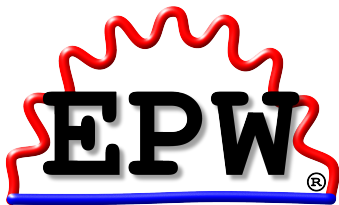


UK Thermoelectric Network Meeting

Kings College London, 1-2 May 2019



Electronic transport and the EPW software

Samuel Poncé

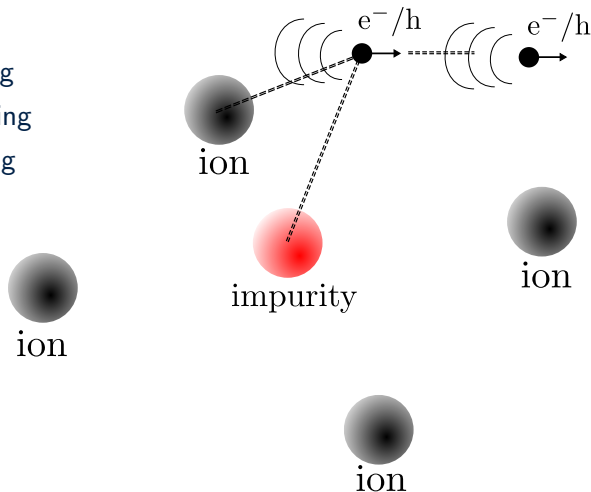
Department of Materials, University of Oxford

Lecture Summary

- Carrier transport
- Quantum Boltzmann equation
- Semiclassical linearized Boltzmann transport equation
- Mobility in real materials
- EPW in a nutshell

Carrier transport

- Lattice scattering
- Impurity scattering
- Ionized scattering



Carrier transport: experimental evidence

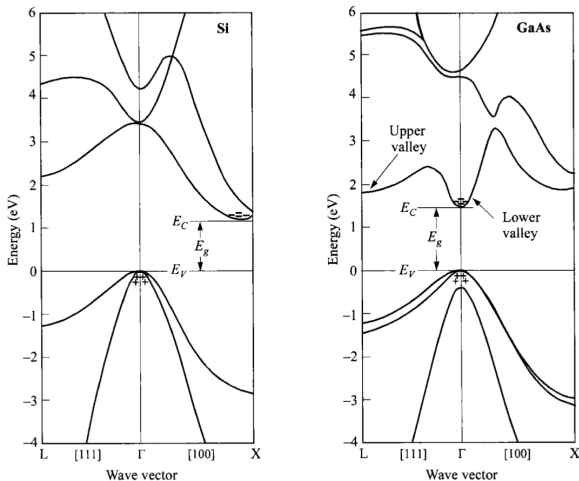
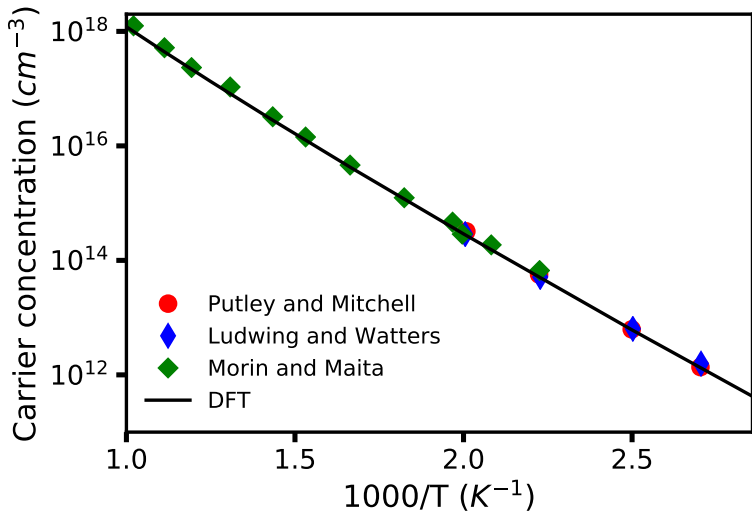
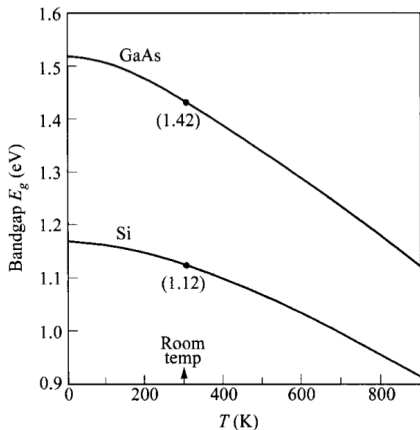


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidence



Carrier transport: experimental evidence



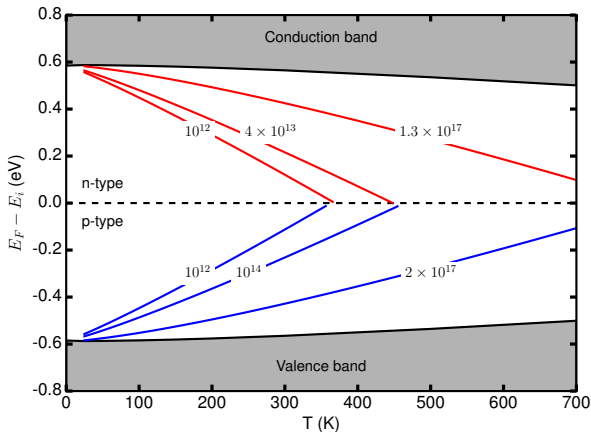
	$E_g(0)$ (eV)	α (eV/K)	β (K)
GaAs	1.519	5.4×10^{-4}	204
Si	1.169	4.9×10^{-4}	655

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

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

Carrier transport

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



Carrier transport: experimental evidence

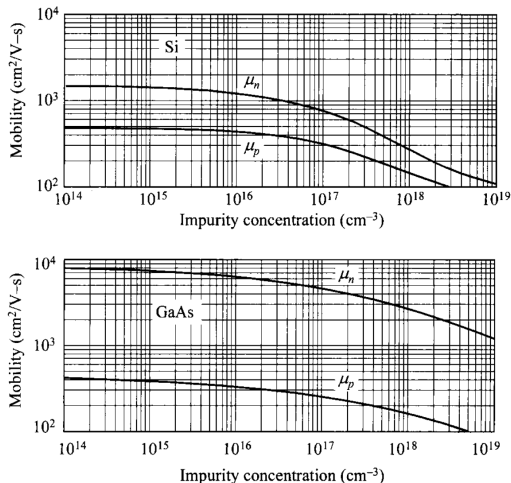


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidence

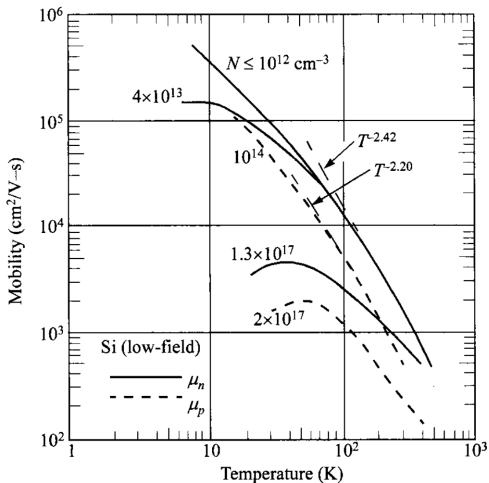


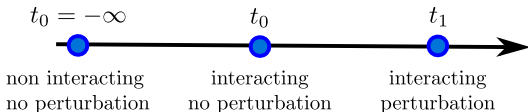
Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Quantum theory of mobility (Heisenberg picture)

Fermion current density

$$j(1) = -\frac{e\hbar^2}{2m} \lim_{2 \rightarrow 1} (\nabla_2 - \nabla_1) G^<(1, 2)$$
$$G^<(1, 2) = \frac{i}{\hbar} \langle \hat{\psi}^\dagger(2) \hat{\psi}(1) \rangle,$$

