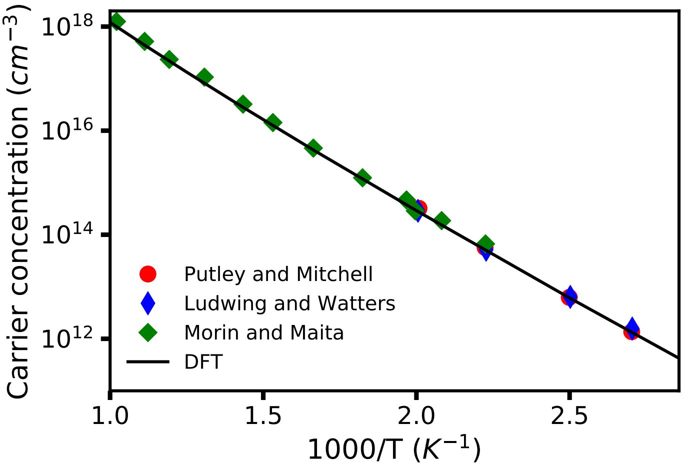


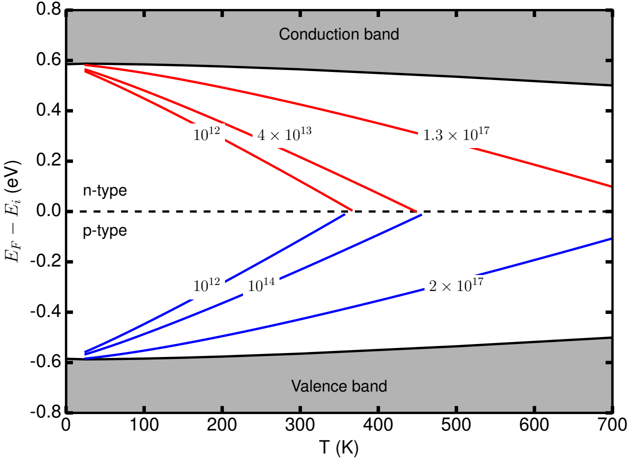
Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences



Carrier transport: experimental evidences

Calculated evolution of the Fermi level of Si as a function of temperature and impurity concentration.



Carrier transport: experimental evidences

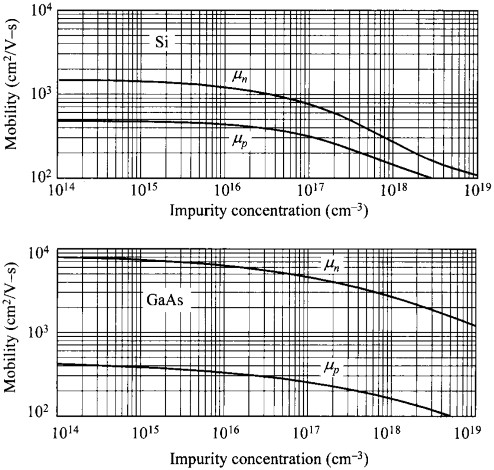


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences

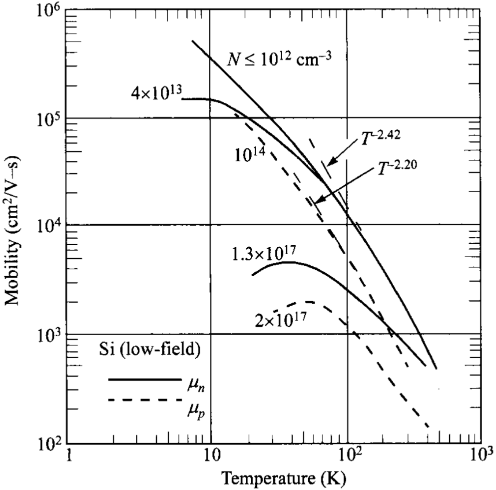


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Quantum theory of mobility

Current density

$$\mathbf{J}(\mathbf{r}_1, t_1) = \frac{-e\hbar^2}{2m} \lim_{\mathbf{r}_2 \to \mathbf{r}_1} (\nabla_2 - \nabla_1) G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_1)$$

$$G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) \equiv \frac{i}{\hbar} \left\langle \hat{\psi}^\dagger_{\mathrm{H}}(\mathbf{r}_2, t_2) \hat{\psi}_{\mathrm{H}}(\mathbf{r}_1, t_1) \right\rangle$$

Current density

$$\mathbf{J}(\mathbf{r}_1, t_1) = \frac{-e\hbar^2}{2m} \lim_{\mathbf{r}_2 \to \mathbf{r}_1} (\nabla_2 - \nabla_1) G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_1)$$

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$$\hat{\psi}_{\mathrm{H}}(\mathbf{r}, t) \equiv \overline{\mathcal{T}} \left[\mathrm{e}^{\frac{i}{\hbar} \int_{t_0}^{t} \mathrm{d}t' \hat{H}(t')} \right] \hat{\psi}(\mathbf{r}) \mathcal{T} \left[\mathrm{e}^{\frac{-i}{\hbar} \int_{t_0}^{t} \mathrm{d}t' \hat{H}(t')} \right]$$

$$\left\langle \hat{O} \right\rangle \equiv \frac{1}{Z} \mathrm{tr} \left[\mathrm{e}^{-\beta \hat{H}(t_0)} \hat{O} \right] \qquad \leftarrow \text{thermodynamical average}$$

$$Z \equiv \mathrm{tr} \left[\mathrm{e}^{-\beta \hat{H}(t_0)} \right] \qquad \leftarrow \text{partition function}$$

Quantum theory of mobility

Current density

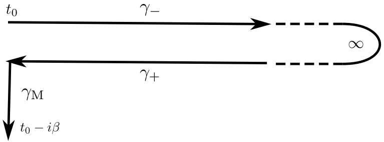
$$\mathbf{J}(\mathbf{r}_1,t_1) = \frac{-e\hbar^2}{2m}\lim_{\mathbf{r}_2\to\mathbf{r}_1}(\nabla_2-\nabla_1)G^<(\mathbf{r}_1,\mathbf{r}_2;t_1,t_1)$$

$$G^<(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2) \equiv \frac{i}{\hbar}\left\langle \hat{\psi}^\dagger_{\mathrm{H}}(\mathbf{r}_2,t_2)\hat{\psi}_{\mathrm{H}}(\mathbf{r}_1,t_1)\right\rangle$$

