ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles

Trieste, 19-23 March 2018

Lecture Wed.2

Introduction to the Boltzmann transport equation

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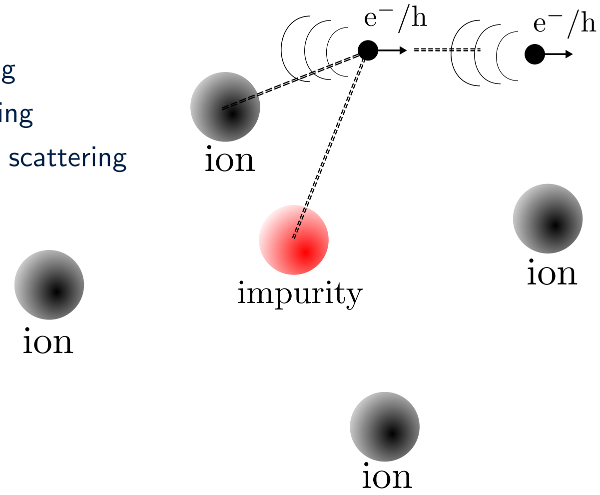
Lecture Summary

- Carrier transport
- Quantum Boltzmann equation
- Boltzmann transport equation
- Self-energy relaxation time approximation
- Lowest-order variational approximation
- Ionized impurity scattering

Carrier transport: experimental evidences

- Lattice scattering
- Impurity scattering
- Ionized impurity scattering



Carrier transport: experimental evidences

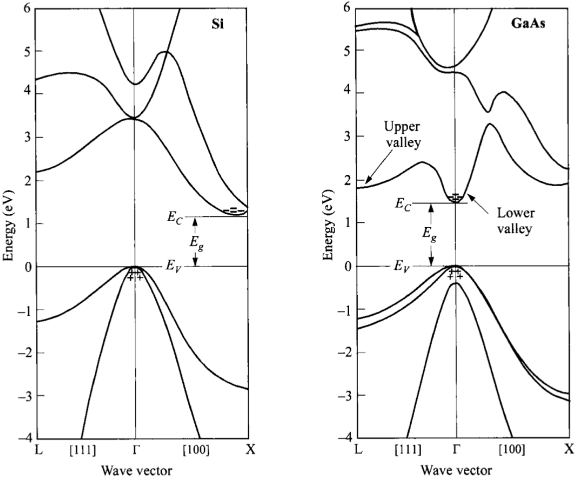
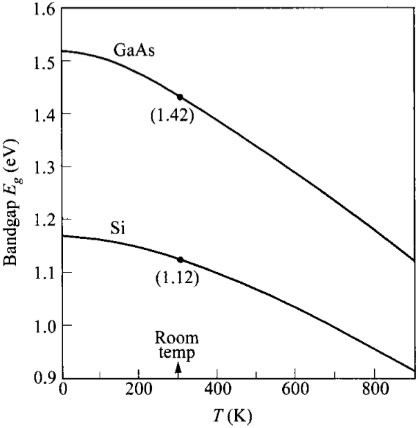


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences



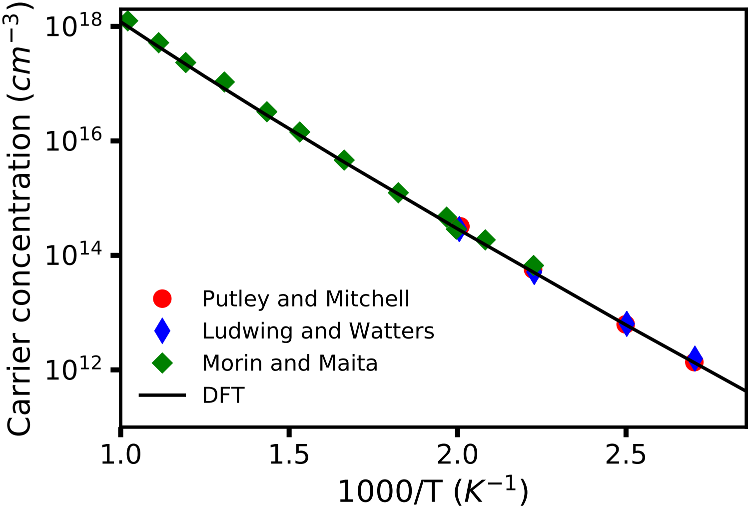
	$E_g(0)$ (eV)	α (eV/K)	β (K)
GaAs	1.519	5.4×10^{-4}	204
Si	1.169	4.9×10^{-4}	655