- $(1) = (\mathbf{r}_1 t_1)$
- $\hat{\psi}$ are field operators



- ${}_0 \langle \cdots \rangle_0 = \frac{1}{Z} \text{Tr} \left[e^{-\beta \hat{H}(t_0 = -\infty)} \right]$ a GS average over the non interacting system
- $\langle \cdots \rangle = \frac{1}{Z} \text{Tr} \left[e^{-\beta \hat{H}(t_0)} \right]$ an average over the interacting system

Quantum theory of mobility (interaction representation)

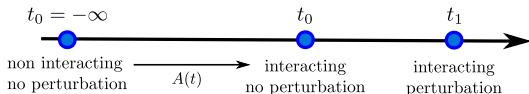
Under an external field $U(1)$ (perturbation), the $\hat{H}$ for EOM can be split into a non-interacting and interacting H :

$$\hat{H}(t) = \hat{H}^0(t) + \hat{H}'(t)$$

$$\hat{H}^0(t) = \int d^3\mathbf{r}_1 \hat{\psi}^\dagger(\mathbf{r}_1) \left[\frac{-\hbar^2}{2m} \nabla_1^2 + U(1) \right] \hat{\psi}(\mathbf{r}_1)$$

$$\hat{H}'(t) = \frac{A(t)}{2} \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1)$$

$A(t)$ is an adiabatic factor.



Time-evolution operators ($t_1 > t_0$)

Interacting and non-interacting time-evolution operators:

$$\hat{U}(t_1, t_0) \triangleq T \exp \left[\frac{-i}{\hbar} \int_{t_0}^{t_1} dt_2 \hat{H}(t_2) \right]$$
$$\hat{U}^0(t_1, t_0) \triangleq T \exp \left[\frac{-i}{\hbar} \int_{t_0}^{t_1} dt_2 \hat{H}^0(t_2) \right]$$

The operators obey Schrödinger EOM:

$$i\hbar \frac{\partial \hat{U}(t_1, t_0)}{\partial t_1} = \hat{H}(t_1) \hat{U}(t_1, t_0).$$

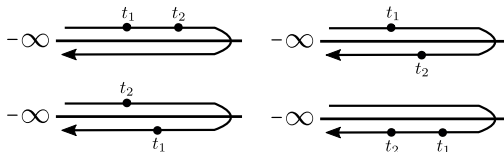
The scattering matrix time-propagate from non-interacting to interacting H:

$$\hat{S}(t_1, t_0) \triangleq \hat{U}^0(t_0, t_1) \hat{U}(t_1, t_0) = T \exp \left[\frac{-i}{\hbar} \int_{t_0}^{t_1} dt_2 \hat{H}'(t_2) \right].$$

Time-loop contour

$$\hat{\psi}(1) = \hat{U}(t_1, t_0) \hat{\psi}(\mathbf{r}_1 t_0)$$

$$\hat{\psi}(1) \hat{\psi}^\dagger(2) = \hat{U}(t_0, t_1) \hat{\psi}(\mathbf{r}_1 t_0) \hat{U}(t_1, t_2) \hat{\psi}^\dagger(\mathbf{r}_2 t_0) \hat{U}^\dagger(t_2, t_0)$$



The real time-loop allows to write the time-ordered Green's function in terms of its GS:

$$G(1^C, 2^C) = -\frac{i}{\hbar} \frac{{}_0 \langle T^C \hat{S}^C \psi(1^C) \psi^\dagger(2^C) \rangle_0}{{}_0 \langle \hat{S}^C \rangle_0}$$

$$\hat{S}^C(t_1^C, t_0^C) \triangleq T^C \exp \left[\frac{-i}{\hbar} \int_{t_0^C}^{t_1^C} dt^C \hat{H}'(t^C) \right]$$

J. Schwinger, J. Math. Phys. **2** 407 (1961)

L. V. Keldysh, Sov. Phys. JETP **20**, 1018 (1965)

Dyson on time loop

To evaluate G we

- Taylor expansion to infinite order

$$\hat{S}^C(t'^C, t^C) \triangleq T^C \exp \left[\frac{-i}{\hbar} \int_{t^C}^{t'^C} dt_1^C \hat{H}'(t_1^C) \right] =$$
$$1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} T^C \int_{t^C}^{t'^C} dt_1^C \int_{t^C}^{t_1^C} dt_2^C \dots \int_{t^C}^{t_{n-1}^C} dt_n^C \hat{H}'(t_1^C) \hat{H}'(t_2^C) \dots \hat{H}'(t_n^C)$$

- Use Wick's decomposition to factorized products of ψ into pairs of ψ in G
- Diagram pairs can be expressed as Feynman diagrams and summed to inf. order

The resulting is called Dyson's equation:

$$\left[i\hbar \frac{\partial}{\partial t_1^C} + \frac{\hbar^2}{2m} \nabla_1^2 - U(1^C) \right] G(1^C, 2^C) - \int d3^C \Sigma(1^C, 3^C) G(3^C, 2^C) = \delta(1^C, 2^C)$$

- Σ is the self-energy which contains the infinite series of distinct diagrams
- Dyson is useful **if we can approximate** Σ by its lowest orders (weak coupling)

F. J. Dyson, Phys. Rev. **75**, 1736 (1949)

G. C. Wick, Phys. Rev. **80**, 268 (1950)

Dyson on ordinary time

Transform Dyson back on ordinary time line $t \in [-\infty, \infty]$ by using a 2×2 matrix form

$$\left[i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1^2 - U(1) \right] \tilde{G}(1, 2) - \int d3 \tilde{\Sigma}(1, 3) \tilde{\tau}_3 \tilde{G}(3, 2) = \tilde{\tau}_3 \delta(1, 2),$$

where $\tilde{\tau}_i$ are Pauli matrices and

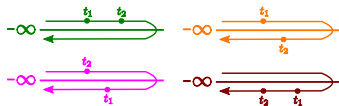
$$\tilde{G}(1, 2) = \begin{bmatrix} G^t(1, 2) & G^<(1, 2) \\ G^>(1, 2) & G^{\bar{t}}(1, 2) \end{bmatrix}$$

$$G^<(1, 2) = \frac{i}{\hbar} \langle \hat{\psi}^\dagger(2) \hat{\psi}(1) \rangle$$

$$G^>(1, 2) = \frac{-i}{\hbar} \langle \hat{\psi}(1) \hat{\psi}^\dagger(2) \rangle$$

$$G^t(1, 2) = \theta(t_1 - t_2) G^>(1, 2) + \theta(t_2 - t_1) G^<(1, 2)$$

$$G^{\bar{t}}(1, 2) = \theta(t_2 - t_1) G^>(1, 2) + \theta(t_1 - t_2) G^<(1, 2)$$



Self-energies

The self-energies are expanded to second-order:

$$\tilde{\Sigma}(1, 2) = \begin{bmatrix} \Sigma^t(1, 2) & \Sigma^<(1, 2) \\ \Sigma^>(1, 2) & \Sigma^{\bar{t}}(1, 2) \end{bmatrix}$$

$$\Sigma^t(1, 2) = \Sigma^{\text{HF}}(1, 2) + \theta(t_2 - t_1)\Sigma^>(1, 2) + \theta(t_1 - t_2)\Sigma^<(1, 2)$$

$$\Sigma^{\bar{t}}(1, 2) = -\Sigma^{\text{HF}}(1, 2) + \theta(t_1 - t_2)\Sigma^>(1, 2) + \theta(t_2 - t_1)\Sigma^<(1, 2)$$

$$\begin{aligned} \Sigma^{<, >}(1, 2) = & (i\hbar)^2 \int d3 \int d4 \bar{V}(1-3)\bar{V}(2-4) \left[G^{<, >}(1, 4)G^{>, <}(4, 3)G^{<, >}(3, 2) \right. \\ & \left. - G^{<, >}(1, 2)G^{<, >}(3, 4)G^{>, <}(4, 3) \right], \end{aligned}$$

$\bar{V}(1-2) = \delta(t_1 - t_2)V(\mathbf{r}_1 - \mathbf{r}_2)$ is the 2-body interaction that **could** contain el-ph.