Keldysh-Schwinger contour formalism

$$G(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) = \frac{-i}{\hbar}\frac{1}{Z}\mathrm{tr}\left\{\mathcal{T}_{\mathrm{C}}\left[\mathrm{e}^{\frac{-i}{\hbar}\int_\gamma \mathrm{d}z\,\hat{H}(z)}[\hat{\psi}(\mathbf{r}_1)]_{z_1}[\hat{\psi}^\dagger(\mathbf{r}_2)]_{z_2}\right]\right\}$$

$$\hat{H}(z) = \hat{H}_0 + \hat{H}_{\mathrm{int}} + \hat{H}_{\mathrm{ext}}(z)$$



Quantum theory of mobility

Perturbative expansion of the GF in powers of $\hat{H}_{\text{int}}$ and $\hat{H}_{\text{ext}}(z)$

$$G(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) = G_0(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) + \sum_{n,m=1}^{\infty}\frac{(-i/\hbar)^{n+m}}{n!m!}\int_\gamma \mathrm{d}z'_1 \dots$$
$$\times \frac{1}{Z}\mathrm{tr}\Big[\mathcal{T}_\mathrm{C}\mathrm{e}^{\frac{-i}{\hbar}\int_\gamma \mathrm{d}z\,[\hat{H}_0]_z}\big[\hat{H}_{\text{int}}\big]_{z'_1}\dots\hat{H}_{\text{ext}}(z''_m)\big[\hat{\psi}(\mathbf{r}_1)\big]_{z_1}\big[\hat{\psi}^\dagger(\mathbf{r}_2)\big]_{z_2}\Big]$$
$$G_0(\mathbf{r}_1,\mathbf{r}_2;z_1,z_2) = \frac{-i}{\hbar}\frac{1}{Z_0}\mathrm{tr}\Big[\mathcal{T}_\mathrm{C}\mathrm{e}^{\frac{-i}{\hbar}\int_\gamma \mathrm{d}z\,[\hat{H}_0]_z}\big[\hat{\psi}(\mathbf{r}_1)\big]_{z_1}\big[\hat{\psi}^\dagger(\mathbf{r}_2)\big]_{z_2}\Big]$$

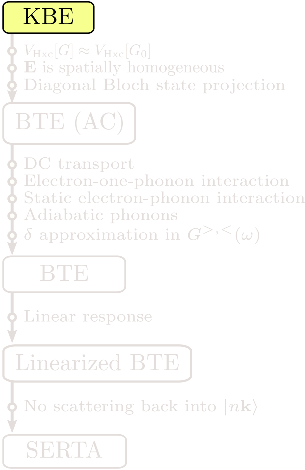
Express $\hat{H}$ in $\hat{\psi}$ $\rightarrow$ Wick's theorem to write G as products of G_0 and then solve the expansion with Feynman diagram $\rightarrow$ Dyson's eq:

$$G(1,2) = G_0(1,2) + \int_\gamma \mathrm{d}3 \int_\gamma \mathrm{d}4\, G_0(1,3)\Sigma[G](3,4)G(4,2)$$
$$1 \equiv (\mathbf{r}_1, z_1)$$

Using Langreth rules, G_0^{-1}, explicit $\hat{H}_0$ and evaluating Dyson at equal time $\rightarrow G^<$ in the limit $t_0 \rightarrow -\infty$:

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}G^<(\mathbf{r}_1,\mathbf{r}_2;t,t) = {} & \left[h_0(\mathbf{r}_1,-i\hbar\nabla_1) - h_0(\mathbf{r}_2,+i\hbar\nabla_2)\right]G^<(\mathbf{r}_1,\mathbf{r}_2;t,t) \\
& + \int \mathrm{d}^3r_3\left[\Sigma^\delta(\mathbf{r}_1,\mathbf{r}_3;t)G^<(\mathbf{r}_3,\mathbf{r}_2;t,t) - G^<(\mathbf{r}_1,\mathbf{r}_3;t,t)\Sigma^\delta(\mathbf{r}_3,\mathbf{r}_2;t)\right] \\
& + \int_{-\infty}^{t}\mathrm{d}t'\int \mathrm{d}^3r_3\Big[\Sigma^>(\mathbf{r}_1,\mathbf{r}_3;t,t')G^<(\mathbf{r}_3,\mathbf{r}_2;t',t) \\
& + G^<(\mathbf{r}_1,\mathbf{r}_3;t,t')\Sigma^>(\mathbf{r}_3,\mathbf{r}_2;t',t) \\
& - \Sigma^<(\mathbf{r}_1,\mathbf{r}_3;t,t')G^>(\mathbf{r}_3,\mathbf{r}_2;t',t) - G^>(\mathbf{r}_1,\mathbf{r}_3;t,t')\Sigma^<(\mathbf{r}_3,\mathbf{r}_2;t',t)\Big]
\end{aligned}
$$

- Unperturbed time-evolution of $G^<$ in static $V(\mathbf{r})$
- Local time self-energy
- Internal dynamical correlations (collisions, scattering)



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

We consider electrons in a solid and choose:

$$h_0(\mathbf{r}, -i\hbar\nabla) = \frac{-\hbar^2\nabla^2}{2m} + V_{\text{lat+Hxc}}(\mathbf{r})$$

$$\rightarrow [h_0(\mathbf{r}_1, -i\hbar\nabla_1) - h_0(\mathbf{r}_2, +i\hbar\nabla_2)]\, G^{<}(\mathbf{r}_1, \mathbf{r}_2; t, t) = 0$$

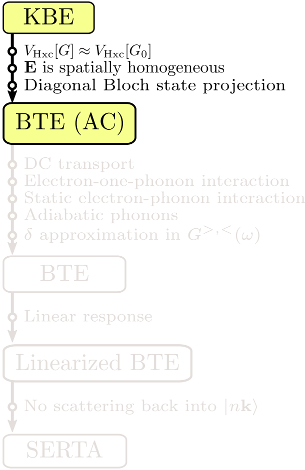
By expanding the Bloch WF in plane waves and taking the diagonal elements we have:

$$\int \mathrm{d}^3 r_3 \left[\Sigma^{\delta}(\mathbf{r}_1, \mathbf{r}_3; t) G^{<}(\mathbf{r}_3, \mathbf{r}_2; t, t) - G^{<}(\mathbf{r}_1, \mathbf{r}_3; t, t)\Sigma^{\delta}(\mathbf{r}_3, \mathbf{r}_2; t)\right]$$

$$\approx -e\mathbf{E}(t) \cdot \frac{1}{\hbar}\frac{\partial f^{<}_{n\mathbf{k}}}{\partial \mathbf{k}}(t, t)$$

where

$$\mp \frac{i}{\hbar} f^{>,<}_{n\mathbf{k}}(t, t') \equiv \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2\, \varphi^{*}_{n\mathbf{k}}(\mathbf{r}_1) G^{>,<}(\mathbf{r}_1, \mathbf{r}_2; t, t') \varphi_{n\mathbf{k}}(\mathbf{r}_2)$$