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

(Lecture Thu.2)

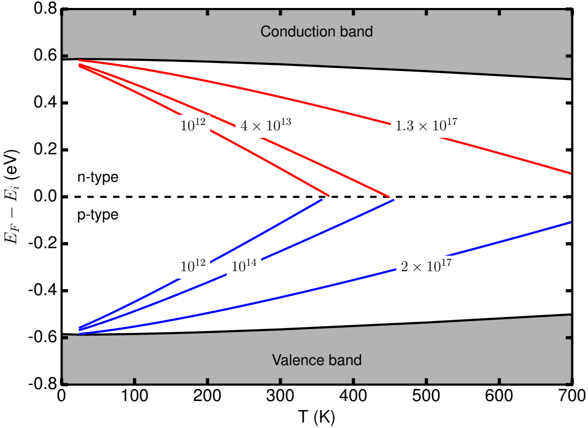
Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences

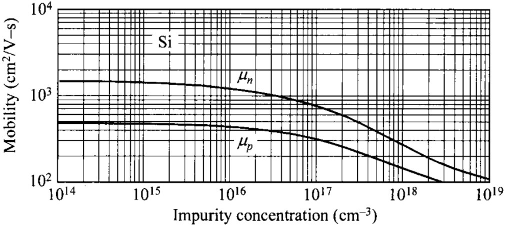


Carrier transport

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



Carrier transport: experimental evidences



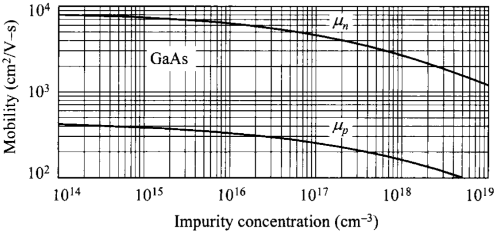


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Carrier transport: experimental evidences

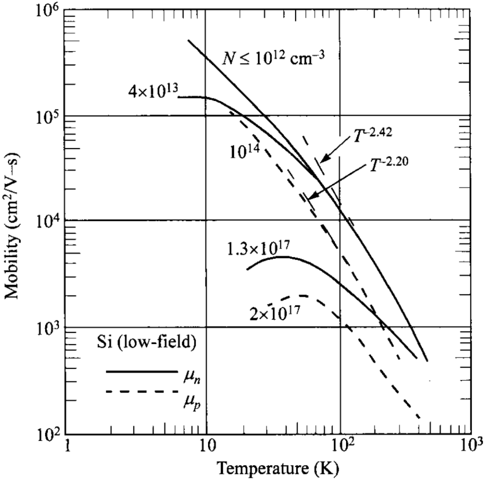


Figure from S. M. Sze, *Physics of Semiconductor Device*, Wiley (2007)

Quantum Boltzmann equation

- Most general transport theory that describes the evolution of the particles distribution function

$$f(\mathbf{k}, \omega, \mathbf{r}, t) = -iG^{<}(\mathbf{k}, \omega, \mathbf{r}, t),$$

where $G^{<}$ is the FT of the lesser Green's function

$$G^{<}(\mathbf{r}, t, \mathbf{R}, T) = i\langle \psi^{\dagger}(\mathbf{R} - 0.5\mathbf{r}, T - 0.5t)\psi(\mathbf{R} + 0.5\mathbf{r}, T + 0.5t)\rangle$$

with $(\mathbf{R}, T)$ for the center of mass.

- Finding $G^{<}$ requires to solve a complex set of 2x2 matrix Green's function [non-equilibrium Keldysh formalism]
- Involves G^{ret} that describes the dissipation of the system
- Valid for out of equilibrium systems

G. D. Mahan, *Many-Particle Physics*, Springer, 2000

Gradient expansion approximation

Assumes

- Homogeneous system ($\nabla_{\mathbf{r}} = 0$)
- In steady state ($\nabla_t = 0$)

energy distribution

el-ph self-energies

$$A(\mathbf{k},\omega)^2 \frac{\partial n_F}{\partial \omega} \mathbf{E} \cdot \{(\mathbf{v_k} + \nabla_{\mathbf{k}} \mathrm{Re}[\Sigma^{\mathrm{ret}}])\Gamma + \sigma \nabla_{\mathbf{k}} \Gamma\} = \Sigma^{>} G^{<} - \Sigma^{<} G^{>}$$

$$A = \frac{2\Gamma}{\sigma^2 + \Gamma^2}, \quad \Gamma = -\mathrm{Im}\Sigma^{\mathrm{ret}}, \quad \sigma = \omega - \varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma^{\mathrm{ret}}$$