HF is the diagonal first-order of the self-energy $\tilde{\Sigma}(1, 2) = \tilde{\tau}_3 \Sigma^{\text{HF}}$

$$\Sigma^{\text{HF}} = -\delta(1, 2) \int d3 \bar{V}(1-3) i\hbar G^<(3, 3) + \bar{V}(1-2) i\hbar G^<(1, 2).$$

Keldysh rotation

The component of $\tilde{G}$ are not linearly independent:

$$\tilde{G}^K(1,2) = \tilde{L}\tilde{\tau}_3\tilde{G}\tilde{L}^\dagger = \begin{bmatrix} G^R(1,2) & G^K(1,2) \\ 0 & G^A(1,2) \end{bmatrix},$$

where the rotation matrix is

$$\tilde{L} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix},$$

where the retarded, advanced and Keldysh Green's function are

$$G^R(1,2) = \theta(t_1 - t_2)[G^>(1,2) - G^<(1,2)]$$

$$G^A(1,2) = -\theta(t_2 - t_1)[G^>(1,2) - G^<(1,2)]$$

$$G^K(1,2) = G^>(1,2) + G^<(1,2).$$

same for $\tilde{\Sigma}$

J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986)

First-order gradient expansion

Wigner center-of-mass representation:

$$G(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) = \int d^3\bar{\mathbf{r}}_{12} d\bar{t}_{12} G(1, 2) e^{-i(\mathbf{k}\bar{\mathbf{r}}_{12} - \omega\bar{t}_{12})},$$

where $\mathbf{r}_{12} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $t_{12} = (t_1 + t_2)/2$, $\bar{\mathbf{r}}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ and $\bar{t}_{12} = t_1 - t_2$.

Dyson's equation

$$[G_0^{-1}(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) \tilde{\mathbf{I}} - \tilde{\Sigma}^K(\mathbf{k}\omega, \mathbf{r}_{12}t_{12})] \star \tilde{G}^K(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) = \tilde{\mathbf{I}}$$

$$G_0^{-1}(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) = \hbar\omega - \frac{\hbar^2 k^2}{2m} - U(\mathbf{r}_{12}t_{12}) \quad \leftarrow \text{non-interacting GF}$$

$$D \star E = DE + \frac{i\hbar}{2} \{D, E\} + \mathcal{O}(\hbar^2) \quad \leftarrow \text{phase-space product}$$

$$\{D, E\} = \frac{\partial D}{\partial \mathbf{r}} \frac{\partial E}{\partial \mathbf{k}} - \frac{\partial D}{\partial t} \frac{\partial E}{\partial \omega} - \frac{\partial D}{\partial \mathbf{k}} \frac{\partial E}{\partial \mathbf{r}} + \frac{\partial D}{\partial \omega} \frac{\partial E}{\partial t} \quad \leftarrow \text{Poisson bracket}$$

H. Groenewold, Physica **12**, 405 (1946)

J. E. Moyal, Math. Proc. Cam. Philo. Soc. **45**, 99124 (1949)

Coupled equation of motion

We use Wigner representation for the first-order gradient expansion approximation:

$$D \star E \approx DE + \frac{i\hbar}{2}\{D, E\}$$

Valid for system where the microscopic space and time length scale are much smaller than the macroscopic inhomogeneities of the system.

The [1,1] and [1,2] components of the Dyson equation gives

$$\begin{aligned} G^R &= [G_0^{-1} - \Sigma^R]^{-1} \\ C &= \{G_0^{-1} - \Re\Sigma^R, G^<\} - \{\Sigma^<, \Re\Sigma^R\}, \end{aligned}$$

where C is the collision matrix:

$$C = \frac{1}{\hbar}(G^>\Sigma^< - G^<\Sigma^>),$$

Quantum transport equations

$$G^R = \left[G_0^{-1} - \Sigma^R \right]^{-1}$$
$$C = \{ G_0^{-1} - \Re \Sigma^R, G^< \} - \{ \Sigma^<, \Re \Sigma^R \}$$
$$C = \frac{1}{\hbar} (G^> \Sigma^< - G^< \Sigma^>)$$

The Schwinger-Keldysh closed real-time formalism can deal with arbitrary time-dependent Hamiltonian in out-of equilibrium system while working at finite temperature through state averaging.

Approximations:

- We assume that we can adiabatically turn on the interaction
- Negligible second-order terms in the gradient expansion

T. Kita, Progress of Theoretical Physics **123**, 581 (2010)

Semiclassical Boltzmann formalism

Approximation:

- **Weak-coupling limit** $\Sigma^R = 0$

$$G^R = \left[G_0^{-1} - \Sigma^R \right]^{-1}$$

$$\{G_0^{-1} - \Re \Sigma^R, G^<\} - \{\Sigma^<, \Re \Sigma^R\} = C$$

Semiclassical Boltzmann formalism

Approximation:

- **Weak-coupling limit** $\Sigma^R = 0$

$$\begin{aligned} G^R &= G_0^R \\ \{G_0^{-1}, G^<\} &= C \end{aligned}$$

Semiclassical Boltzmann formalism

Approximation:

- **Weak-coupling limit** $\Sigma^R = 0$

$$G^R(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) = \left[\omega - \frac{k^2}{2m} - U(\mathbf{r}_{12}t_{12}) \right]^{-1}$$
$$\frac{\partial G^<}{\partial t} + \frac{\mathbf{k}}{m} \cdot \frac{\partial G^<}{\partial \mathbf{r}} + \frac{\partial U}{\partial t} \frac{\partial G^<}{\partial \omega} - \frac{\partial U}{\partial \mathbf{r}} \cdot \frac{\partial G^<}{\partial \mathbf{k}} = C$$

Semiclassical Boltzmann formalism

Approximation:

- Weak-coupling limit $\Sigma^R = 0$

$$G^R(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) = \left[\omega - \frac{k^2}{2m} - U(\mathbf{r}_{12}t_{12}) \right]^{-1}$$

$$\frac{\partial G^<}{\partial t} + \frac{\mathbf{k}}{m} \cdot \frac{\partial G^<}{\partial \mathbf{r}} + \frac{\partial U}{\partial t} \frac{\partial G^<}{\partial \omega} - \frac{\partial U}{\partial \mathbf{r}} \cdot \frac{\partial G^<}{\partial \mathbf{k}} = C$$

We define the semiclassical distribution function f :

$$f(\mathbf{k}, \mathbf{r}_{12}t_{12}) = \frac{-i\hbar}{(2\pi\hbar)^3} \int \frac{d\omega}{2\pi} G^<(\mathbf{k}\omega, \mathbf{r}_{12}t_{12})$$

which gives

$$\frac{\partial f}{\partial t} + \frac{\mathbf{k}}{m} \cdot \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial U}{\partial \mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{k}} = I$$

where $I = \int C d\omega / 2\pi$ is the collision integral.

Semiclassical Boltzmann formalism

$$\frac{\partial f}{\partial t} + \frac{\mathbf{k}}{m} \cdot \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial U}{\partial \mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{k}} = I$$

The semiclassical approximation does not stem from $\int \omega$ but from the weak-coupling approximation which allows a frequency independent function f to fulfill the quantum EOM.

Without the weak-coupling approximation, one cannot find a closed equation for f .