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

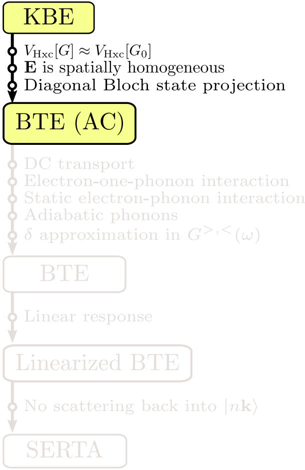
$$\frac{\partial f^{<}_{n\mathbf{k}}}{\partial t}(t,t) - e\mathbf{E}(t)\cdot\frac{1}{\hbar}\frac{\partial f^{<}_{n\mathbf{k}}}{\partial \mathbf{k}}(t,t) = -\Gamma^{(\mathrm{co})}_{n\mathbf{k}}(t)$$

where the *collision rate* is defined as:

$$\Gamma^{(\mathrm{co})}_{n\mathbf{k}}(t) \equiv \int_{-\infty}^{t} \mathrm{d}t' \, \Big[\Gamma^{>}_{n\mathbf{k}}(t,t') f^{<}_{n\mathbf{k}}(t',t) + f^{<}_{n\mathbf{k}}(t,t')\Gamma^{>}_{n\mathbf{k}}(t',t) - \Gamma^{<}_{n\mathbf{k}}(t,t') f^{>}_{n\mathbf{k}}(t',t) - f^{>}_{n\mathbf{k}}(t,t')\Gamma^{<}_{n\mathbf{k}}(t',t)\Big]$$

and

$$\mp i\hbar\Gamma^{>,<}_{n\mathbf{k}}(t,t') \equiv \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \, \varphi^{*}_{n\mathbf{k}}(\mathbf{r}_1)\Sigma^{>,<}(\mathbf{r}_1,\mathbf{r}_2;t,t')\varphi_{n\mathbf{k}}(\mathbf{r}_2)$$

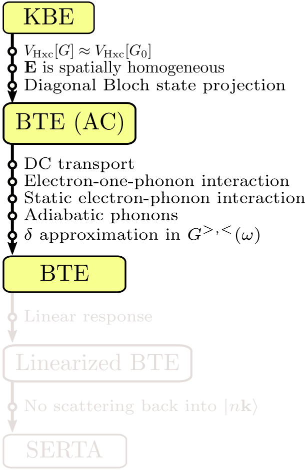


S. Poncé *et al.*,
Rep. Prog. Phys. **83**, 036501 (2020)

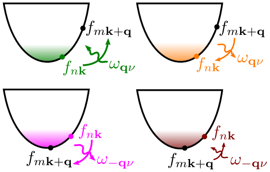
For time-independent $\mathbf{E}$ (DC) we can do a FT:

$$-e\mathbf{E}\cdot\frac{1}{\hbar}\frac{\partial f_{n\mathbf{k}}}{\partial\mathbf{k}} = -\int\frac{\mathrm{d}\omega}{2\pi}\Big[f^{<}_{n\mathbf{k}}(\omega)\Gamma^{>}_{n\mathbf{k}}(\omega) - f^{>}_{n\mathbf{k}}(\omega)\Gamma^{<}_{n\mathbf{k}}(\omega)\Big]$$

$$f_{n\mathbf{k}} \equiv \int\frac{\mathrm{d}\omega}{2\pi} f^{<}_{n\mathbf{k}}(\omega) \quad \leftarrow \text{occupation function}$$



Approximate the self-energy:



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

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

The electron-phonon matrix element

(Lecture Tue.1)

Variation of the Kohn-Sham potential

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} | u_{n\mathbf{k}} \rangle_{\mathrm{uc}}$$

Lattice-periodic part of wavefunction

Incommensurate modulation

$$\Delta_{\mathbf{q}\nu} v_{\mathrm{SCF}} = \sum_{\kappa\alpha p} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_p)} \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}}}\, e_{\kappa\alpha,\nu}(\mathbf{q}) \frac{\partial V_{\mathrm{SCF}}(\mathbf{r})}{\partial \tau_{\kappa\alpha p}}$$

Zero-point amplitude

Phonon polarization

Displacement of a single ion

κ Atom in the unit cell
α Cartesian direction
p Unit cell in the equivalent supercell

KBE
- $V_{\mathrm{Hxc}}[G] \approx V_{\mathrm{Hxc}}[G_0]$
- $\mathbf{E}$ is spatially homogeneous
- Diagonal Bloch state projection

BTE (AC)
- DC transport
- Electron-one-phonon interaction
- Static electron-phonon interaction
- Adiabatic phonons
- δ approximation in $G^{>,<}(\omega)$

BTE
- Linear response

Linearized BTE
- No scattering back into $|n\mathbf{k}\rangle$

SERTA

F. Giustino,
Rev. Mod. Phys. **89**, 015003 (2017)

Macroscopic average of the current density is

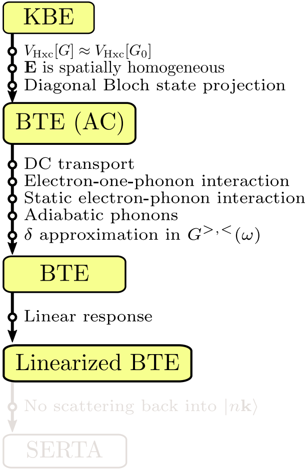
$$\mathbf{J}_{\mathrm{M}}(\mathbf{E}) = \frac{-e\hbar^2}{2m}\frac{1}{V}\int \mathrm{d}^3 r \lim_{\mathbf{r}_2\to\mathbf{r}_1}(\nabla_2 - \nabla_1)G^{<}(\mathbf{r}_1,\mathbf{r}_2;t,t;\mathbf{E})$$
$$= \frac{-e}{V_{\mathrm{uc}}}\sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}}\,\mathbf{v}_{n\mathbf{k}}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

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

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

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

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

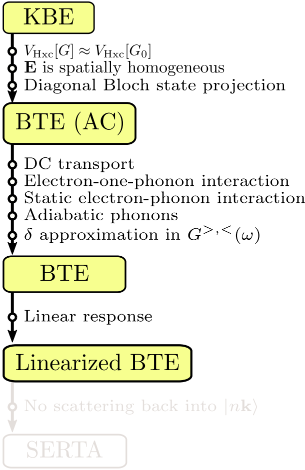
where

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

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

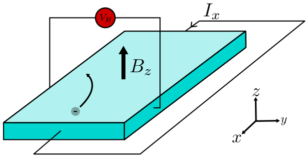
where the scattering rate is:

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



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

`bfieldz = 1.0d-10`



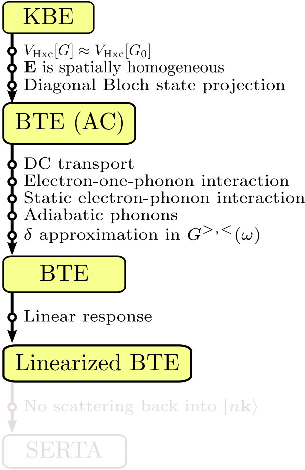
$$\mu^{\mathrm{H}}_{\alpha\beta\gamma} = \frac{-e}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma)$$

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:

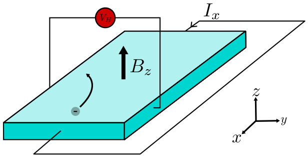
$$\mu^{\mathrm{H}}_{\alpha\beta\gamma} = r^{\mathrm{H}}_{\alpha\beta\gamma}\mu^{\mathrm{d}}_{\alpha\beta}$$
$$r^{\mathrm{H}}_{\alpha\beta\gamma} \equiv \sum_{\delta\epsilon} \frac{(\mu^{\mathrm{d}}_{\alpha\delta})^{-1}\, \mu^{\mathrm{H}}_{\delta\epsilon\gamma}\, (\mu^{\mathrm{d}}_{\epsilon\beta})^{-1}}{B_\gamma},$$