L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Benjamin, 1962

Electric current

- The steady-state electric current $\mathbf{J}$ is related to the driving electric field $\mathbf{E}$ via the mobility tensors $\boldsymbol{\mu}$ as:

$$
\begin{aligned}
J_\alpha &= e\,(n_{\rm e}\,\mu_{{\rm e},\alpha\beta} + n_{\rm h}\,\mu_{{\rm h},\alpha\beta})E_\beta \\
&= -e\,\Omega^{-1}\sum_n \Omega_{\rm BZ}^{-1}\int d\mathbf{k}\, f_{n\mathbf{k}}\, v_{n\mathbf{k},\alpha}
\end{aligned}
$$

  where $v_{n\mathbf{k},\alpha} = \hbar^{-1}\partial\varepsilon_{n\mathbf{k}}/\partial k_\alpha$ is the band velocity.

- We need to find the occupation function $f_{n\mathbf{k}}$ which reduces to the Fermi-Dirac distribution $f^0_{n\mathbf{k}}$ in the absence of the electric field

Mobility

- Experimentalists prefers to measure mobility as it is independent of the carrier concentration n

$$\mu_{\mathrm{e},\alpha\beta} = \frac{\sigma_{\alpha\beta}}{n_e} = \frac{1}{n_e}\frac{\partial J_\alpha}{\partial E_\beta}$$
$$= -\sum_{n\in\mathrm{CB}}\int d\mathbf{k}\ v_{n\mathbf{k},\alpha}\,\partial_{E_\beta} f_{n\mathbf{k}} \Big/ \sum_{n\in\mathrm{CB}}\int d\mathbf{k}\, f^0_{n\mathbf{k}}.$$

(similar expression for hole mobility)

- We need to evaluate the linear response of the distribution function $f_{n\mathbf{k}}$ to the electric field $\mathbf{E}$.

Boltzmann transport equation (BTE)

Electron can be treated as classical particle but electron scattering is the result of short-range forces and must be treated quantum mechanically.

The BTE is a *semi-classical* treatment which

- describes carrier dynamics using Newton's law without treating explicitly the crystal potential. The influence of the crystal potential is treated indirectly through the electronic bandstructure (= effective masses).
- carrier scattering is treated quantum mechanically.

M. Lundstrom, *Fundamentals of Carrier Transport*, Cambridge (2000)

Boltzmann transport equation

Like in QBE, we start from the carrier distribution function $f(\mathbf{k}, \omega, \mathbf{r}, t)$. At equilibrium $df/dt = 0$ the change of the distribution function is given by the Boltzmann equation:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\partial \mathbf{k}}{\partial t} \cdot \frac{\partial f}{\partial \mathbf{k}} + \frac{\partial T}{\partial t} \cdot \frac{\partial f}{\partial T} + \frac{\partial f}{\partial t}\bigg|_{\text{scatt}} = 0$$

Approximations:

G. D. Mahan, *Many-Particle Physics*, Springer, 2000

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Approximations:

- Homogeneous field (independent of $\mathbf{r}$)

G. D. Mahan, *Many-Particle Physics*, Springer, 2000

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Approximations:

- Homogeneous field (independent of $\mathbf{r}$)
- Constant temperature

G. D. Mahan, *Many-Particle Physics*, Springer, 2000

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Approximations:

- Homogeneous field (independent of $\mathbf{r}$)
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Approximations:

- Homogeneous field (independent of $\mathbf{r}$)
- Constant temperature
- DC conductivity
- No magnetic field $\frac{\partial \mathbf{k}}{\partial t} = -(-e)\mathbf{E} - \frac{1}{137}\mathbf{v} \times \mathbf{H}$

G. D. Mahan, *Many-Particle Physics*, Springer, 2000

Boltzmann transport equation

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$$\text{Quantum} \rightarrow \left.\frac{\partial f_{n\mathbf{k}}(T)}{\partial t}\right|_{\text{scatt}} = (-e)\mathbf{E} \cdot \frac{\partial f_{n\mathbf{k}}(T)}{\partial \mathbf{k}} \leftarrow \text{Semi-classical}$$

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Linearized Boltzmann transport equation

$$\text{Quantum} \rightarrow \left.\frac{\partial f_{n\mathbf{k}}(T)}{\partial t}\right|_{\text{scatt}} = (-e)\mathbf{E} \cdot \frac{\partial f_{n\mathbf{k}}(T)}{\partial \mathbf{k}} \leftarrow \text{Semi-classical}$$