BTE in a crystal

Approximations:

- Homogeneous field (independent of r)
- Direct current regime (independent of t)

$$-\frac{\partial U}{\partial \mathbf{r}} \frac{\partial f_{n\mathbf{k}}}{\hbar \partial \mathbf{k}} = I_{n\mathbf{k}}$$
$$-e\mathbf{E} \frac{\partial f_{n\mathbf{k}}}{\hbar \partial \mathbf{k}} = I_{n\mathbf{k}}.$$

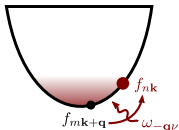
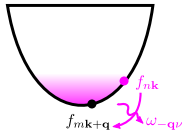
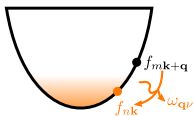
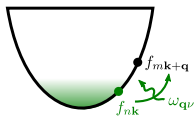
Collision integral

$$I = \int C d\omega / 2\pi$$

$$C = \frac{1}{\hbar} (G^> \Sigma^< - G^< \Sigma^>)$$

We use the local approximation of neglecting the space-time derivatives and obtain:

$$I_{n\mathbf{k}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 \left[f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) n_{\mathbf{q}\nu} \right. \\ \left. + f_{n\mathbf{k}}(1 - f_{m\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) (1 + n_{\mathbf{q}\nu}) \right. \\ \left. - (1 - f_{n\mathbf{k}}) f_{m\mathbf{k}+\mathbf{q}} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) (1 + n_{\mathbf{q}\nu}) \right. \\ \left. - (1 - f_{n\mathbf{k}}) f_{m\mathbf{k}+\mathbf{q}} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) n_{\mathbf{q}\nu} \right]$$

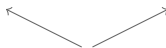


The electron-phonon matrix element

Variation of the Kohn-Sham potential



$$g_{mn,\nu}(\mathbf{k}, \mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} V | u_{n\mathbf{k}} \rangle$$



Lattice-periodic part of wavefunction

Incommensurate modulation



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

κ Atom in the unit cell

α Cartesian direction

p Unit cell in the equivalent supercell

Zero-point amplitude

Phonon polarization

Displacement of a single ion

Linearized Boltzmann transport equation

We take the derivative wrt electric field

$$\frac{\partial}{\partial E_\beta} \left[e\mathbf{E} \cdot \frac{\partial f_{n\mathbf{k}}}{\hbar \partial \mathbf{k}} \right]_{\mathbf{E}=0} = \frac{\partial I_{n\mathbf{k}}}{\partial E_\beta}$$

$$\begin{aligned} \frac{\partial}{\partial E_\beta} \left[e\mathbf{E} \cdot \frac{\partial f_{n\mathbf{k}}}{\hbar \partial \mathbf{k}} \right]_{\mathbf{E}=0} &= e \frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\beta} \\ \frac{\partial I_{n\mathbf{k}}}{\partial E_\beta} &= \tau_{n\mathbf{k}}^{-1} \partial_{E_\beta} f_{n\mathbf{k}} - \frac{2\pi}{\hbar} \sum_{m\nu\sigma} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \delta(\Delta\varepsilon_{\mathbf{k},\mathbf{q}}^{mn} + \sigma\hbar\omega_{\mathbf{q}\nu}) \\ &\quad \times [(1+\sigma)/2 - \sigma f_{n\mathbf{k}}^0 + n_{\mathbf{q}\nu}] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}} \\ \tau_{n\mathbf{k}}^{-1} &= -2\text{Im}\Sigma_{n\mathbf{k}}^{\text{R}} = \frac{2\pi}{\hbar} \sum_{m\nu\sigma} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \\ &\quad \times [(1+\sigma)/2 - \sigma f_{m\mathbf{k}+\mathbf{q}}^0 + n_{\mathbf{q}\nu}] \delta(\Delta\varepsilon_{\mathbf{k},\mathbf{q}}^{mn} - \sigma\hbar\omega_{\mathbf{q}\nu}), \end{aligned}$$

where $\sigma \pm 1$ for phonon absorption/emission and $\Delta\varepsilon_{\mathbf{k},\mathbf{q}}^{mn} = \varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}}$.

Linearized Boltzmann transport equation

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

Current density: $j(1) = -\frac{e\hbar^2}{2m} \lim_{2 \rightarrow 1} (\nabla_2 - \nabla_1) G^<(1, 2)$

$$= -\frac{e\hbar}{2} \int \frac{d(\hbar\mathbf{k})^3}{(2\pi\hbar)^3} (-2i\frac{\hbar\mathbf{k}}{m}) \int d\omega G^<(\mathbf{k}\omega, \mathbf{r}_{12}t_{12}) \leftarrow \text{Wigner transform}$$

Macro current: $J_\alpha = \int \frac{d\mathbf{r}_1}{V} j(1)$

$$= -\frac{e}{\Omega} \sum_n \frac{1}{\Omega_{\text{BZ}}} \int d\mathbf{k} f_{n\mathbf{k}} v_{n\mathbf{k},\alpha},$$

The electron drift mobility is:

$$\mu_{e,\alpha\beta}^d = \frac{\sigma_{e,\alpha\beta}}{n_e} = \left. \frac{\partial \mathbf{J}}{\partial E_\beta} \right|_{\mathbf{E}=0} = \frac{-1}{n_e \Omega} \sum_{n \in \text{CB}} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} v_{n\mathbf{k},\alpha} \partial_{E_\beta} f_{n\mathbf{k}}$$

Self energy relaxation time approximation (SERTA)

We can approximate IBTE by neglecting $\partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}$

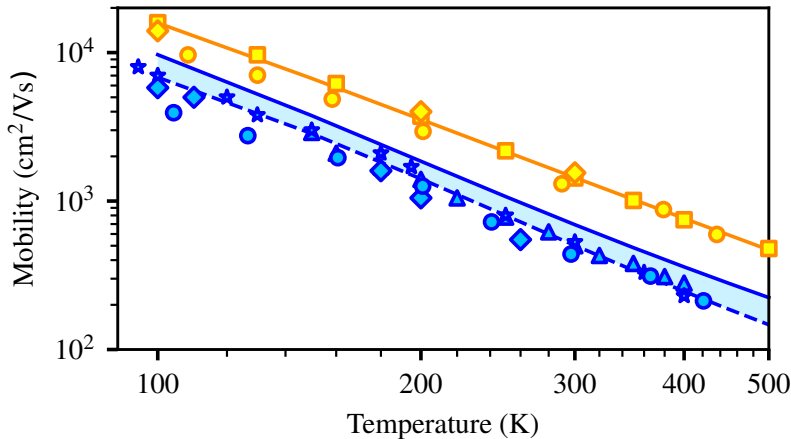
$$\partial_{E_\beta} f_{n\mathbf{k}} = e \frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\beta} \tau_{n\mathbf{k}}$$

The intrinsic electron mobility is therefore:

$$\begin{aligned} \mu_{e,\alpha\beta}^d &= - \sum_{n \in \text{CB}} \int d\mathbf{k} \, v_{n\mathbf{k},\alpha} \partial_{E_\beta} f_{n\mathbf{k}} / \sum_{n \in \text{CB}} \int d\mathbf{k} \, f_{n\mathbf{k}}^0 \\ &= \frac{-e}{n_e \Omega} \sum_{n \in \text{CB}} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} \frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\alpha} v_{n\mathbf{k},\beta} \tau_{n\mathbf{k}} \end{aligned}$$

Intrinsic carrier mobility

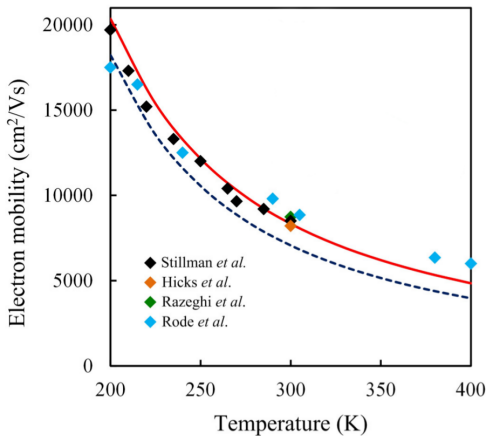
Electron and hole mobility in silicon (EPW)