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

Self energy relaxation time approximation

`scattering_serta = .true.`



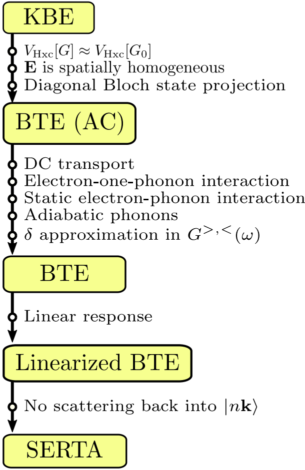
$$\mu^{\mathrm{H}}_{\alpha\beta\gamma} = \frac{-e}{V_{\mathrm{uc}} n_{\mathrm{c}}} \sum_n \int \frac{\mathrm{d}^3 k}{\Omega_{\mathrm{BZ}}} v^{\alpha}_{n\mathbf{k}} \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma)$$

BTE:

$$\left[1 - \frac{e}{\hbar} \tau_{n\mathbf{k}} (\mathbf{v}_{n\mathbf{k}} \times \mathbf{B}) \cdot \nabla_{\mathbf{k}} \right] \partial_{E_\beta} f_{n\mathbf{k}}(B_\gamma) = e v^{\beta}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \tau_{n\mathbf{k}}$$

Linked with the imaginary part of the electron-phonon self-energy:

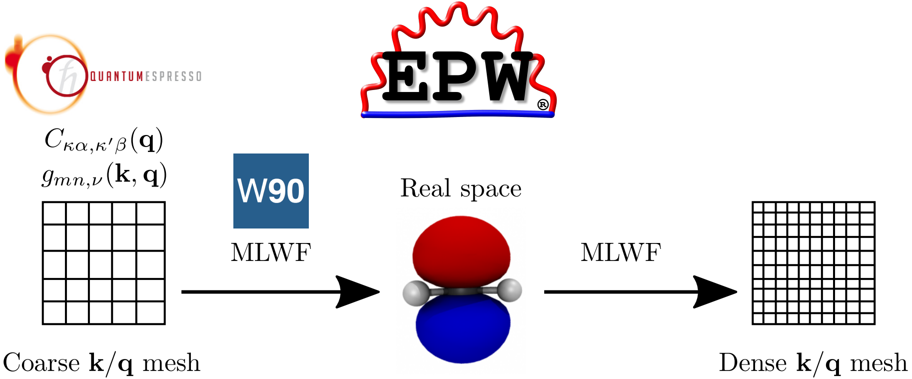
$$\tau_{n\mathbf{k}} = \frac{1}{2 \Im \Sigma_{n\mathbf{k}}}$$



S. Poncé *et al.*,
Phys. Rev. B **97**, 121201 (2018)

Electron-phonon interpolation

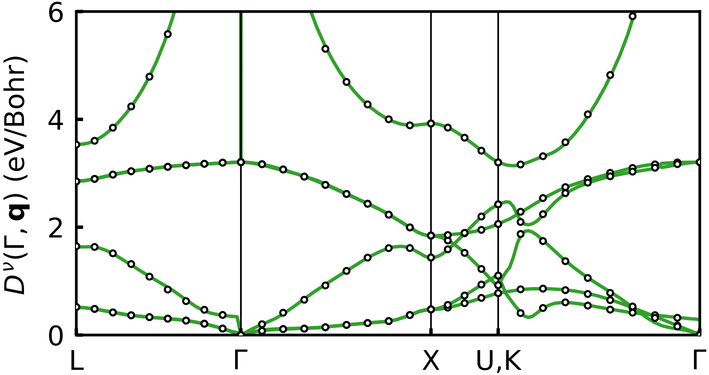
EPW relies on Maximally Localized Wannier Function to interpolate electron-phonon matrix elements.



S. Poncé *et al.*, Comp. Phys. Commun. **209**, 116 (2016)

Deformation potential of c-BN

$$D^{\nu}(\Gamma,\mathbf{q}) = \frac{1}{\hbar N_{\mathrm{w}}}\left[2\rho V_{\mathrm{uc}}\hbar\omega_{\mathbf{q}\nu}\sum_{nm}|g_{mn\nu}(\Gamma,\mathbf{q})|^2\right]^{1/2}$$



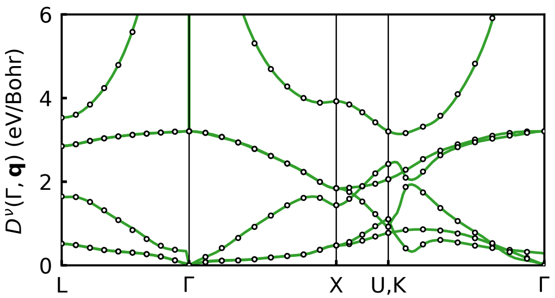
S. Poncé *et al.*, arXiv:2105.04192 (2021)

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

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

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

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)

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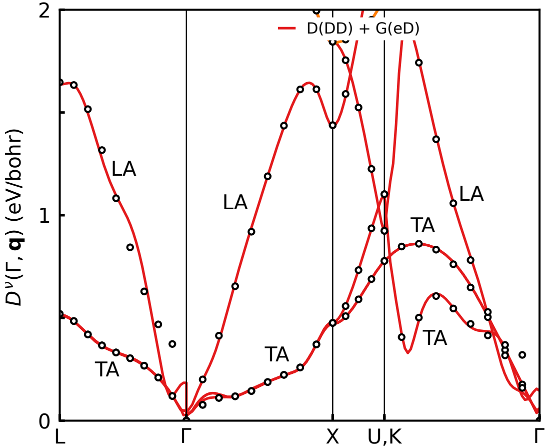
$$g^{\mathcal{L},\mathrm{D}}_{mn\nu}(\mathbf{k},\mathbf{q}) = i\frac{4\pi}{V_{\mathrm{uc}}}\frac{e^2}{4\pi\varepsilon^0}\sum_{\kappa}\left[\frac{\hbar}{2N_{p'}M_\kappa\omega_{\mathbf{q}\nu}}\right]^{\frac{1}{2}}\sum_{\mathbf{G}\neq-\mathbf{q}} \times \frac{(\mathbf{G}+\mathbf{q})\cdot\mathbf{Z}^*_\kappa\cdot\mathbf{e}_{\kappa\mathbf{q}\nu}}{(\mathbf{G}+\mathbf{q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