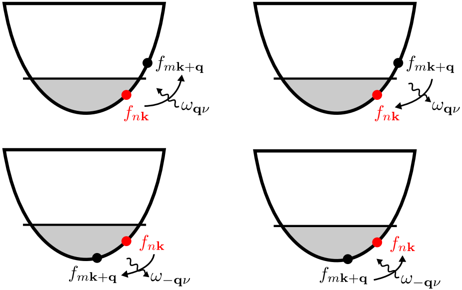
If $\mathbf{E}$ is small, $f_{n\mathbf{k}}$ can be expanded into $f_{n\mathbf{k}} = f^0_{n\mathbf{k}} + \mathcal{O}(\mathbf{E})$. Keeping only the linear term in $\mathbf{E}$ becomes

$$(-e)\mathbf{E} \cdot \frac{\partial f_{n\mathbf{k}}(T)}{\partial \mathbf{k}} = (-e)\mathbf{E} \cdot \mathbf{v}_{n\mathbf{k}} \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}$$

This is the collisionless term of Boltzmann's equation for a uniform and constant electric field, in the absence of temperature gradients and magnetic fields

Linearized Boltzmann transport equation

$$\left.\frac{\partial f_{n\mathbf{k}}(T)}{\partial t}\right|_{\text{scatt}} = (-e)\mathbf{E}\cdot\mathbf{v}_{n\mathbf{k}}\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}$$



This is the modification of the distribution function arising from electron-phonon scattering in and out of the state $|n\mathbf{k}\rangle$, via emission or absorption of phonons with frequency $\omega_{\mathbf{q}\nu}$

Linearized Boltzmann transport equation

$$\left.\frac{\partial f_{n\mathbf{k}}(T)}{\partial t}\right|_{\text{scatt}} = (-e)\mathbf{E}\cdot\mathbf{v}_{n\mathbf{k}}\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}$$

$$\begin{aligned}\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}\mathbf{v}_{n\mathbf{k}}\cdot(-e)\mathbf{E} = \frac{2\pi}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\text{BZ}}}\,|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \\ \times\Big\{(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})(1+n_{\mathbf{q}\nu}) \\ +(1-f_{n\mathbf{k}})f_{m\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu} \\ -f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}\nu})(1+n_{\mathbf{q}\nu}) \\ -f_{n\mathbf{k}}(1-f_{m\mathbf{k}+\mathbf{q}})\delta(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}\nu})n_{\mathbf{q}\nu}\Big\}\end{aligned}$$

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

The electron-phonon matrix element

Variation of the Kohn-Sham potential

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

Lattice-periodic part of wavefunction

Incommensurate modulation

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

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

(`Lecture Tue.1`)

Linearized Boltzmann transport equation

We take the derivatives of the Boltzmann equation with respect to $\mathbf{E}$ to obtain the iterative Botlzmann transport equation (IBTE):

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

having defined the relaxation time:

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

Self energy relaxation time approximation (SERTA)

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

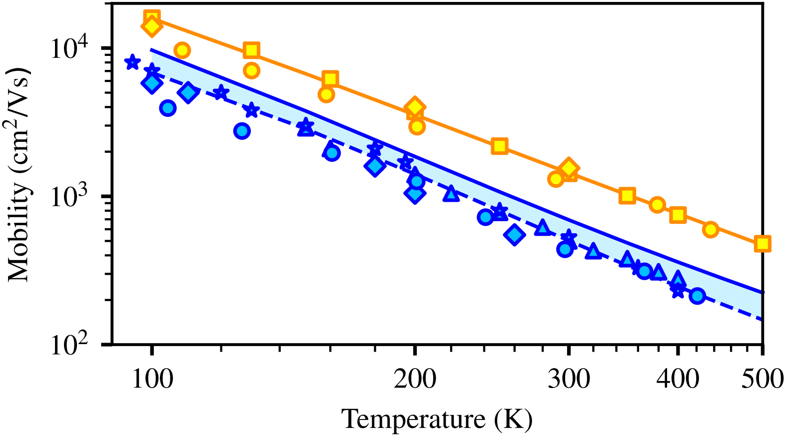
$$\partial_{E_\beta} f_{n\mathbf{k}} = e \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\beta} \tau^0_{n\mathbf{k}}$$

