Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.5.19 Lecture 06

10:25 – 11:55

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Review of lecture in the last week

- Optical absorption with inter-band transition
- Photon emission from inter-band transition
- Optical absorption with exciton formation
- Photon emission from exciton recombination
- Concept of exciton-polariton

Contents today

Concept of exciton-polariton (continued)

Chapter 5 Semi-classical treatment of transport

Transport coefficient

Classical transport: Boltzmann equation

Currents: particle flows

Drude formula, Diffusion current, Hall effect

Various scatterings

Heat transport, Thermoelectric effect

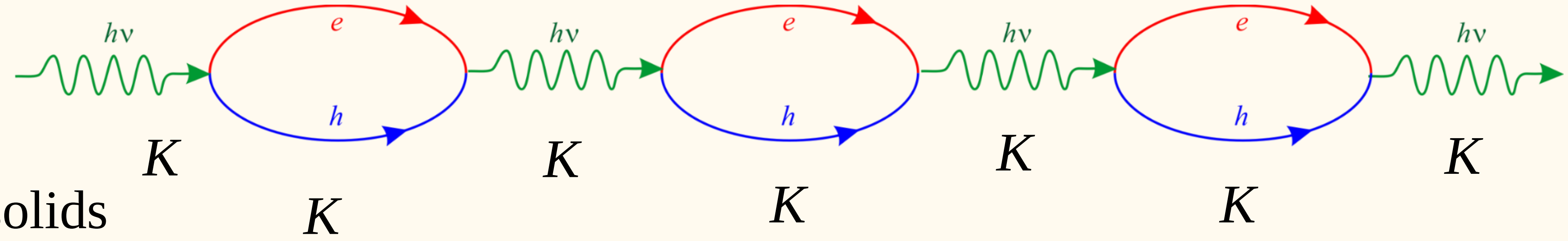
Exciton-polariton

Concept of exciton-polariton

Chain of photon-exciton

1 cycle $\sim$ few fs

coherent propagation in solids



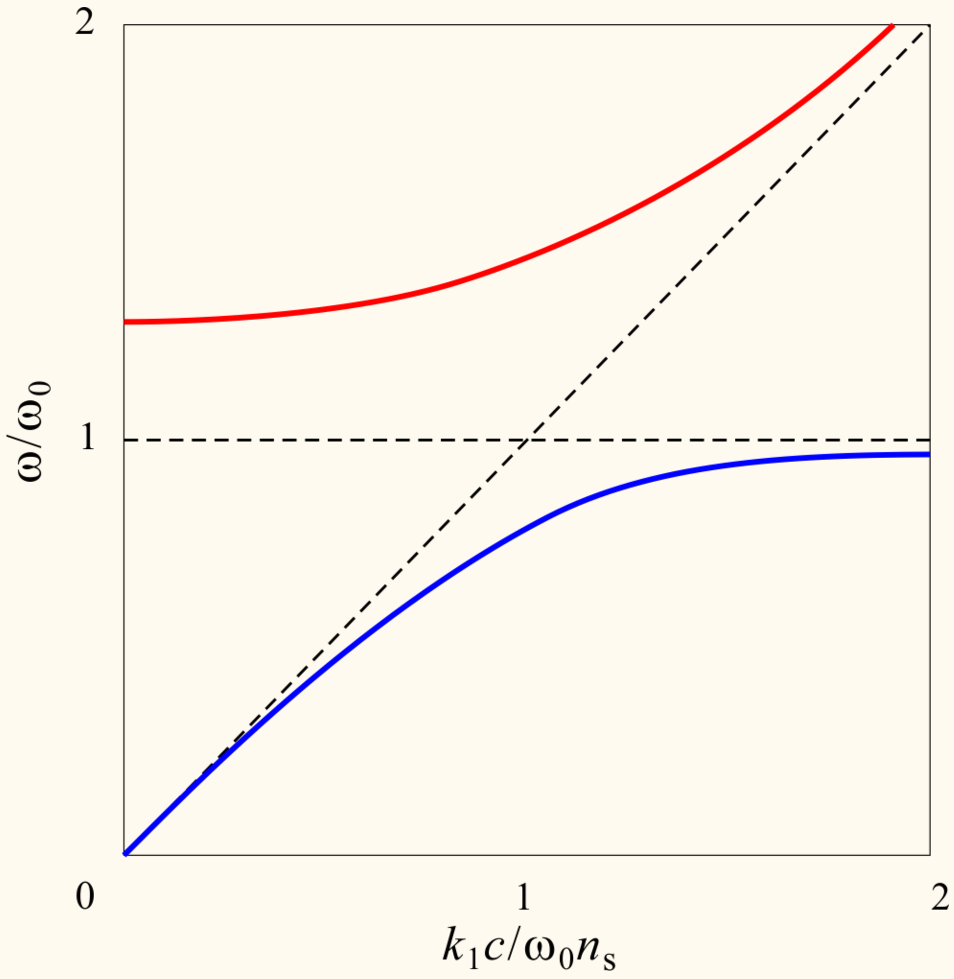
ϵ_{s}: contributions other than from excitons $\epsilon_{\mathrm{r}}(\omega) = \epsilon_{\mathrm{s}} \left(1 + \frac{\Delta_{\mathrm{ex}}}{\omega_0 - \omega - i\gamma}\right)$

transverse wave: $\left.\begin{matrix} \boldsymbol{k} \cdot \boldsymbol{E} = 0 \\ \omega_{\mathrm{t}} = \omega_0 \end{matrix}\right\}$ polariton equation $c^2 \boldsymbol{k}^2 = \omega_0^2 \epsilon_{\mathrm{r}}(\omega_0, \boldsymbol{k})$

Longitudinal wave: $\omega_{\mathrm{l}} = \omega_0 + \Delta_{\mathrm{ex}} = \omega_{\mathrm{t}} + \Delta_{\mathrm{ex}}$

Δ_{ex} : longitudinal-transverse splitting

Exciton-polariton (2)