S. Ponc  et al., Physical Review B **97**, 121201 (2018)

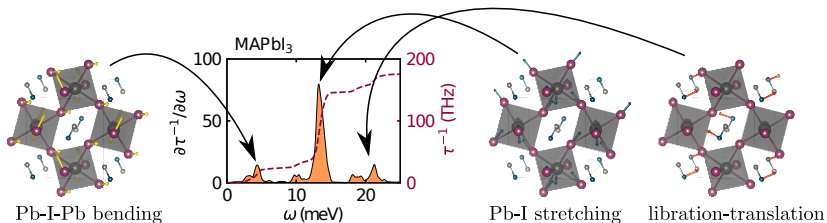
Intrinsic carrier mobility

Electron mobility in GaAs using IBTE and SERTA (dashed)



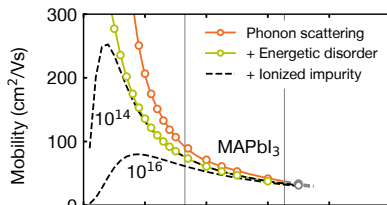
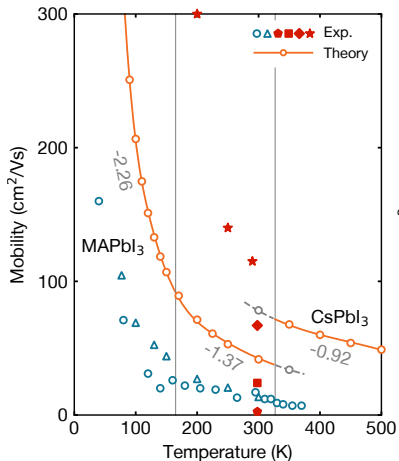
T.-H. Liu *et al.*, Phys. Rev. B **95**, 075206 (2017)

Spectral decomposition in MAPbI₃



ACS Energy Letters **4**, 456 (2019)

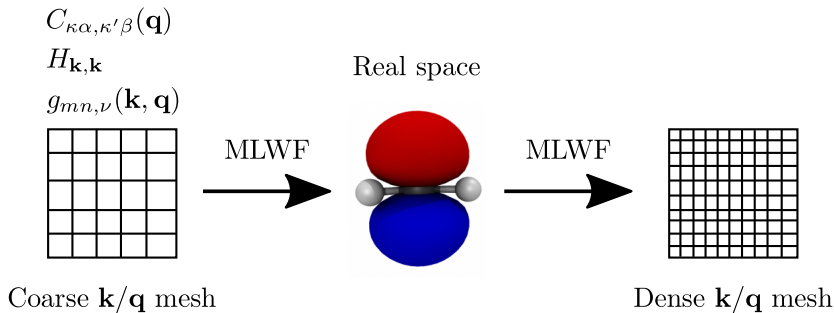
Mobility in MAPbI₃



ACS Energy Letters 4, 456 (2019)

What is EPW?

Electron-phonon Wannier (EPW) is a free GPL Fortran software, part of QE, that relies on MLWF to interpolate electron-phonon matrix elements.



What can EPW do for you



- Interpolate el-ph matrix element on ultra dense momentum grids
- Compute electron and phonon linewidths, scattering rates & lifetimes
- Electron and phonon spectral functions
- Electron-phonon coupling strength
- Superconducting properties
- Transport properties (mobility & resistivity)

Recent EPW developments

- Fully integrated into QE
- Optimization & scalability
- Stability: Buildbot test-farm
- SOC and USPP support
- Transport module



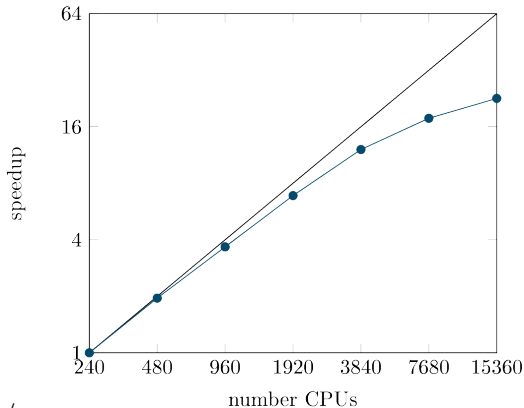
<http://epw.org.uk>



<http://epwforum.uk>



<https://gitlab.com/QEF/q-e>



CsPbI₃ on MareNostrum 4

Comput. Phys. Commun. **209**, 116 (2016)

Structure of the code

```
sponce@mauve:~/program/q-e/EPW$ ls  
bin  epw.md  examples  Ford  License  
    Makefile  README  src  tests
```

Structure of the code

```
sponce@mauve:~/program/q-e/EPW$ ls
bin  epw.md  examples  Ford  License
     Makefile  README  src  tests
```

- bin: Contains the epw.x soft link to the EPW executable.
- examples: Contains examples from the tutorials on [\[Link\]](#)
- Ford: Automatic documentation [\[Link\]](#)
- src: Contains all the EPW source files
- tests: Deprecated → replaced by q-e/test-suite/epw_*

Structure of the code

The epw.f90 file:

```
1 CALL epw_readin
2 CALL allocate_epwq
3 CALL epw_setup
4 CALL wann_run()
5 CALL elphon_shuffle_wrap()
6 CALL deallocate_epw
7 CALL close_epw()
```

Structure of the code

The epw.f90 file:

```
1 CALL epw_readin
2 CALL allocate_epwq
3 CALL epw_setup
4 CALL wann_run() <--
5 CALL elphon_shuffle_wrap()
6 CALL deallocate_epw
7 CALL close_epw()
```

Restart option:

- `wannierize = .false.`

Structure of the code

The wannierize.f90 file:

```
1 ! write the short input file for the wannier90 code
2 CALL write_winfile
3 ! run the wannier90 code to create MLWFs
4 CALL pw2wan90epw
5 --> CALL setup_nnkp
6 --> CALL ylm_expansion
7 --> CALL compute_amn_para
8 --> CALL compute_mmn_para
```

Files created:

```
1 prefix.win ! w90 input file
2 prefix.wout ! w90 output file
3 prefix.nnkp ! Contains initial projections and the nearest
               neighbors of each k-points to compute  $M_{mn}(k,b)$  matrix
               elements
4 prefix.ukk ! Contains rotation matrix  $U(k)$  for interpolation
5 prefix.bvec ! Contains next k-points if  $v_{me} > v_3$  (wannier > v3)
6 prefix.mmn ! Contains the overlap matrix
```

Structure of the code

The epw.f90 file:

```
1 CALL epw_readin
2 CALL allocate_epwq
3 CALL epw_setup
4 CALL wann_run()
5 CALL elphon_shuffle_wrap() <--
6 CALL deallocate_epw
7 CALL close_epw()
```

Restart option:

- `kmaps = .false.`
- `epbwrite = .false.`
- `epbread = .true.`

Structure of the code

The `elphon_shuffle_wrap.f90` file:

```
1 ! compute coarse grid dipole matrix elements.  
2 CALL compute_pmn_para
```

$\hat{v}_\alpha = i[\hat{H}, \hat{r}_\alpha]$ with matrix elements:

$$v_{mn\mathbf{k}\mathbf{k}'\alpha} = \langle \psi_{m\mathbf{k}'} | \hat{v}_\alpha | \psi_{n\mathbf{k}} \rangle = \langle \psi_{m\mathbf{k}'} | \hat{p}_\alpha + i[\hat{V}_{\text{NL}}, \hat{r}_\alpha] | \psi_{n\mathbf{k}} \rangle,$$

where $\hat{p}_\alpha = -i\nabla_\alpha$ is the momentum operator. In the *local approximation* we neglect $\hat{V}_{\text{NL}}$:

$$\tilde{v}_{mn\mathbf{k}} = \mathbf{k}\delta_{mn} + \sum_{\mathbf{G}} c_{m\mathbf{k}}(\mathbf{G})^* c_{n\mathbf{k}}(\mathbf{G}) \mathbf{G}.$$