The intrinsic electron mobility is therefore:

$$\begin{aligned}\mu_{\mathrm{e},\alpha\beta} &= -\sum_{n\in\mathrm{CB}} \int d\mathbf{k}\; v_{n\mathbf{k},\alpha}\, \partial_{E_\beta} f_{n\mathbf{k}} \Big/ \sum_{n\in\mathrm{CB}} \int d\mathbf{k}\; f^0_{n\mathbf{k}} \\ &= \frac{-e}{n_\mathrm{e}\,\Omega} \sum_{n\in\mathrm{CB}} \int \frac{d\mathbf{k}}{\Omega_\mathrm{BZ}}\; \frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\alpha}\, v_{n\mathbf{k},\beta}\, \tau^0_{n\mathbf{k}}\end{aligned}$$

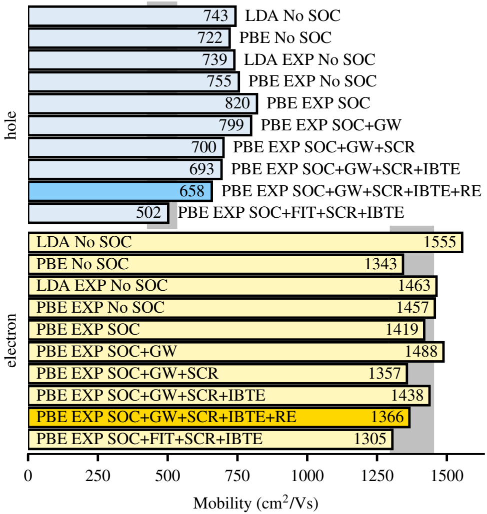
Intrinsic carrier mobility

Electron and hole mobility in silicon (`EPW`)



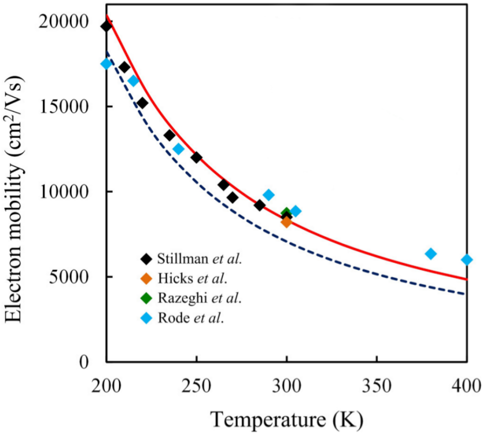
S. Poncé *et al.*, Physical Review B, in press (2018) and can be found on arXiv:1803.05462

Intrinsic Si carrier mobility at 300K



S. Poncé *et al.*, Physical Review B, in press (2018) and can be found on arXiv:1803.05462

Electron mobility in GaAs using IBTE and SERTA (dashed)



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

Lowest-order variational approximation (LOVA)

From Eliashberg theory of phonon-driven superconductivity, Pinkski, Butler and Allen developed a framework based on this variational principle to compute electrical and thermal resistivities of metals.

One can go from the BTE to the LOVA introducing energy integrals and using the following approximations:

- Isotropic relaxation time τ
- Assume the DOS at the Fermi level is slowly varying $\delta(\varepsilon_{n\mathbf{k}} - \varepsilon) \approx \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F) \rightarrow$ valid for metals only !

P. B. Allen, Phys. Rev. B **13**, 1416 (1976)
P. B. Allen, Phys. Rev. B **17**, 3725 (1978)
F. J. Pinski, P. B. Allen, and W. H. Butler, Phys. Rev. B **23**, 5080 (1981)

Lowest-order variational approximation (LOVA)

Carrier resistivity:

$$\rho_{\alpha\beta}^{\mathsf{LOVA}} = \frac{2\pi\Omega_{\mathsf{BZ}} k_B T}{e^2\hbar\mathfrak{n}(\varepsilon_F)\langle v_\alpha(\varepsilon_F) v_\beta(\varepsilon_F)\rangle} \int_0^\infty \frac{d\omega}{\omega} \frac{(\omega/2T)^2 \alpha_{\mathsf{tr}}^2 F(\omega)}{\sinh^2(\omega/2T)}$$