For transverse wave

$$k = k_1 + ik_2$$

Real-imaginary comparison

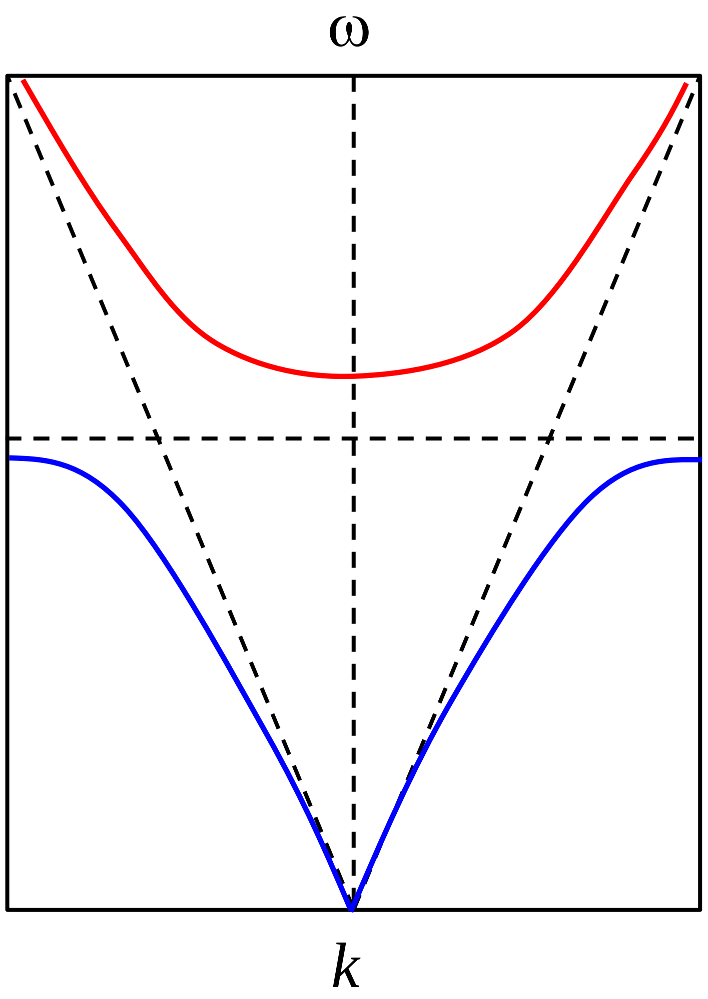
$$\begin{cases} \dfrac{\omega^2 \epsilon_s}{c^2}\left(1 + \dfrac{\Delta_{ex}}{\omega_0 - \omega}\right) = k_1^2 - k_2^2, \\ \pi\delta(\omega - \omega_0)\dfrac{\omega_0^2 \epsilon_s}{c^2} = 2k_1 k_2 \end{cases}$$

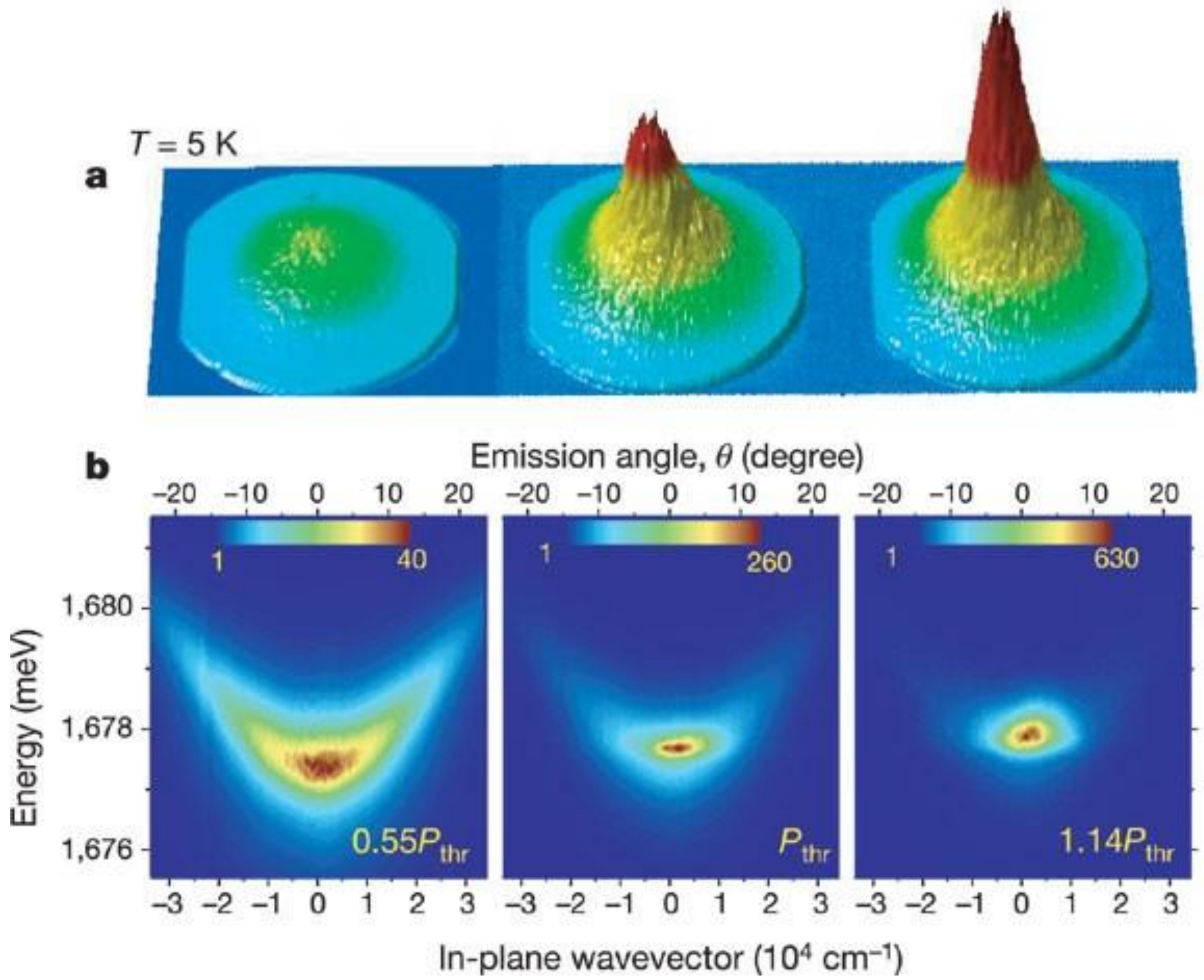
Resonance

Dispersion relation

$$\omega\sqrt{\frac{\omega - \omega_{-}\Delta_{ex}}{\omega - \omega_0}} = \frac{ek_1}{\sqrt{\epsilon_s}}$$