New: `vme == .true.`

Structure of the code

The `elphon_shuffle_wrap.f90` file:

```
1 ! compute coarse grid dipole matrix elements.  
2 CALL compute_pmn_para  
3 CALL createkmap_pw2(xk_all,nkstot, xq0)  
4 CALL createkmap ( xq )
```

Files created:

```
1 prefix.kmap ! Store the index of k+q on the coarse k-grid.  
2 prefix.kgmap ! G-vectors needed to fold the k+q grid into the  
   k grid
```

Structure of the code

The elphon_shuffle_wrap.f90 file:

```
1  ! compute coarse grid dipole matrix elements.
2  CALL compute_pmn_para
3  CALL createkmap_pw2(xk_all,nkstot, xq0)
4  CALL createkmap ( xq )
5  ! Find crystal symmetry
6  CALL find_sym ( nat, tau, ityp, .false., m_loc )
7  ! Find symmetry for the specific q-point
8  CALL star_q2(xq, at, bg, nsym, s, invs, nq, sxq, isq, imq, .
    true., sym_smallq )
9  CALL elphon_shuffle ( iq_irr, nqc_irr, nqc, gmapsym, eigv,
    isym, xq0, .false. )
10 CALL rotate_epmat ( cz1, cz2, xq, nqc, lwin, lwinq )
```

Unfolding from the IBZ to full BZ

$$\begin{aligned} g_{mn,\nu}(\mathbf{k}, \mathbf{q}) &= \frac{1}{\sqrt{2\omega_{\mathbf{q}\nu}}} \langle \psi_{m\mathbf{k}+\mathbf{q}}(\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{scf}}(\mathbf{r}) | \psi_{n\mathbf{k}}(\mathbf{r}) \rangle \\ &= \frac{1}{\sqrt{2\omega_{\mathbf{q}\nu}}} \left[\langle \psi_{m\mathbf{k}+\mathbf{q}}(\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{el}}(\mathbf{r}) | \psi_{n\mathbf{k}}(\mathbf{r}) \rangle \right. \\ &\quad + \sum_{\mathbf{G}\mathbf{G}'} \langle \psi_{m\mathbf{k}+\mathbf{q}}(\mathbf{r}) | \mathbf{k} + \mathbf{q} + \mathbf{G}(\mathbf{r}) \rangle \\ &\quad \times \langle \mathbf{k} + \mathbf{q} + \mathbf{G}(\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{ion}}(\mathbf{r}) | \mathbf{k} + \mathbf{G}'(\mathbf{r}) \rangle \langle \mathbf{k} + \mathbf{G}'(\mathbf{r}) | \psi_{n\mathbf{k}}(\mathbf{r}) \rangle \Big] \end{aligned}$$

Unfolding from the IBZ to full BZ

$$\begin{aligned}
 g_{mn,\nu}(\mathbf{k}, \mathbf{S}\mathbf{q}) = & \frac{1}{\sqrt{2\omega_{\mathbf{q}\nu}}} \left[\langle \psi_{m\mathbf{k}+\mathbf{S}\mathbf{q}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{el}}(\mathbf{r}) | \psi_{n\mathbf{k}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \right. \\
 & + \sum_{\mathbf{G}\mathbf{G}'} \langle \psi_{m\mathbf{k}+\mathbf{S}\mathbf{q}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \mathbf{k} + \mathbf{S}\mathbf{q} + \mathbf{G}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \\
 & \times \langle \mathbf{S}^{-1}\mathbf{k} + \mathbf{q} + \mathbf{G}(\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{ion}}(\mathbf{r}) | \mathbf{S}^{-1}\mathbf{k} + \mathbf{G}'(\mathbf{r}) \rangle \\
 & \left. \times \langle \mathbf{k} + \mathbf{G}'(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \psi_{n\mathbf{k}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \right]
 \end{aligned}$$

Unfolding from the IBZ to full BZ

$$\begin{aligned}
 g_{mn,\nu}(\mathbf{k}, \mathbf{S}\mathbf{q}) &= \frac{1}{\sqrt{2\omega_{\mathbf{q}\nu}}} \left[\langle \psi_{m\mathbf{k}+\mathbf{S}\mathbf{q}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{el}}(\mathbf{r}) | \psi_{n\mathbf{k}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \right. \\
 &\quad + \sum_{\mathbf{G}\mathbf{G}'} \langle \psi_{m\mathbf{k}+\mathbf{S}\mathbf{q}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \mathbf{k} + \mathbf{S}\mathbf{q} + \mathbf{G}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \\
 &\quad \times \langle \mathbf{S}^{-1}\mathbf{k} + \mathbf{q} + \mathbf{G}(\mathbf{r}) | \partial_{\mathbf{q}\nu} V^{\text{ion}}(\mathbf{r}) | \mathbf{S}^{-1}\mathbf{k} + \mathbf{G}'(\mathbf{r}) \rangle \\
 &\quad \left. \times \langle \mathbf{k} + \mathbf{G}'(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \psi_{n\mathbf{k}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \right] \\
 g_{mn,\nu}(\mathbf{k}, -\mathbf{S}\mathbf{q}) &= \frac{1}{\sqrt{2\omega_{\mathbf{q}\nu}}} \left[\langle \psi_{m\mathbf{k}-\mathbf{S}\mathbf{q}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \left(\partial_{\mathbf{q}\nu} V^{\text{el}}(\mathbf{r}) \right)^* | \psi_{n\mathbf{k}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \right. \\
 &\quad + \sum_{\mathbf{G}\mathbf{G}'} \langle \psi_{m\mathbf{k}-\mathbf{S}\mathbf{q}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \mathbf{k} - \mathbf{S}\mathbf{q} + \mathbf{G}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \\
 &\quad \times \langle \mathbf{S}^{-1}\mathbf{k} - \mathbf{q} + \mathbf{G}(\mathbf{r}) | \partial_{-\mathbf{q}\nu} V^{\text{ion}}(\mathbf{r}) | \mathbf{S}^{-1}\mathbf{k} + \mathbf{G}'(\mathbf{r}) \rangle \\
 &\quad \left. \times \langle \mathbf{k} + \mathbf{G}'(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) | \psi_{n\mathbf{k}}(\{\mathbf{S}|\mathbf{v}\}\mathbf{r}) \rangle \right]
 \end{aligned}$$

Structure of the code

The elphon_shuffle_wrap.f90 file:

```
1  ! compute coarse grid dipole matrix elements.
2  CALL compute_pmn_para
3  CALL createkmap_pw2(xk_all,nkstot, xq0)
4  CALL createkmap ( xq )
5  ! Find crystal symmetry
6  CALL find_sym ( nat, tau, ityp, .false., m_loc )
7  ! Find symmetry for the specific q-point
8  CALL star_q2(xq, at, bg, nsym, s, invs, nq, sxq, isq, imq, .
    true., sym_smallq )
9  CALL elphon_shuffle ( iq_irr, nqc_irr, nqc, gmapsym, eigv,
    isym, xq0, .false. )
10 CALL rotate_epmat ( cz1, cz2, xq, nqc, lwin, lwinq )
11 CALL ephwann_shuffle ( nqc, xqc ) <--
```

Files created:

```
1  prefix.epbX  ! Contains unfolded matrix elements
```

Structure of the code

The epw.f90 file:

```
1 CALL epw_readin
2 CALL allocate_epwq
3 CALL epw_setup
4 CALL wann_run()
5 CALL elphon_shuffle_wrap()
6 --> CALL ephwann_shuffle ( nqc, xqc ) <--
7 CALL deallocate_epw
8 CALL close_epw()
```

Restart option:

- epwwrite = .false.
- epwread = .true.