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

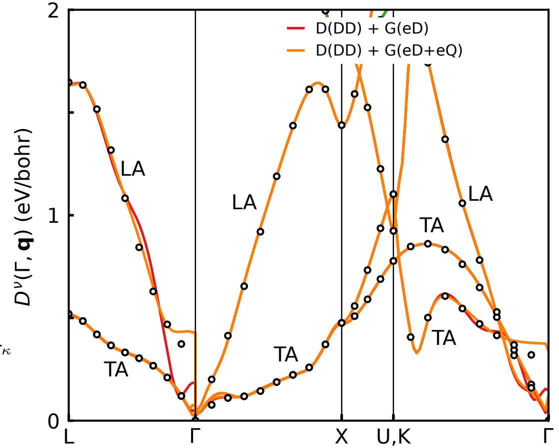
`quadrupole.fmt`

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

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

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

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

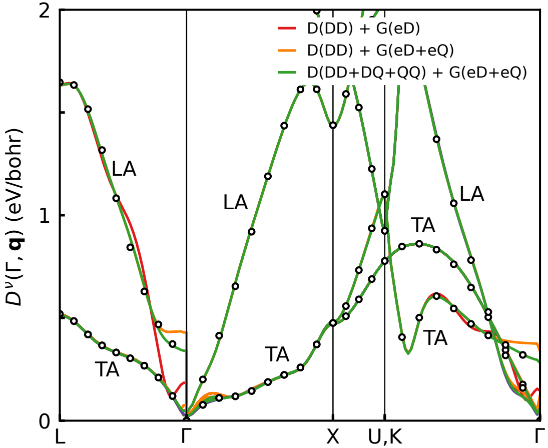


C. Verdi *et al.*, Phys. Rev. Lett. **115**, 176401 (2015)
J. Sjakste *et al.*, Phys. Rev. B **92**, 054307 (2015)
G. Brunin *et al.*, Phys. Rev. Lett. **125**, 136601 (2020)
V.A. Jhalani *et al.*, Phys. Rev. Lett. **125**, 136602 (2020)

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

Long-range interaction: dynamical matrix

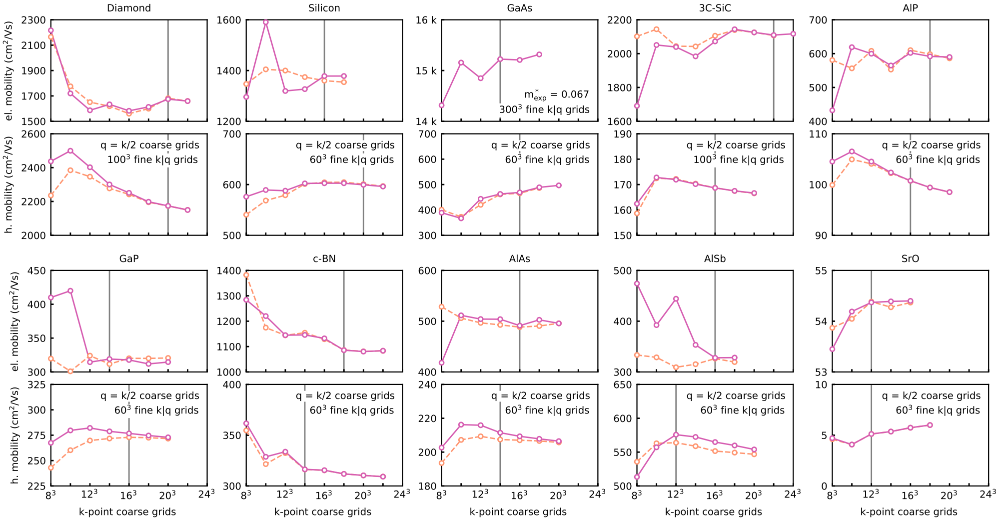
$$D^{\mathcal{L},\mathrm{D+Q}}_{\kappa\alpha,\kappa'\beta}(\mathbf{q}) = \frac{e^{i\mathbf{q}\cdot(\boldsymbol{\tau}_\kappa - \boldsymbol{\tau}_{\kappa'})} e^{\frac{-\mathbf{q}\cdot\boldsymbol{\varepsilon}^\infty\cdot\mathbf{q}}{4\Lambda^2}}}{\mathbf{q}\cdot\boldsymbol{\varepsilon}^\infty\cdot\mathbf{q}}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



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

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

Mobility convergece with coarse BZ grids

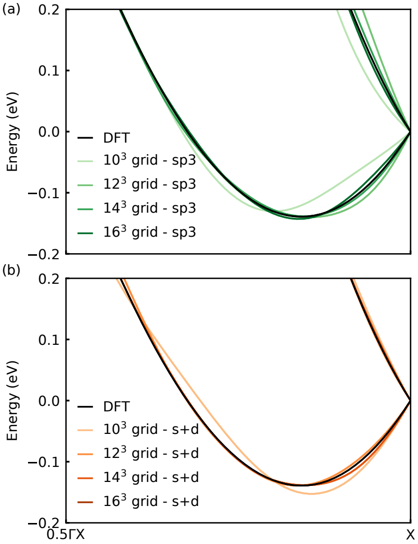


S. Poncé *et al.*, arXiv:2105.04192 (2021)

Convergence of Wannier functions

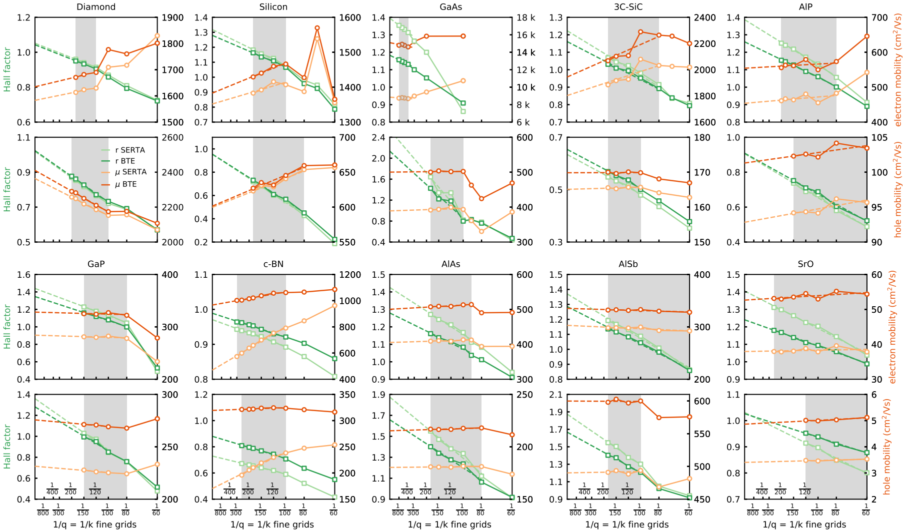
Slower convergence of Wannier function when:

- CBM/VBM not at a high symmetry point
- SOC is used
- conduction manifold only is Wannierized
- Ex: CB of silicon with SOC



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

Mobility convergence with fine BZ grids



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

Gaussian or adaptative smearings - [c-BN]

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

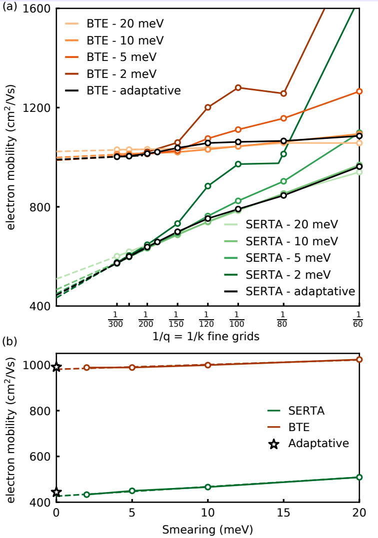
Adaptative broadening:

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

where the phonon velocity is:

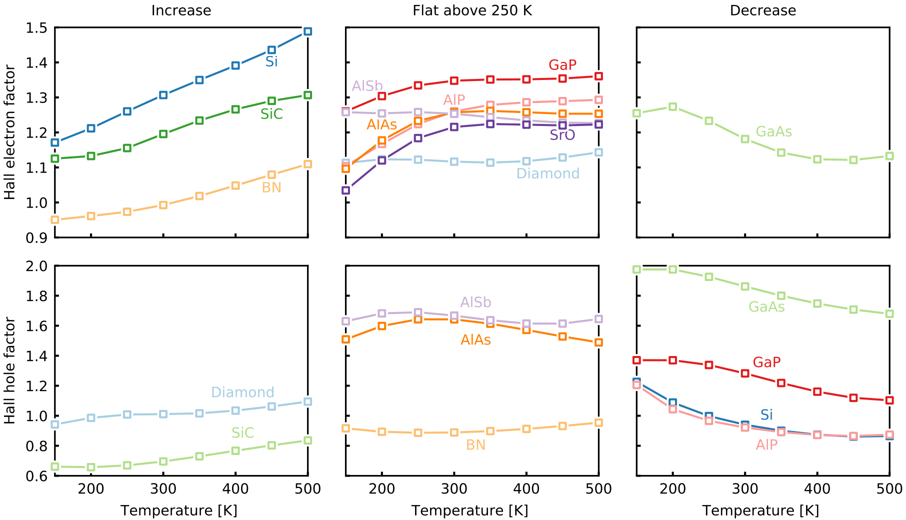
$$v_{\mathbf{q}\mu\nu\beta} = \frac{1}{2\omega_{\mathbf{q}\nu}}\frac{\partial D_{\mu\nu}(\mathbf{q})}{\partial q_\beta} = \frac{1}{2\omega_{\mathbf{q}\nu}}\sum_{\mathbf{R}} iR_\beta e^{i\mathbf{q}\cdot\mathbf{R}}D_{\mu\nu}(\mathbf{R}).$$

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



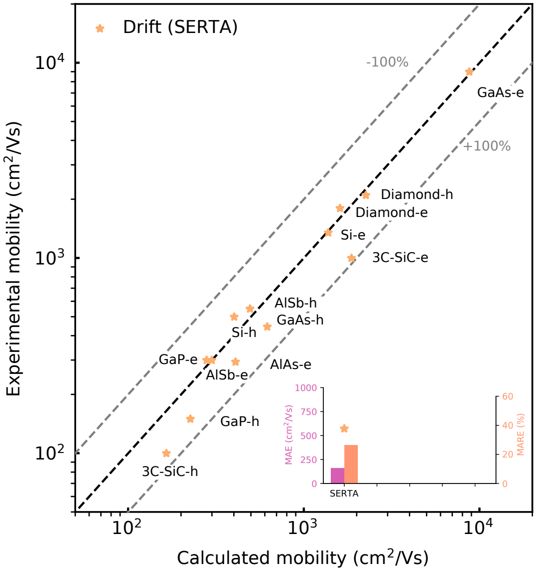
S. Poncé *et al.*, arXiv:2105.04192 (2021)

Hall factor is not unity



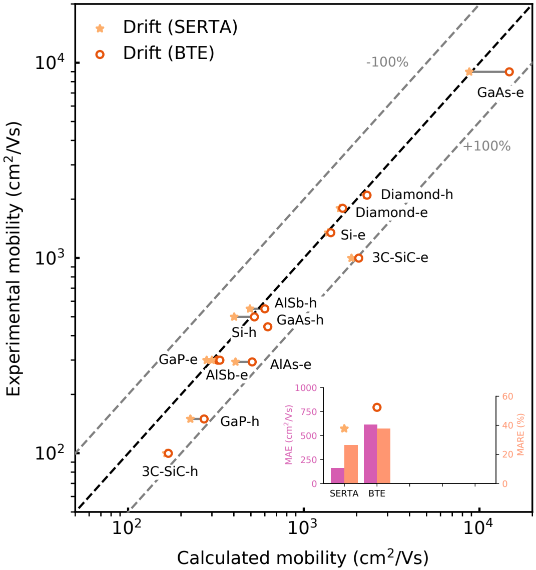
S. Poncé *et al.*, arXiv:2105.04192 (2021)

Experimental comparison



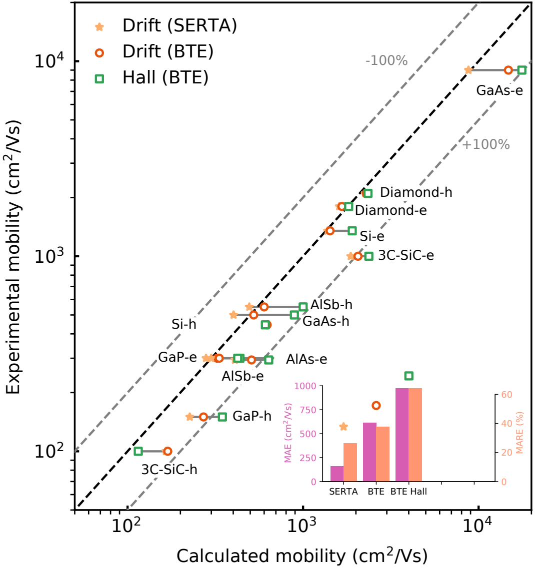
S. Poncé *et al.*,
arXiv:2105.04192 (2021)