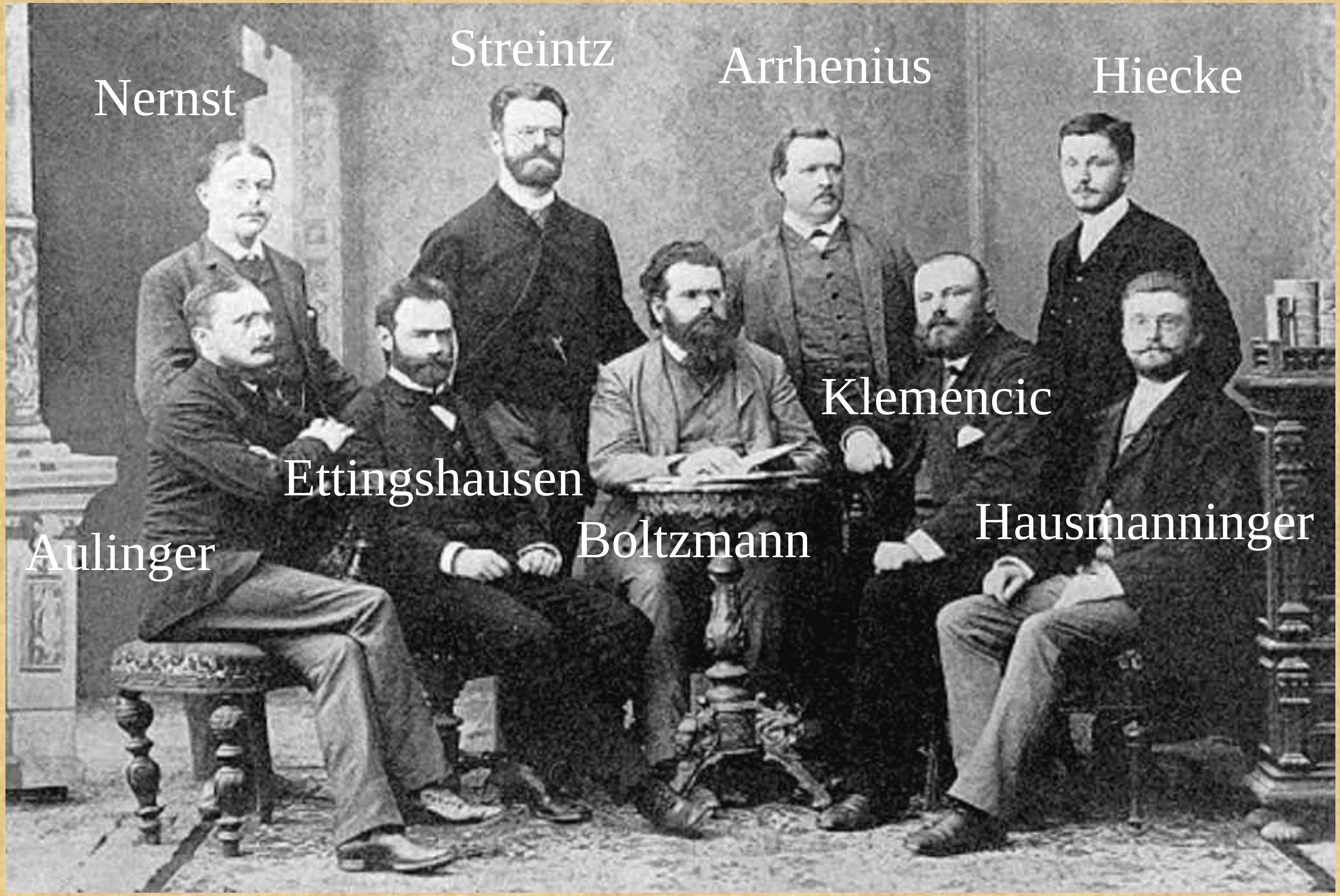
Bose-Einstein condensation of exciton-polaritons





J. Kasprzak *et al.*, Nature **443**, 409 (2006).

Chapter 5 Semi-classical treatment of transport



Ludwig Boltzmann
1844 - 1906

From Wikipedia

Classical, semi-classical transport, transport coefficient

Transport in condensed matter: Charge, heat, spin carriers
- electrons : most electric devices
- ions : batteries, sensors

Classical, semi-classical transport ⟷ Quantum transport (quantum mechanical nature in transport)

Semi-classical: quantum mechanics affects energy distribution function

Classical semi-classical boundary Fermi degenerate temperature

$$T_{\mathrm{F}} = \frac{\hbar^2}{2mk_{\mathrm{B}}}(3\pi^2 n)^{2/3}$$ for 3-dimensional systems

$$T_{\mathrm{F}} = \frac{\hbar^2}{16\pi m k_{\mathrm{B}}} n$$ for 2-dimensional systems

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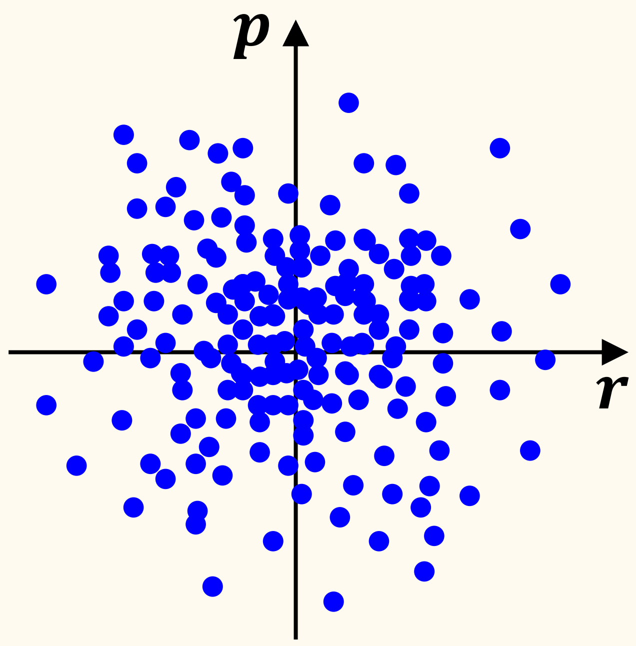
External perturbation → Linear response: Transport coefficient Conductance, Resistance

current density $\boldsymbol{j} = \boldsymbol{\sigma}\mathbf{E}$ electric field

$\mathbf{E} = \boldsymbol{\rho}\boldsymbol{j} = \boldsymbol{\sigma}^{-1}\boldsymbol{j}$

conductivity tensor

resistivity tensor



$(\boldsymbol{r}, \boldsymbol{p})$ 6-dimensional phase space

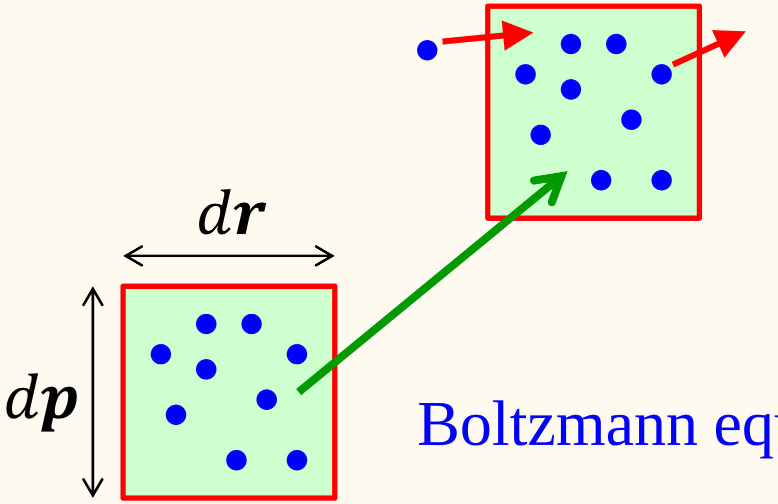
Distribution function $f(\boldsymbol{r}, \boldsymbol{p}, t)$ $\quad \dfrac{d\boldsymbol{r}}{dt} = \boldsymbol{v} = \dfrac{\boldsymbol{p}}{m}, \quad \dfrac{d\boldsymbol{p}}{dt} = \boldsymbol{F}$

No collision: $f(\boldsymbol{r} + \boldsymbol{v}dt, \boldsymbol{p} + \boldsymbol{F}dt, t + dt) = f(\boldsymbol{r}, \boldsymbol{p}, t)$

Introduction of collision: $(\partial f/\partial t)_c$

$$f\left(\boldsymbol{r} + \frac{\boldsymbol{p}}{m^*}dt, \boldsymbol{p} + \boldsymbol{F}dt, t + dt\right) + \left(\frac{\partial f}{\partial t}\right)_c dt = f(\boldsymbol{r}, \boldsymbol{p}, t)$$

$$\rightarrow f(\boldsymbol{r}, \boldsymbol{p}, t) + \left[\frac{\partial f}{\partial \boldsymbol{r}}\frac{d\boldsymbol{r}}{dt} + \frac{\partial f}{\partial \boldsymbol{p}}\frac{d\boldsymbol{p}}{dt} + \frac{\partial f}{\partial t}\right] dt$$



Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = -\left(\frac{\partial f}{\partial t}\right)_c$$

Currents: Particle flows

Boltzmann equation $$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = -\left(\frac{\partial f}{\partial t}\right)_c$$

Relaxation time approximation: $$-\left(\frac{\partial f}{\partial t}\right)_c = -\frac{f - f_0}{\tau}$$

$\boldsymbol{p}$: Anisotropic distribution = Current

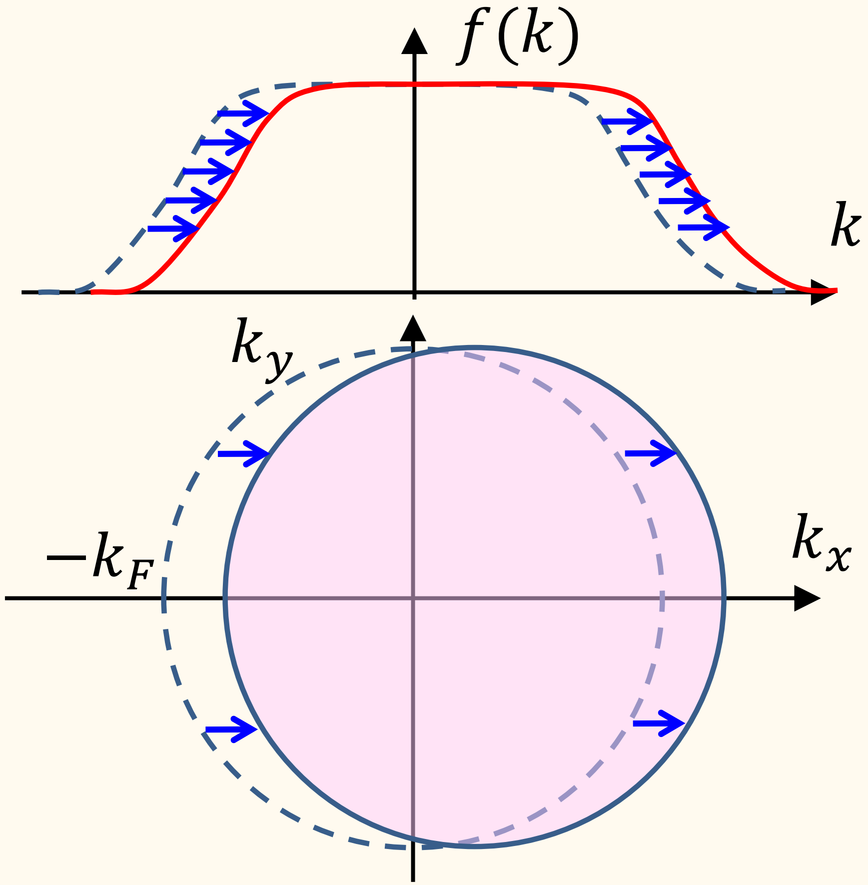
f_0: isotropic in $\boldsymbol{p}$-space → the collision term leads to current

$\frac{\partial f}{\partial t}$: time derivative of the distribution, zero for steady states

$\frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}}$: velocity times spatial gradient in the particle density → Diffusion current

$\boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}}$: force on the particles times gradient of f in $\boldsymbol{p}$-space → Drift current

Drift current by electric field



$$-e\mathbf{E}\cdot\frac{\partial f}{\partial \boldsymbol{p}} = -\frac{f-f_0}{\tau(\boldsymbol{p})}$$

$$\therefore f(\boldsymbol{p}) = f_0(\boldsymbol{p}) + e\tau(\boldsymbol{p})\mathbf{E}\cdot\frac{\partial f}{\partial \boldsymbol{p}} \approx f_0(\boldsymbol{p}) + e\tau(\boldsymbol{p})\mathbf{E}\cdot\frac{\partial f_0}{\partial \boldsymbol{p}} \approx f_0(\boldsymbol{p}+e\tau\mathbf{E})$$

$$\mathbf{E} = (\mathcal{E}_x, 0, 0)$$

$$\langle v\rangle = \int\frac{d^3k}{(2\pi)^3}\boldsymbol{v}(\boldsymbol{k})\left(f_0 + e\tau\mathbf{E}\cdot\frac{\partial f_0}{\hbar\partial\boldsymbol{k}}\right) = \int\frac{d^3k}{(2\pi)^3}\frac{\hbar k_x}{m}e\tau\mathcal{E}_x\frac{\partial f_0}{\hbar\partial k_x}$$
$$= \frac{e\mathcal{E}_x}{m}\int\mathscr{D}(E)\tau(E)\frac{\hbar^2k_x^2}{m}\frac{\partial f_0}{\partial E}dE$$

Density of states: $\mathscr{D}(E)\propto\sqrt{E}(=A\sqrt{E})$

Kinetic energy: $\frac{\hbar^2k_x^2}{m}\to 2\cdot\frac{E}{3}$

law of equipartition of energy

Drude formula

Paul Drude (1863 – 1906)

For metals ($T_F \gg 300$ K) Low temperature approximation: $\frac{\partial f_0}{\partial E} \approx -\delta(E - E_\mathrm{F})$

$$\langle v_x \rangle = -A \frac{e\mathcal{E}_x}{m} \frac{2\tau(E_\mathrm{F})}{3} E_\mathrm{F}^{3/2} \qquad n = \int_0^{E_\mathrm{F}} \mathscr{D}(E) dE = A \frac{2}{3} E_\mathrm{F}^{3/2}$$

$$\sigma = -e \frac{\langle v_x \rangle}{\mathcal{E}_x} = \frac{e^2 n \tau(E_\mathrm{F})}{m}$$

Drude formula for metals

For Maxwell distribution $(f_0 \approx A_\mathrm{F} \exp(-E/k_\mathrm{B} T))$

$$-\frac{\partial f_0}{\partial E} = -\frac{A_\mathrm{F}}{k_\mathrm{B} T} \exp\left[-\frac{E}{k_\mathrm{B} T}\right] = -\frac{f_0}{k_\mathrm{B} T} = -\frac{f_0}{(2\langle E \rangle / 3n)}$$

$$\sigma = e^2 \int \tau(E) \mathscr{D}(E) \frac{2E}{3m} \frac{3nf_0}{2\langle E \rangle} dE = \frac{ne^2 \langle \tau \rangle_E}{m}$$

Drude-like formula

$$\langle \tau \rangle_E \equiv \frac{\langle \tau E \rangle}{\langle E \rangle} = \int_0^\infty \tau(E) E^{3/2} f_0 dE \Big/ \int_0^\infty E^{3/2} f_0 dE$$

Diffusion current

No external force: $\boldsymbol{F} = \vec{0}, \quad f = f_0 + f_1$

Relaxation time approximation: $\boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} = -\frac{f_1}{\tau} \quad f_1 \approx \tau \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}}$

$$\boldsymbol{J} = (-e) \int_V \tau \boldsymbol{v}(\boldsymbol{v} \cdot \boldsymbol{\nabla} f) d\boldsymbol{r}$$

