Irreversible Thermodynamics & Transport

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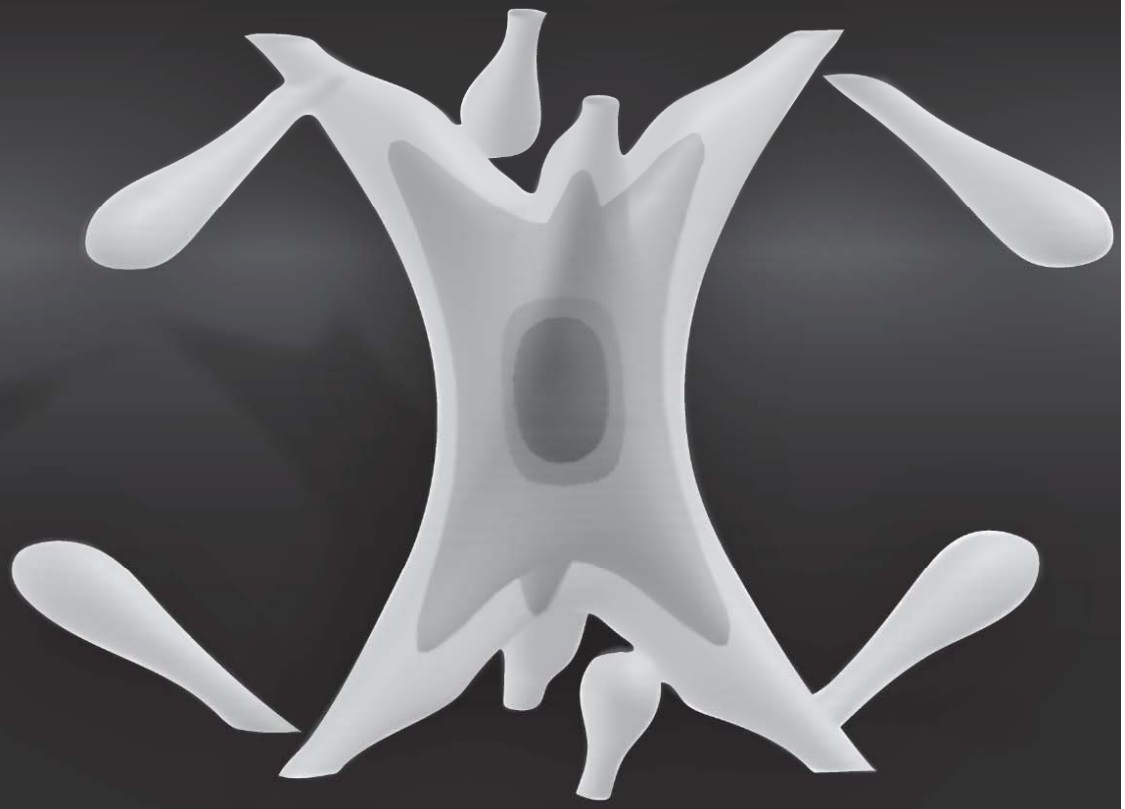
CEM Miniworkshop
Wednesday May 24 2017



Center for Emerging Materials
NSF MRSEC DMR 1420451

Art: Fermi surface of Bi_2Se_3, by Renee Ripley

Structure of the lecture

1. Introduction (20%)
    - Thermodynamics
    - Transport what? Mass, entropy, charge, magnetization, ...
    - Onsager
2. Electrons (50%)
    - Types of transport
    - Charge, spin, heat fluxes
    - Band transport
    - Multicarrier transport
    - Transport of spins on conduction electrons
3. Magnons (30%)
    - Fluxes of spins on localized electrons: magnons
    - Spin and heat fluxes
    - Advective transport
    - Spin Seebeck effect

Thermodynamics

U is the internal energy

$U(X_0, X_1, \ldots X_\mu, \ldots)$ is a macroscopic function of size of the system

S is the entropy.

Entropy is the function that, by definition, gets maximized as the system tends to equilibrium

$S(X_0, X_1, \ldots X_\mu, \ldots)$ is a macroscopic function of size of the system

The ensemble of the **extensive properties X_i** fully define the internal energy and the entropy of the system

If $S(X)$ or $U(X)$ are known, all thermodynamic properties of the system are known. They are the fundamental equations for the state of the system.