Structure of the code

The ephwann_shuffle.f90 file:

```
1 CALL loadumat           ! Rotation matrix
2 CALL hambloch2wan(...)  ! Hamiltonian
3 CALL dmebloch2wan(...)  ! Dipole
4 CALL dynbloch2wan(...)  ! Dynamical matrix
5 CALL ephbloch2wane(...) ! Bloch el and Bloch ph -> Wannier el
                        and Bloch ph
6 CALL ephbloch2wanp(...) ! Wannier el and Bloch ph -> Wannier
                        el and Wannier ph
```

Files created (used for restart):

```
1 prefix.epmatwe1 ! Deleted when the run is finished
2 prefix.epmatwp1 ! Contains matrix element in real space
3 crystal.fmt     ! Formatted crystal information
4 dmedata.fmt     ! Formatted dipole (for velocities)
5 epwdata.fmt     ! Formatted eigenenergies, zstar, dielectric
                    function, real-space Ham+dyn
```

From coarse Bloch space to localized real space

The Hamiltonian

CALL `hambloch2wan(...)`

$$H_{mn}(\mathbf{R}_p - \mathbf{R}'_p) = \frac{1}{N_p} \sum_{m'n', \mathbf{k}} e^{-i\mathbf{k} \cdot (\mathbf{R}'_p - \mathbf{R}_p)} U_{mm', \mathbf{k}}^\dagger H_{m'n', \mathbf{k}} U_{nn', \mathbf{k}}$$

The Dynamical matrix

CALL `dynbloch2wan(...)`

$$D_{mn\kappa\alpha}(\mathbf{R}_{p'} - \mathbf{R}'_{p'}) = \frac{1}{N_{p'}} \sum_{\mathbf{q}\nu} e^{-i\mathbf{q} \cdot (\mathbf{R}'_{p'} - \mathbf{R}_{p'})} e_{\kappa\alpha, \nu}^*(\mathbf{q}) D_{\nu\kappa\alpha}(\mathbf{q}) e_{\kappa\alpha, \nu}(\mathbf{q})$$

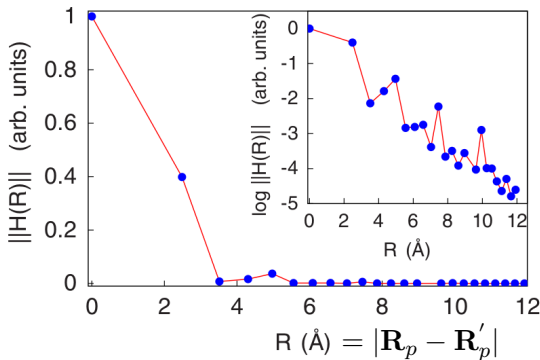
$N_p, N_{p'}$ are the number of BvK supercells for el and ph.

F. Giustino *et al.*, Phys. Rev. B **76**, 165108 (2007)

From coarse Bloch space to localized real space

Files created:

```
1 decay.H          ! Real-space decay of the Hamiltonian
2 decay.dynmat     ! Real-space decay of the dynamical matrix
```

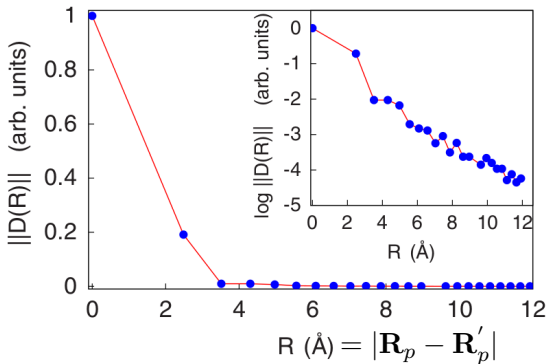


F. Giustino *et al.*, Phys. Rev. B **76**, 165108 (2007)

From coarse Bloch space to localized real space

Files created:

```
1 decay.H          ! Real-space decay of the Hamiltonian
2 decay.dynmat     ! Real-space decay of the dynamical matrix
```



F. Giustino *et al.*, Phys. Rev. B **76**, 165108 (2007)

From coarse Bloch space to localized real space

The electron-phonon matrix element

$$g_{nm\kappa\alpha}(\mathbf{R}_p, \mathbf{R}_{p'}) = \frac{1}{N_p N_{p'}} \sum_{\mathbf{k}, \mathbf{q}} \sqrt{\frac{2M_\kappa \omega_{\mathbf{q}\nu}}{\hbar}} e^{-i(\mathbf{k} \cdot \mathbf{R}_p + \mathbf{q} \cdot \mathbf{R}_{p'})} \\ \times \sum_{m'n'\nu} e_{\kappa\alpha, \nu}^*(\mathbf{q}) U_{mm', \mathbf{k}+\mathbf{q}}^\dagger g_{m'n'\nu}(\mathbf{k}, \mathbf{q}) U_{n'n\mathbf{k}}$$

↑
on the coarse grids (prefix.epbX files)

$N_p, N_{p'}$ are the number of BvK supercells for el and ph.

From coarse Bloch space to localized real space

$$g_{nm\kappa\alpha}(\mathbf{R}_p, \mathbf{R}_{p'}) = \frac{1}{N_p N_{p'}} \sum_{\mathbf{k}, \mathbf{q}} \sqrt{\frac{2M_{\kappa}\omega_{\mathbf{q}\nu}}{\hbar}} e^{-i(\mathbf{k}\cdot\mathbf{R}_p + \mathbf{q}\cdot\mathbf{R}_{p'})} \\ \times \sum_{m'n'\nu} e_{\kappa\alpha,\nu}^*(\mathbf{q}) U_{mm',\mathbf{k}+\mathbf{q}}^{\dagger} g_{m'n'\nu}(\mathbf{k}, \mathbf{q}) U_{n'n\mathbf{k}}$$

CALL ephbloch2wane(...)

$$g_{nm\nu}(\mathbf{R}_p, \mathbf{q}) = \frac{1}{N_p} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_p} \sum_{m'n'} U_{mm',\mathbf{k}+\mathbf{q}}^{\dagger} g_{m'n'\nu}(\mathbf{k}, \mathbf{q}) U_{n'n\mathbf{k}}$$

CALL ephbloch2wanp(...)

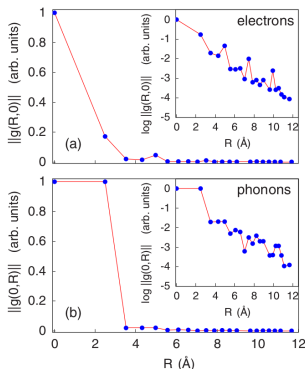
$$g_{nm\kappa\alpha}(\mathbf{R}_p, \mathbf{R}_{p'}) = \frac{1}{N_{p'}} \sum_{\mathbf{q}} \sqrt{\frac{2M_{\kappa}\omega_{\mathbf{q}\nu}}{\hbar}} e^{-i\mathbf{q}\cdot\mathbf{R}_{p'}} \sum_{\nu} e_{\kappa\alpha,\nu}^*(\mathbf{q}) g_{mn\nu}(\mathbf{R}_p, \mathbf{q})$$

F. Giustino, Rev. Mod. Phys. **89**, 1 (2017)

From coarse Bloch space to localized real space

Files created:

```
1 decay.epwane      ! Real-space decay of the electronic part  
    of the el-ph  
2 decay.epmat_wanep ! Real-space decay of the el-ph
```