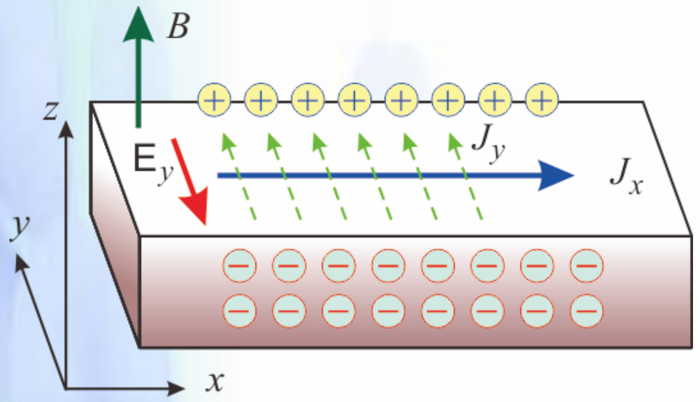
Take the x-direction to that of ∇f: $j_x = -e \int_{\mathrm{uv}} \tau v_x^2 \frac{\partial f}{\partial x} d\boldsymbol{r} = -e \left\langle \frac{\tau v^2}{3} \right\rangle \frac{\partial n}{\partial x}$

$$\boldsymbol{j} = (-e) D \boldsymbol{\nabla} n, \quad D = \left\langle \frac{\tau v^2}{3} \right\rangle$$

Einstein relation: $D = \frac{\tau}{3}\langle v^2 \rangle = \frac{\tau k_{\mathrm{B}} T}{m^*} = \frac{\mu}{e} k_{\mathrm{B}} T$

$\mu = \frac{e\tau}{m^*}$: mobility

The Hall effect



Galvanomagnetic effect: Force on electrons ← Lorentz force

$\boldsymbol{B} \parallel z$-axis

$$\boldsymbol{j} = \frac{ne^2}{m^*} \left(\begin{array}{cc|c} A_l & -A_t & 0 \\ A_t & A_i & 0 \\ \hline 0 & 0 & A_z \end{array} \right) \mathbf{E}$$

A_t term creates j_y hence E_y : Hall voltage (electric field)

The Hall coefficient is defined as $R_\mathrm{H} = \frac{\mathcal{E}_y}{J_x B_z}$ $\quad \mathcal{E}_y = -\frac{A_t}{A_l}\mathcal{E}_x$

With cyclotron frequency $\omega_c = \frac{eB}{m^*}$ $\quad \sigma_{xx} = \frac{ne^2}{m^*}A_l = \frac{ne^2}{m^*}\left\langle \frac{\tau}{1+(\omega_c\tau)^2} \right\rangle_E, \quad \sigma_{xy} = \frac{ne^2}{m^*}\left\langle \frac{\omega_c\tau^2}{1+(\omega_c\tau)^2} \right\rangle_E$

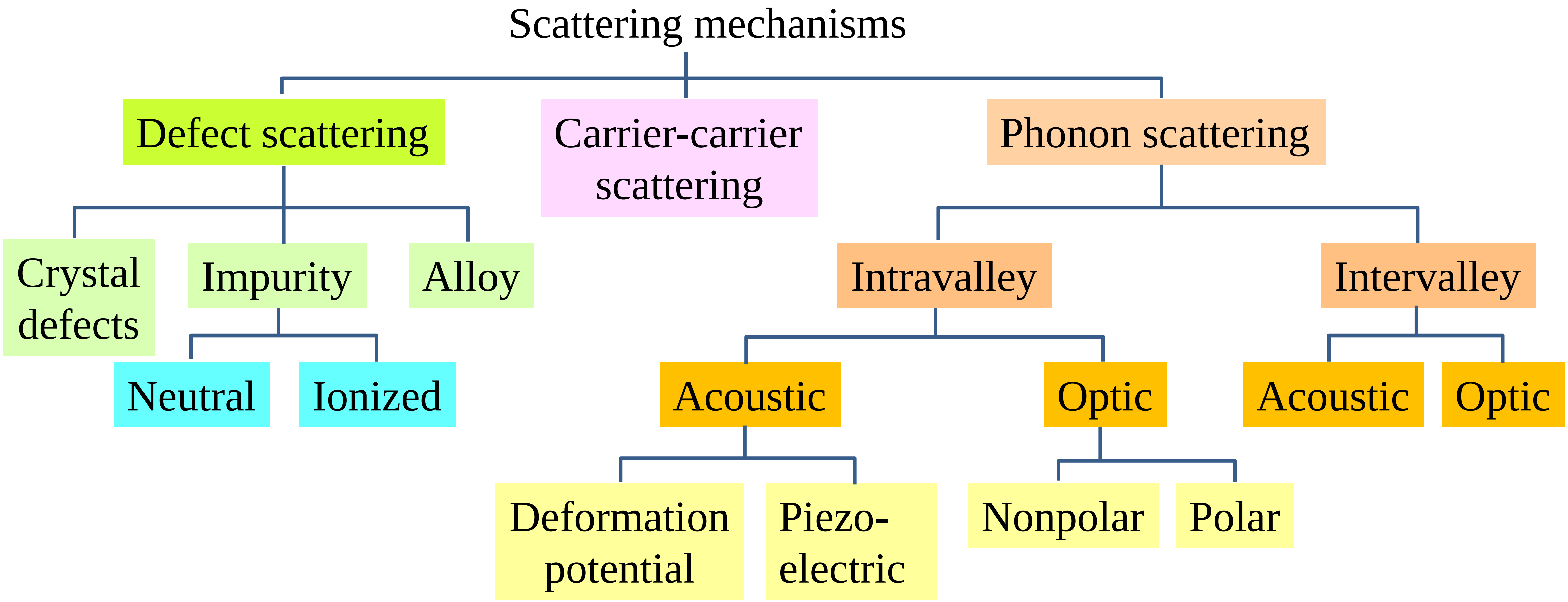
In case $\omega_c\tau \ll 1$

$$R_\mathrm{H} = -\frac{1}{ne}\frac{\langle\tau^2\rangle_E}{\langle\tau\rangle_E^2} = \frac{1}{n(-e)}\frac{\Gamma(2s+5/2)\Gamma(5/2)}{(\Gamma(s+5/2))^2} = \frac{r_\mathrm{H}}{n(-e)}$$

$r_\mathrm{H} \sim 1$ is called Hall factor

Mobility is defined and expressed as $\mu = \frac{v}{|\mathcal{E}|} = \frac{nev}{ne|\mathcal{E}|} = \frac{j}{ne|\mathcal{E}|} = \frac{\sigma}{ne} = \sigma|R_\mathrm{H}| = \frac{e\tau}{m^*}$