Thermodynamic potentials

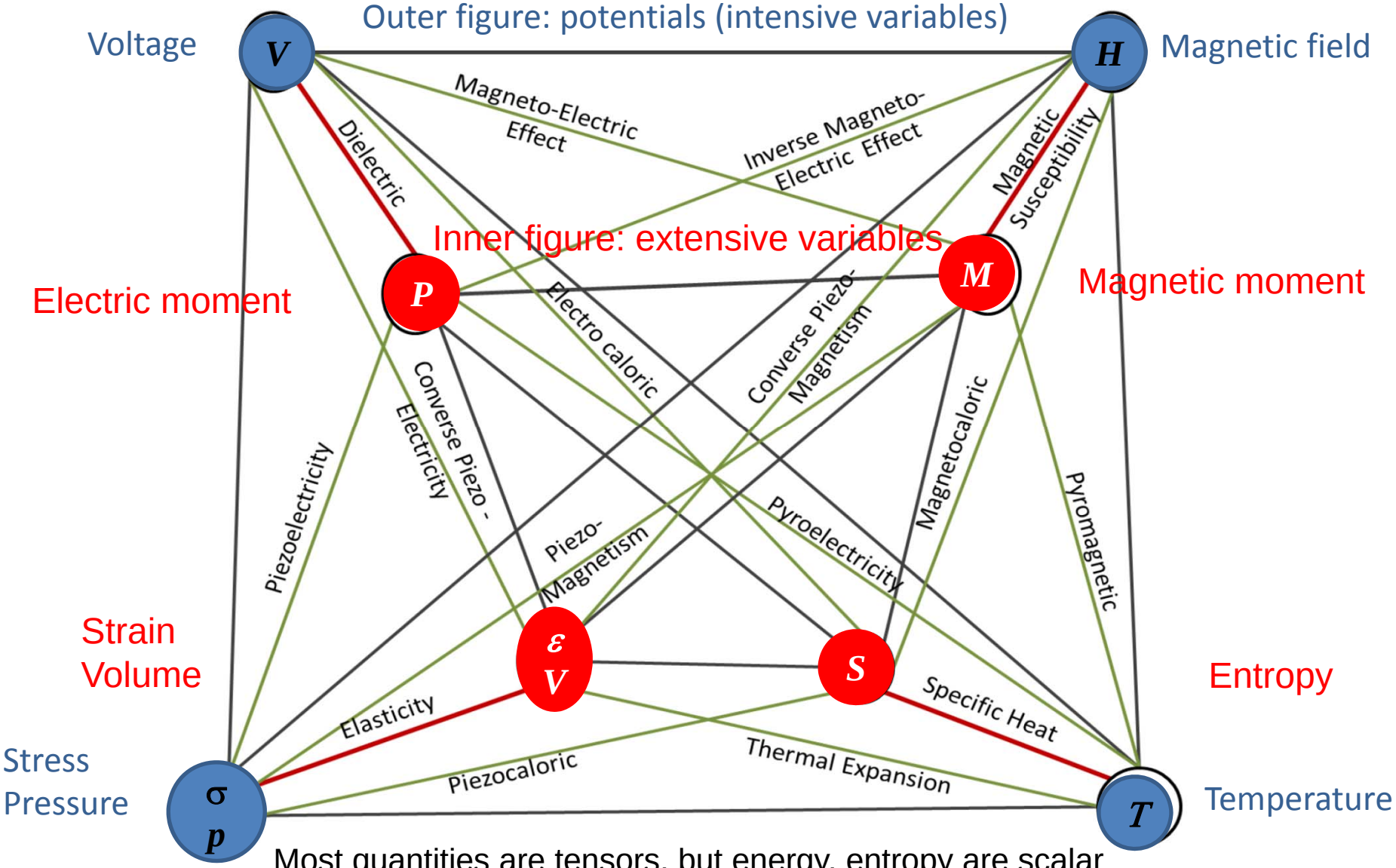
The potentials are related to the derivatives of the entropy vis-à-vis their respective extensive properties

$$T \equiv \left(\frac{\partial S}{\partial U} \right)_{X_i}^{-1} \qquad \phi_i \equiv -T^{-1} \left(\frac{\partial S}{\partial X_i} \right)_{X_{j \neq i}}$$

Effect	Intensive Potential (ϕ_μ)	Extensive (X_μ)	Specific Extensive
Thermal	Temperature T	Entropy S	Spec. Entropy
Electrical	Electrochemical potential μ_ϕ	Electric moment $\vec{P}$	Polarization density
Magnetic	Magnetic field $\vec{H}$	Magnetic moment $\vec{M}$	Magnetization density
Mechanical	Stress $\vec{\sigma}$	Deformation ($\Delta x\ \Delta y\ \Delta z$)	Strain $\vec{\varepsilon}$
Mechanical (gas or liquid)	Pressure p	Volume V	1
Chemical	Electrochemical potential μ_ϕ	Number of particles N	Density (N/V)