With the isotropic transport spectral function:

$$\alpha_{\mathsf{tr}}^2 F(\omega) = \frac{1}{\mathfrak{n}(\varepsilon_F)\langle \mathbf{v}(\varepsilon_F)\rangle^2} \sum_{nm\nu} \iint_{\mathsf{BZ}} \frac{d\mathbf{k}d\mathbf{q}}{\Omega_{\mathsf{BZ}}^2} |g_{mn,\nu}(\mathbf{k},\mathbf{q})|^2$$
$$\Big[\mathbf{v}_{n\mathbf{k}} \cdot \mathbf{v}_{n\mathbf{k}} - \mathbf{v}_{n\mathbf{k}} \cdot \mathbf{v}_{m\mathbf{k}+\mathbf{q}}\Big] \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F)\delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_F)\delta(\omega - \omega_{\mathbf{q}\nu})$$

P. B. Allen, Phys. Rev. B **13**, 1416 (1976)
P. B. Allen, Phys. Rev. B **17**, 3725 (1978)
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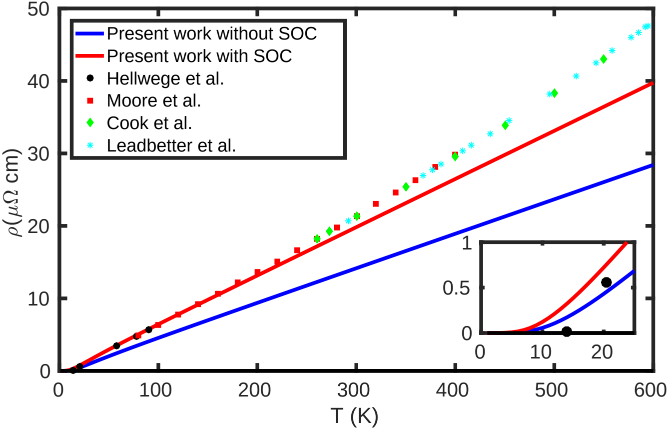
Lowest-order variational approximation (LOVA)

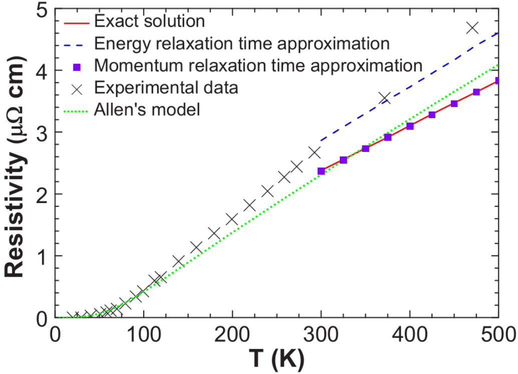
Resistivity of Pb with and without spin-orbit coupling



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

Lowest-order variational approximation (LOVA)

Resistivity of Al with IBTE , SERTA (dashed line) and LOVA (dotted line)



W. Li, Phys. Rev. B **92**, 075405 (2015)

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

H. Brooks, Phys. Rev. **83**, 879 (1951)
S. S. Li and W. R. Thurber, 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:

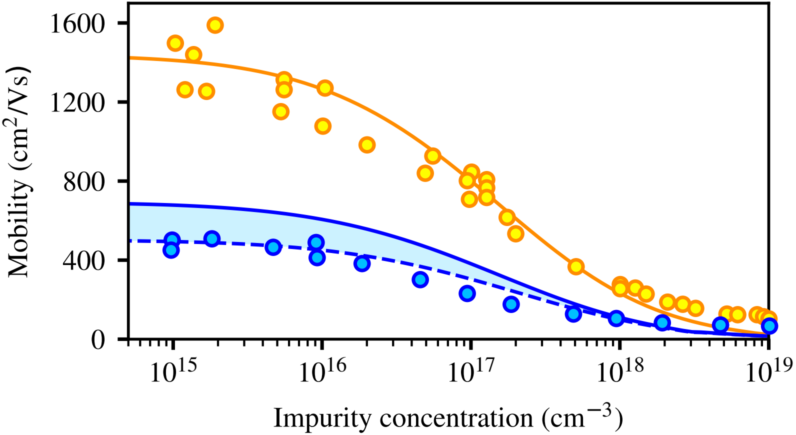
$$\mu = \mu_l \Big[1 + X^2 \{\mathsf{ci}(X)\cos(X) + \sin(X)(\mathsf{si}(X) - \frac{\pi}{2})\}\Big]$$

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

P. Norton, T. Braggins, and H. Levinstein, Phys. Rev. B **8**, 5632 (1973)

Ionized impurity scattering

Electron and hole mobility in silicon (EPW)



S. Poncé *et al.*, Physical Review B, in press (2018) and can be found on arXiv:1803.05462

References: insightful books

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