Carrier scattering mechanisms



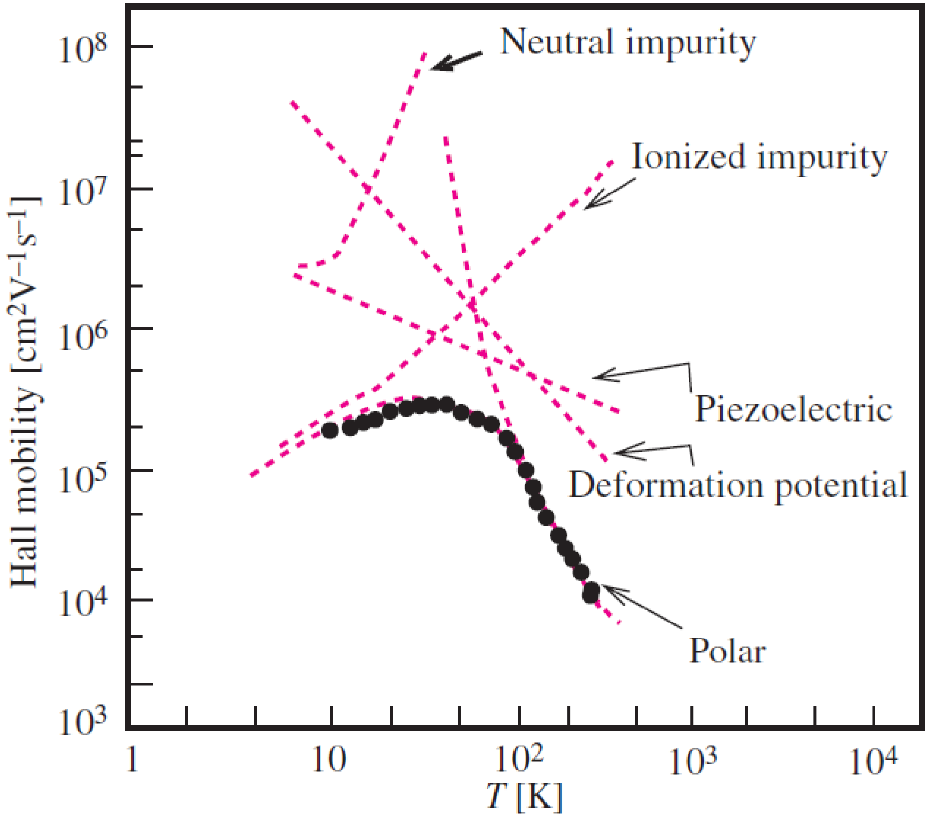
The parameter which represents the scattering mechanism
= averaged time interval of scattering

Scattering time: τ_β β : scattering mechanism

Matthiessen's rule and effect of scattering on the electric transport

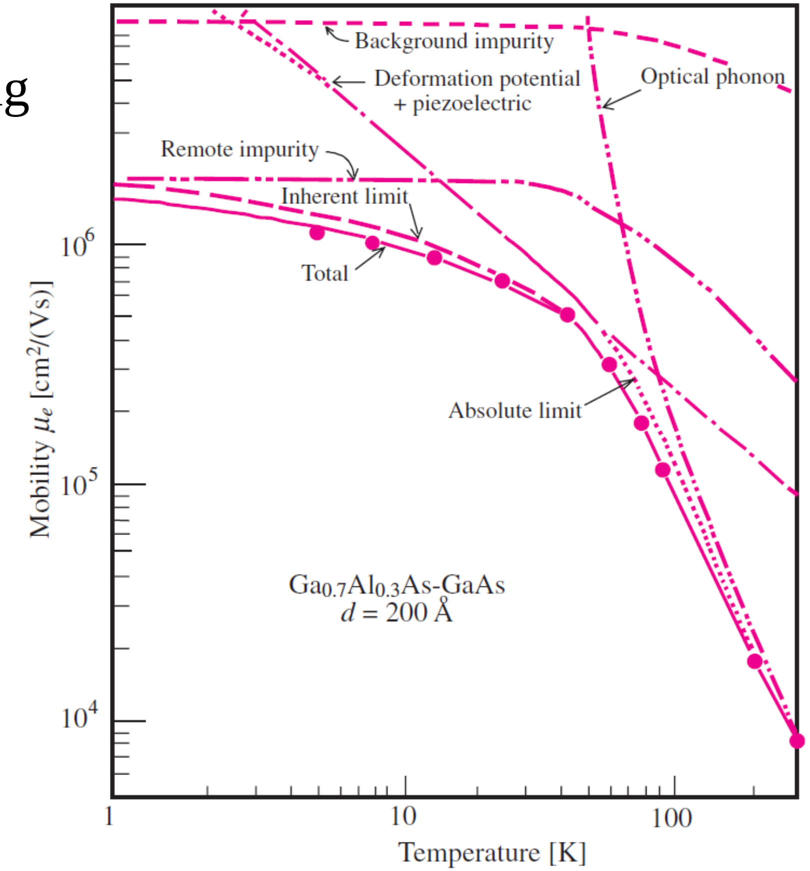
Matthiessen's rule (series connection of scattering)

$$\frac{1}{\tau_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\tau_\beta} = \frac{1}{\tau_{\mathrm{defects}}} + \frac{1}{\tau_{\mathrm{cattier}}} + \frac{1}{\tau_{\mathrm{lattice}}} + \cdots \qquad \frac{1}{\mu_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\mu_\beta} = \frac{1}{\mu_{\mathrm{defects}}} + \frac{1}{\mu_{\mathrm{cattier}}} + \frac{1}{\mu_{\mathrm{lattice}}} + \cdots$$



Fletcher *et al.*, J. Phys. C **5**, 212 (1972)

Reduction of impurity scattering by modulation doping structure



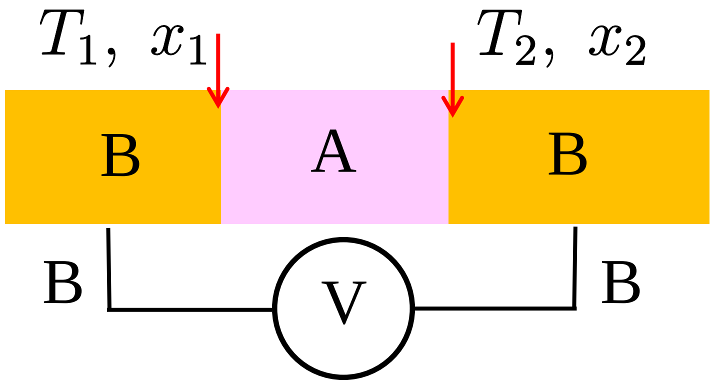
Walukiewicz *et al.* Phys. Rev. B **30**, 4571 (1984).