Experimental comparison

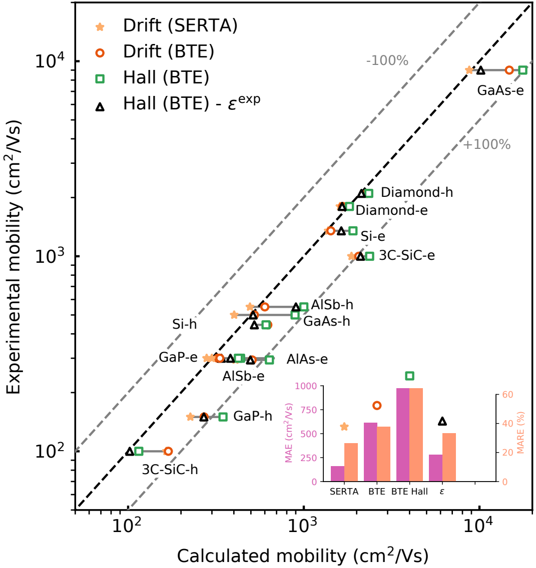


S. Poncé *et al.*,
arXiv:2105.04192 (2021)

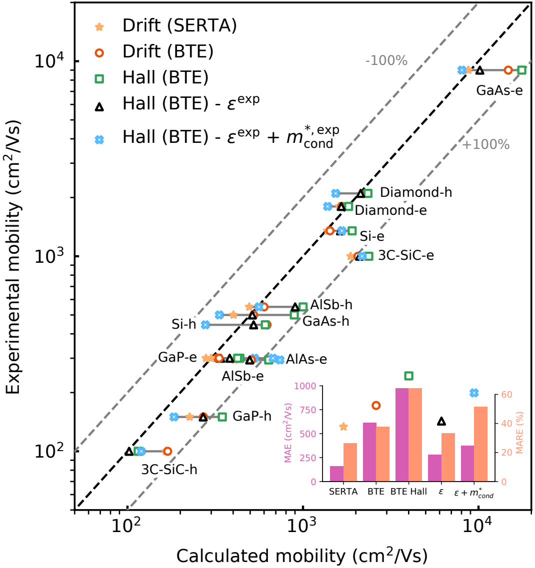
Experimental comparison



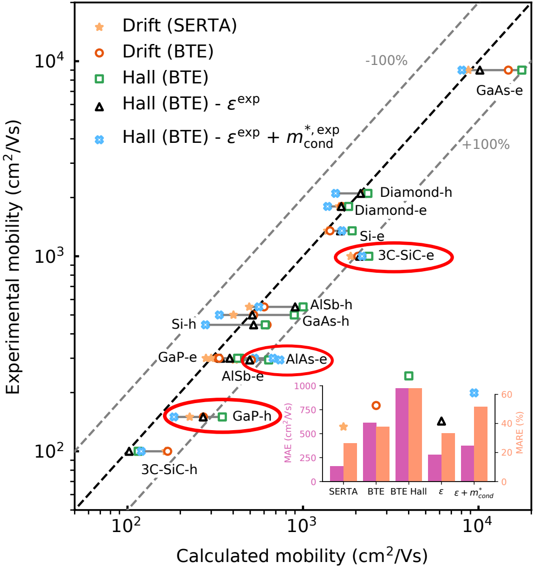
S. Poncé *et al.*,
arXiv:2105.04192 (2021)



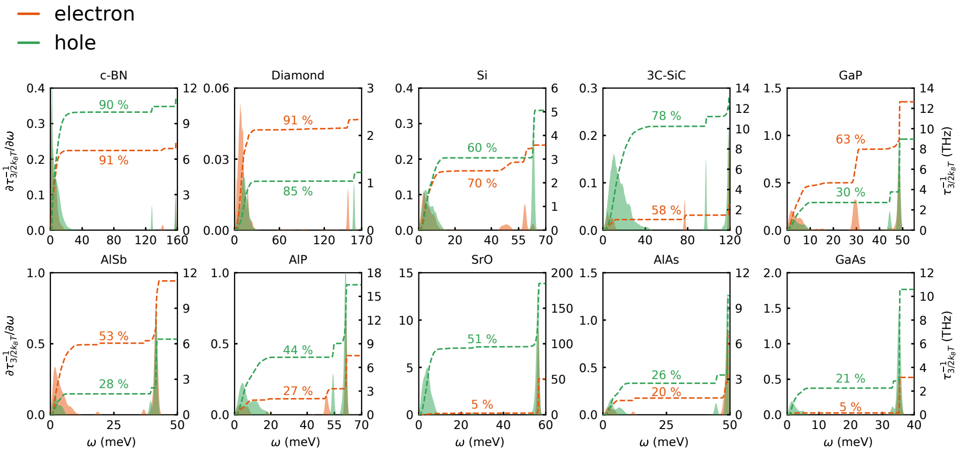
S. Poncé *et al.*,
arXiv:2105.04192 (2021)



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

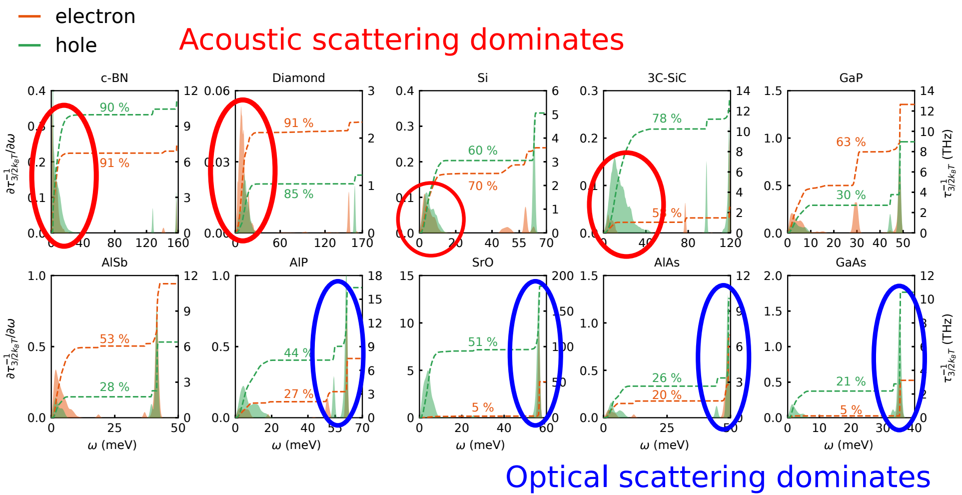


S. Poncé *et al.*,
arXiv:2105.04192 (2021)



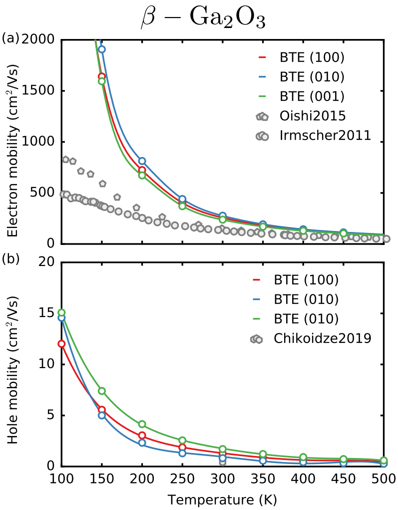
S. Poncé *et al.*, arXiv:2105.04192 (2021)

Spectral decomposition: dominant scattering



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

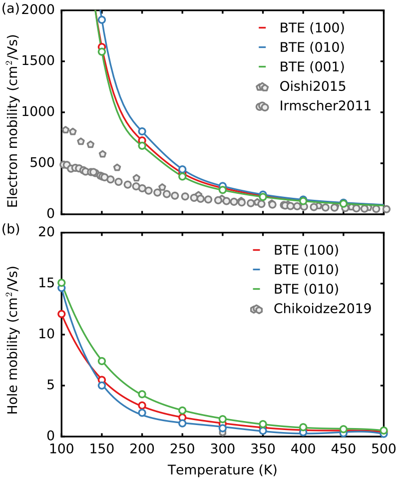
Examples of mobility with T done with EPW



S. Poncé *et al.*,
Phys. Rev. Res. **2**, 033102 (2020)

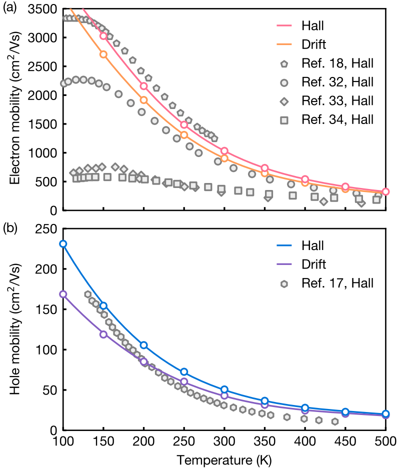
Examples of mobility with T done with EPW