F. Giustino *et al.*, Phys. Rev. B **76**, 165108 (2007)

Structure of the code

The ephwann_shuffle.f90 file:

```
1 CALL dynwan2bloch(...) ! Dynamical matrix
2 CALL ephwan2blochp(...) ! Wannier el and Wannier ph ->
   Wannier el and Bloch ph
3 CALL hamwan2bloch(...) ! Hamiltonian
4 CALL dmewan2bloch(...) ! Dipole
5 CALL ephwan2bloch(...) ! Wannier el and Bloch ph -> Bloch el
   and Bloch ph
6 IF (prtgkk ) CALL print_gkk( iq )
7 IF (phonselfen ) CALL selfen_phon_q( iq )
8 IF (elecselfen ) CALL selfen_elec_q( iq, first_cycle )
9 IF (plselfen ) CALL selfen_pl_q( iq )
10 IF (nest_fn ) CALL nesting_fn_q( iq )
11 IF (specfun_el ) CALL spectral_func_q( iq )
12 IF (specfun_ph ) CALL spectral_func_ph( iq )
13 IF (specfun_pl ) CALL spectral_func_pl_q( iq )
14 IF (scattering) CALL scattering_rate_q( ... )
15 IF (.not. iterative_bte) CALL transport_coeffs (ef0,efcb)
```

Fan-Migdal electron self-energy

Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

$$\Sigma_{n\mathbf{k}}^{\text{FM}}(\omega, T) = \frac{1}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \\ \times \left[\frac{1 - f_{m\mathbf{k}+\mathbf{q}}(T) + n_{\mathbf{q}\nu}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar - \omega_{\mathbf{q}\nu} + i\eta} + \frac{f_{m\mathbf{k}+\mathbf{q}}(T) + n_{\mathbf{q}\nu}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar + \omega_{\mathbf{q}\nu} + i\eta} \right]$$

Fan-Migdal electron self-energy

Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

Summation over all phonon
branches and wavevectors

$$\Sigma_{n\mathbf{k}}^{\text{FM}}(\omega, T) = \frac{1}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \quad \text{Extension to finite temperature}$$
$$\times \left[\frac{1 - f_{m\mathbf{k}+\mathbf{q}}(T) + n_{\mathbf{q}\nu}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar - \omega_{\mathbf{q}\nu} + i\eta} + \frac{f_{m\mathbf{k}+\mathbf{q}}(T) + n_{\mathbf{q}\nu}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar + \omega_{\mathbf{q}\nu} + i\eta} \right]$$

Dynamical structure on the scale
of the phonon energy

Fan-Migdal phonon self-energy

$$\Pi_{\mathbf{q}\nu}(\omega, T) = 2 \sum_{mn} \int_{\text{BZ}} \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} |g_{mn,\nu}(\mathbf{k}, \mathbf{q})|^2 \frac{f_{n\mathbf{k}}(T) - f_{m\mathbf{k}+\mathbf{q}}(T)}{\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \omega - i\delta}$$

Structure of the code

Input variables:

```
1 elecselven      = .true.          scattering = .true.
2 nest_fn         = .true.          scattering_serta = .true.
3 phonselven      = .true.          int_mob     = .true.
4 a2f             = .true.          carrier     = .true.
5                                     ncarrier    = 1E13
6 specfun_el      = .true.          nstemp      = 3
7 wmin_specfun    = -4              tempsmin   = 100
8 wmax_specfun    = 1               tempsmax   = 500
9 nw_specfun      = 20
```

Files created:

```
1 linewidth.phself ! Im electron self-energy = linewidths
2 lambda.phself    ! Lambda phonon self-energy
3 linewidth.elfself ! Im electron self-energy = linewidths
4 specfun.elfself  ! Electron spectral function
5 specfun_sup.elfself ! Supporting file for spectral function
6 specfun.phon     ! Phonon spectral function
7 specfun_sup.phon ! Supporting file for spectral function
```

Polar divergence

Input variables:

```
1 lpolar      = .true.
```

In polar materials, $g_{mn,\nu}(\mathbf{k}, \mathbf{q})$ diverge as $1/|\mathbf{q}|$ for $|\mathbf{q}| \rightarrow 0$
Split the electron-phonon matrix elements into a short- ($\mathcal{S}$) and a long-range ($\mathcal{L}$) contribution:

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

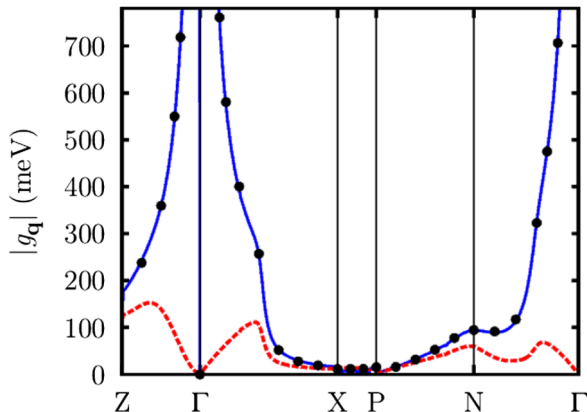
$$g_{mn,\nu}^{\mathcal{L}}(\mathbf{k}, \mathbf{q}) = i \sum_{\kappa} \left(\frac{\hbar}{2M_{\kappa}\omega_{\mathbf{q}\nu}} \right)^{1/2} \times \sum_{\mathbf{G} \neq -\mathbf{q}} \frac{(\mathbf{q} + \mathbf{G}) \cdot \mathbf{Z}_{\kappa}^* \cdot \mathbf{e}_{\kappa,\nu}(\mathbf{q})}{(\mathbf{q} + \mathbf{G}) \cdot \boldsymbol{\varepsilon}^{\infty} \cdot (\mathbf{q} + \mathbf{G})} \langle \psi_{m\mathbf{k}+\mathbf{q}} | e^{i(\mathbf{q}+\mathbf{G}) \cdot (\mathbf{r}-\boldsymbol{\tau}_{\kappa})} | \psi_{n\mathbf{k}} \rangle$$

S. Ponc  et al., J. Chem. Phys. **143**, 102813 (2015)

C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015)

Polar divergence

Wannier interpolation of the electron-phonon matrix elements for anatase TiO_2



C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015)

Crystal acoustic sum rule

Input variables:

```
1 lifc           = .true.
2 asr_typ        = 'simple'    ! freq. at Gamma for 3 acoustic
   modes = 0
3 asr_typ        = 'crystal'  ! Lagrangian approach
```

Requires to run q2r.x and to copy the prefix.fc file into save/ifc.q2r before EPW calculation

N. Mingo *et al.*, Phys. Rev. B **77**, 033418 (2008)

N. Mounet, PhD thesis, MIT (2005) [\[link\]](#)

Miscellaneous

Input variables:

```
1 fsthick      = 1.0 ! eV   ! Windows around the Fermi level.  
    Some properties requires large values  
2 eptemp       = 1      ! K    ! Temperature at which the  
    calculation is performed. Not to be confused with  
    tempsmin\max which is used for mobility and supersedes  
    eptemp  
3 degaussw     = 0.01 ! eV   ! Gaussian broadening for the delta  
    functions. Should be small  
4 degaussq     = 0.05 ! meV  ! Gaussian broadening for the \  
    lambda and a2f phonons
```

Convergence must be made for:

```
1 nk1,nk2,nk3  
2 nq1,nq2,nq3  
3 nkf1,nkf2,nkf3 or filkf  
4 nqf1,nqf2,nqf3 or filqf  
5 ecut  
6 fsthick
```

References

- F. Giustino *et al.*, Phys. Rev. B **76**, 165108 (2007) [\[link\]](#)
- T. Kita, Prog. Th. Phys. **123**, 581 (2010) [\[link\]](#)
- C. Verdi *et al.*, Phys. Rev. Lett. **115**, 176401 (2015) [\[link\]](#)
- S. Poncé *et al.*, Comput. Phys. Commun. **209**, 116 (2016) [\[link\]](#)
- F. Giustino, Rev. Mod. Phys. **89**, 1 (2017) [\[link\]](#)
- S. Poncé *et al.*, Phys. Rev. B **97**, 121201 (2018) [\[link\]](#)
- 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