Heat transport, thermoelectric effect

Heat flux density: $j_{qx} = \langle n v_x (E-\mu) \rangle = \int_0^{\infty} v_x (E-\mu) f(E) \mathscr{D}(E) dE$

Temperature gradient ∇T Carrier thermal conductivity $\kappa_n = -\dfrac{j_{qx}}{\partial T/\partial x}$ $(\boldsymbol{j}_q = -\hat{\kappa}\nabla T)$

Seebeck effect



J: current, V: voltage, T: temperature, Q: heat flow

$S_{\mathrm{AB}} = \dfrac{V_{\mathrm{AB}}}{\Delta T}$ Seebeck coefficient

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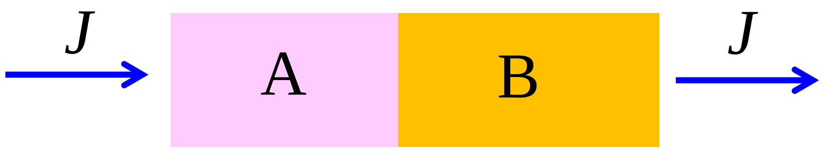
Peltier effect



$\Pi_{\mathrm{AB}} = \dfrac{Q_{\mathrm{AB}}}{J}$ Peltier coefficient

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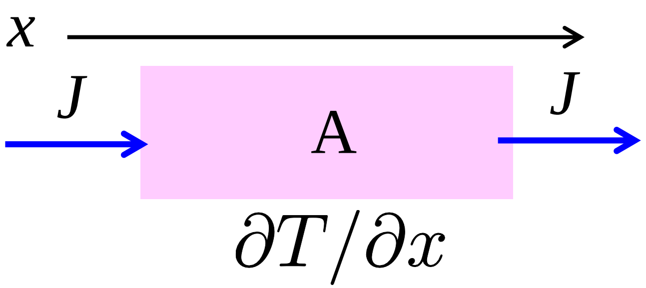
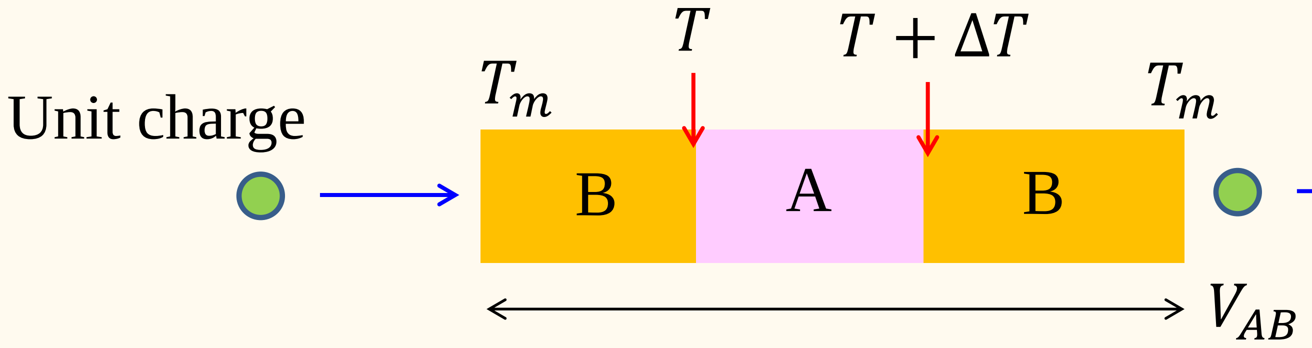
Thomson effect



$\tau = \dfrac{\partial Q/\partial x}{J(\partial T/\partial x)}$ Thomson coefficient

can be obtained from single material

The Kelvin relations



Quasi-static process → Thermodynamics can be applied

First law of thermodynamics $$V_{\mathrm{BA}} + \Pi_{\mathrm{BA}}(T) - \Pi_{\mathrm{BA}}(T+\Delta T) + (\tau_{\mathrm{B}} - \tau_{\mathrm{A}})\Delta T = 0$$

Second law of thermodynamics $$\frac{\Pi_{\mathrm{BA}}(T)}{T} - \frac{\Pi_{\mathrm{BA}}(T+\Delta T)}{T+\Delta T} + \frac{\tau_{\mathrm{B}} - \tau_{\mathrm{A}}}{T}\Delta T = 0$$

Taking $\Delta T \to 0$, these two become $$\frac{dV_{\mathrm{BA}}}{dT} - \frac{d\Pi_{\mathrm{BA}}}{dT} + \tau_{\mathrm{B}} - \tau_{\mathrm{A}} = 0, \quad \frac{d}{dT}\left(\frac{\Pi_{\mathrm{BA}}}{T}\right) = \frac{\tau_{\mathrm{B}} - \tau_{\mathrm{A}}}{T}$$

The second equation becomes $$\tau_{\mathrm{B}} - \tau_{\mathrm{A}} = T\frac{d}{dT}\left(\frac{\Pi_{\mathrm{BA}}}{T}\right) = \frac{d\Pi_{\mathrm{BA}}}{dT} - \frac{\Pi_{\mathrm{BA}}}{T}$$

The Kelvin relations are obtained as $$\therefore S_{\mathrm{AB}} = \frac{\Pi_{\mathrm{AB}}}{T}, \quad \frac{dS_{\mathrm{AB}}}{dT} = \frac{\tau_{\mathrm{A}} - \tau_{\mathrm{B}}}{T}$$

The absolute Seebeck, Peltier coefficients can be obtained from the relations.

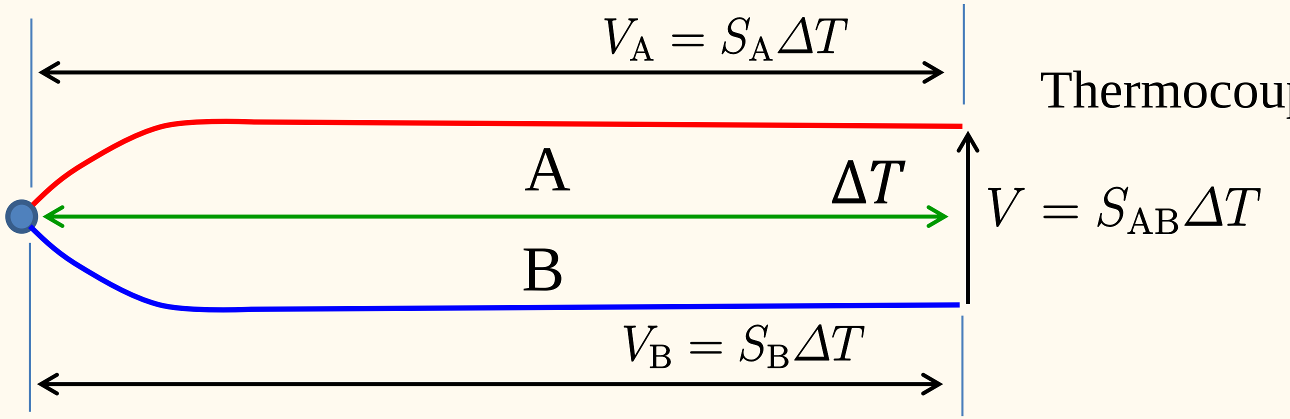
Seebeck coefficient as material constant

Material specific (absolute) constant can be experimentally obtained from

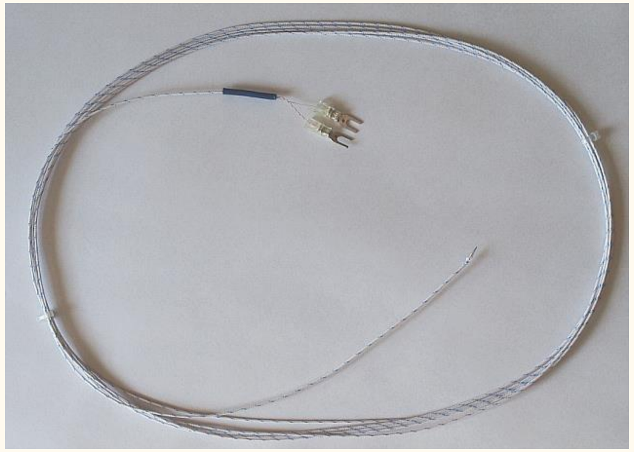
$$S_{\mathrm{A}}(T) \equiv \int_0^T \frac{\tau_{\mathrm{A}}(T')}{T'} dT'$$