$\beta - Ga_2O_3$



S. Poncé *et al.*,
Phys. Rev. Res. **2**, 033102 (2020)

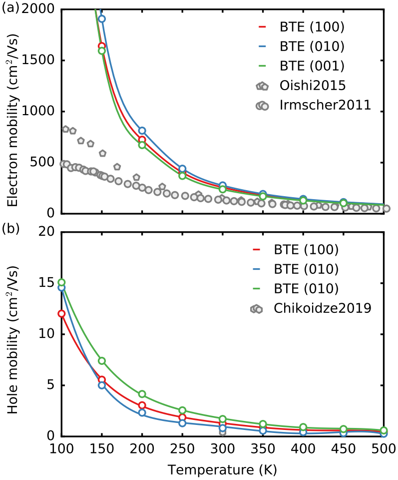
w-GaN



S. Poncé *et al.*,
Phys. Rev. Lett. **123**, 096602 (2019)

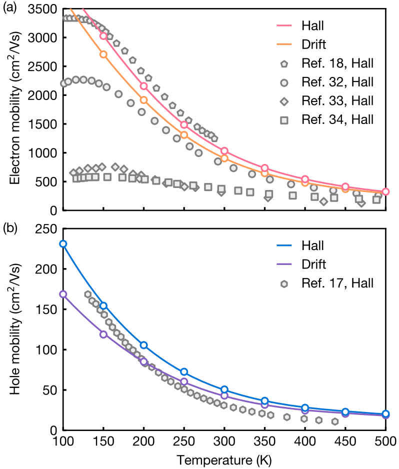
Examples of mobility with T done with EPW

$\beta - Ga_2O_3$



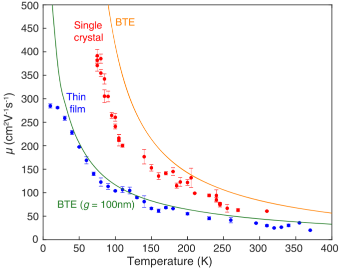
S. Poncé *et al.*,
Phys. Rev. Res. **2**, 033102 (2020)

w-GaN



S. Poncé *et al.*,
Phys. Rev. Lett. **123**, 096602 (2019)

$CH_3NH_3PbI_3$



C.Q. Xia *et al.*,
J. Phys. Chem. Lett. **12**, 3607 (2021)

`assume_metal = .true.`

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

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

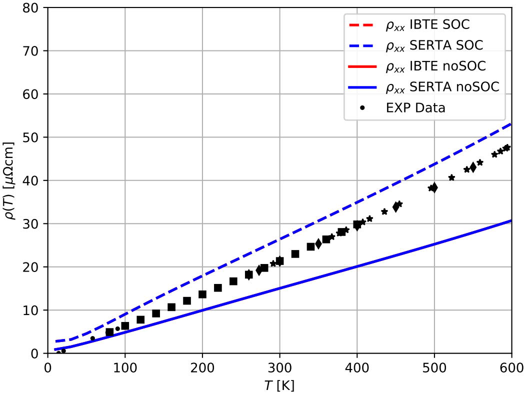


Figure courtesy of Félix Goudreault

Brooks-Herring model for impurity scattering

Semi-empirical Brooks-Herring model for the hole of silicon:

$$\mu_{\mathrm{i}} = \frac{2^{7/2}\epsilon_s^2 (k_{\mathrm{B}}T)^{3/2}}{\pi^{3/2} e^3 \sqrt{m_d^*}\, n_{\mathrm{i}} G(b)} \quad \left[\frac{\mathrm{cm}^2}{\mathrm{Vs}}\right],$$

where $G(b) = \ln(b+1) - b/(b+1)$, $b = 24\pi m_d^* \epsilon_s (k_{\mathrm{B}}T)^2 / e^2 h^2 n'$, and $n' = n_{\mathrm{h}}(2 - n_{\mathrm{h}}/n_{\mathrm{i}})$.
Here $m_d^* = 0.55 m_0$ is the silicon hole density-of-state effective mass.

H. Brooks, Phys. Rev. **83**, 879 (1951)
S. S. Li *et al.*, Solid-State Electronics **20**, 609 (1977)

Brooks-Herring model for impurity scattering

Because the electron mass is anisotropic in silicon, we used the Long-Norton model:

$$\mu_{\mathrm{i}}^{\mathrm{LN}} = \frac{7.3 \cdot 10^{17} T^{3/2}}{n_i G(b)} \quad \left[\frac{\mathrm{cm}^2}{\mathrm{Vs}}\right],$$

The mobility total phonon (μ_l) and impurity (μ_i) mobility is:

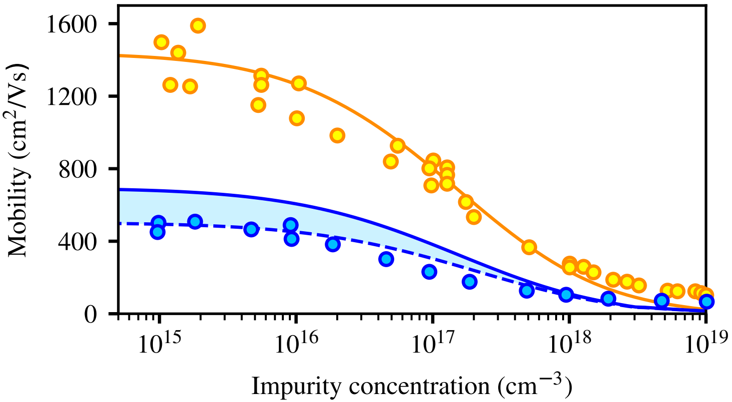
$$\mu = \mu_l \Big[1 + X^2 \{\mathsf{ci}(X)\cos(X) + \sin(X)(\mathsf{si}(X) - \frac{\pi}{2})\}\Big]$$

$X^2 = 6\mu_l/\mu_i$ and ci(X) and si(X) are the cosine and sine integrals.

P. Norton *et al.*, Phys. Rev. B **8**, 5632 (1973)

Brooks-Herring model for impurity scattering

Electron and hole mobility in silicon (EPW)



S. Poncé *et al.*, Phys. Rev. B **97**, 121201 (2018)

References [books and reviews]

- S. Poncé, W. Li, S. Reichardt and F. Giustino, Rep. Prog. Phys. **83**, 036501 (2020)
- F. Giustino, Rev. Mod. Phys. **89**, 015003 (2017)
- J. M. Ziman, *Electrons and Phonons*, Oxford (1960)
- L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Benjamin (1962)
- G. Grimvall, *The electron-phonon interaction in metals*, North-Holland (1981)
- G. D. Mahan, *Many-Particle Physics*, Springer (2000)
- M. Lundstrom, *Fundamentals of Carrier Transport*, Cambridge (2000)
- S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Supplemental Slides

A supplemental slide

Some extra information.