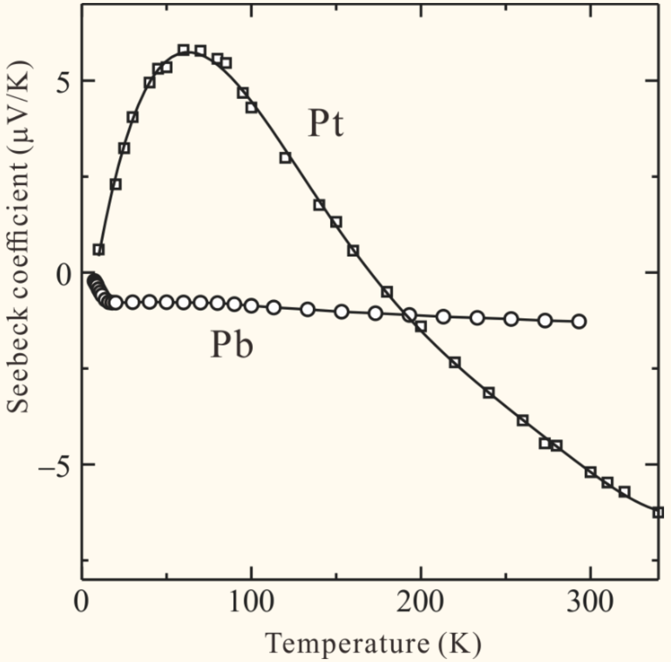
Then for other materials

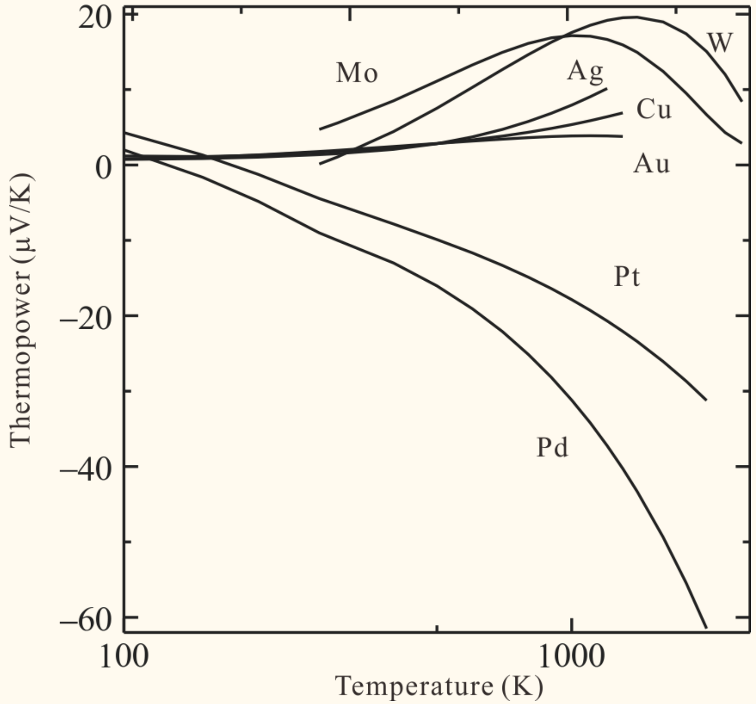
$$S_{\mathrm{AB}} = S_{\mathrm{A}} - S_{\mathrm{B}}$$



Thermocouple







Boltzmann equation and thermoelectric constants

For the thermoelectric effect, we need to consider (only) ∇T

The distribution function in lhs is replaced with unperturbed one.

$$\boldsymbol{v}\cdot\nabla f+\frac{\boldsymbol{F}}{m^*}\nabla_v f=-\frac{f-f_0}{\tau(E)}\approx\left[\boldsymbol{v}\cdot\nabla+\frac{\boldsymbol{F}}{m^*}\nabla_{\boldsymbol{v}}\right]f_0$$

With $a\equiv-\dfrac{E-E_{\mathrm{F}}}{k_{\mathrm{B}}T}$

$$\frac{\partial f_0}{\partial T}=\frac{\partial f_0}{\partial E}\frac{\partial E}{\partial a}\frac{\partial a}{\partial T}=\frac{\partial f_0}{\partial E}(-k_{\mathrm{B}}T)\left(\frac{E-E_{\mathrm{F}}}{k_{\mathrm{B}}T^2}\right)=\frac{\partial f_0}{\partial E}\frac{E_{\mathrm{F}}-E}{T}$$

From the above we can rewrite

$$\nabla f_0=\nabla T\frac{E_{\mathrm{F}}-E}{T}\frac{\partial f_0}{\partial E},\qquad \nabla_v f_0=\nabla_v E\frac{\partial f_0}{\partial E}=m\boldsymbol{v}\frac{\partial f_0}{\partial E}$$

Then the Boltzmann equation gives

$$f=f_0-\tau(E)\boldsymbol{v}\cdot\left[-e\mathbf{E}+\frac{E_{\mathrm{F}}-E}{T}\nabla T\right]\frac{\partial f_0}{\partial E}$$

Substituting the above and $\mathbf{E}=(\mathcal{E}_x,0,0)$ into the current expression

$$j_x=-e\langle nv_x\rangle=-e\int_0^\infty v_x f(E)\mathscr{D}(E)dE$$

$$=e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x+\frac{E_{\mathrm{F}}-E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE$$

Boltzmann equation and thermoelectric constants (2)

$$j_x = e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x + \frac{E_F - E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE = 0$$

$j_x = 0$ means the balancing of the drift current and the diffusion current

Then the Seebeck coefficient is calculated as

$$S = \frac{\mathcal{E}_x}{\partial T/\partial x} = \int_0^\infty v_x^2\tau\frac{E_F - E}{eT}\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE \Big/ \int_0^\infty v_x^2\tau\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE$$

$$= \frac{1}{eT}\left[E_F - \int_0^\infty \tau E^2\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE \Big/ \int_0^\infty \tau E\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE\right]$$

$$= \langle\tau E\rangle_E/\langle\tau\rangle_E$$

Maxwell approximation

$$\frac{\partial f_0}{\partial E} = -\frac{f_0}{k_B T}$$

Energy dependence of relaxation time

$$\tau \propto E^s$$

$$S = -\frac{1}{eT}\left[\frac{\langle\tau E\rangle_E}{\langle\tau\rangle_E} - E_F\right] = -\frac{1}{eT}\left[\left(\frac{5}{2}+s\right)k_B T - E_F\right]$$

Seebeck measurement provides information on E_F and scattering mechanisms

Peltier device

$$S = \frac{1}{qT}\left[\left(\frac{5}{2}+s\right)k_{\mathrm{B}}T - E_{\mathrm{F}}\right] \qquad \Pi = ST$$

Sign of the coefficient changes with carrier charge