Equilibrium thermodynamics

not describing compositional changes, i.e. no chemistry



Most quantities are tensors, but energy, entropy are scalar

J. F. Nye, "Physical properties of crystals", Oxford, Clarendon (1960)

Irreversible thermodynamics = transport

Flux $\mathbf{j}_i$ of extensive property X_i:

- mass
- particle number
- charge
- entropy
- spin (magnetic moment)

Driven by **thermodynamic force $\mathcal{F}_i = -\nabla\phi_i$ gradient of a potential,**

Gradient in:

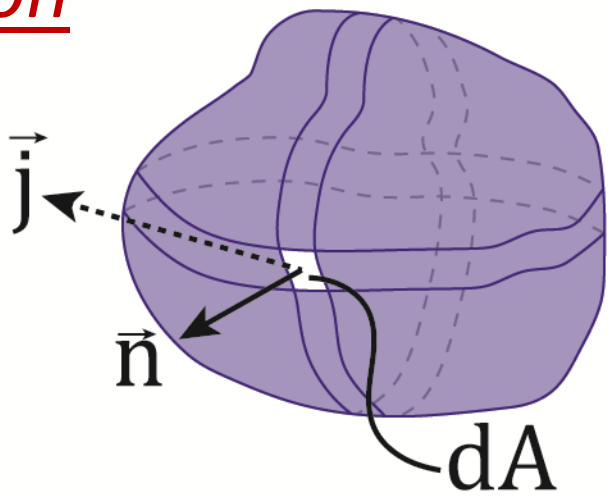
- pressure => mechanical force drives water through a pipe
- chemical potential => force that drives diffusion
- electrochemical potential => electric field drives current
- temperature => thermal gradients drive heat flow
- magnetization => magnetic force keeps your magnet on your refrigerator door

$$\vec{F} = \nabla(\vec{M} \cdot \vec{H})$$

Continuity equation

Integral $$\frac{dX_i}{dt} + \oiint_A \mathbf{j}_i . d\mathbf{A} = \Sigma_i$$

Differential (Gauβ) $$\frac{\partial X_i / V}{\partial t} + \nabla \bullet \mathbf{j}_i = \Sigma_i / V$$



$\mathbf{A}$ is any imaginary closed surface, that encloses a volume V

$\oiint_A \square d\mathbf{A}$ denotes a surface integral over that closed surface,

X is the total amount of the quantity in the volume V,
$\mathbf{j_X}$ is the flux of X,
t is time,
Σ is the net rate that X is being generated inside the volume V.

When X is being generated, it is called a "source" and it makes Σ more positive.
When X is being destroyed, it is called a "sink" and it makes Σ more negative.

Continuity equation

2. Is the quantity transported conserved?

YES:

- mass m
- charge c

$$\frac{dX_i}{dt} + \oiint_S \mathbf{j}_i . d\mathbf{S} = 0$$

=> **results in flow lines and equipotential lines in a real medium**

NO:

- entropy Q/T
- spin s
- photoexcited electron-hole pairs in semiconductors

$$\frac{dX_i}{dt} + \oiint_S \mathbf{j}_i . d\mathbf{S} = \Sigma$$

=> **results in "drift-diffusion equation"**

The Onsager Relation

A force $\mathcal{F}_i$ that arises from one of the potentials - $\nabla\phi_i$ can affect the flux **j** of any extensive X :

$$\vec{\mathbf{j}}_i = \vec{\mathbf{j}}_i(\mathcal{F}_0, \mathcal{F}_1, \ldots \mathcal{F}_i, ..)$$

1. **Only applies if relation between forces and fluxes is linear.**

2. **Includes mixed conduction effects**

   1.1 Temperature gradients can create concentration gradients and mass transport: **thermal diffusion and Soret effect**

   1.2 Electric fields can push electrically charged ions: **electrophoresis**

   1.3 Temperature gradients can create gradients in electron concentrations and thus voltages: **thermoelectric effects**

2. **Covers Advection or Drag:** a specie A in a mixture of A and B can be affected by a force, where specie B is much less affected. When A-B interactions are stronger than A-A or B-B interactions, the force acting on A results in a flux of B

   2.1 Mud dragged by water (2-phased flow)

   2.2 Phonon-Electron, Magnon-Electron or Phonon-Magnon Drag

Onsager is the 1st term of a series expansion (Linear transport)

Expand this into powers of the forces (here only for the x-direction flux vector):

$$j_i^x(\mathcal{F}_0, \mathcal{F}_1, \ldots \mathcal{F}_i, ..) = \sum_j \mathcal{L}_{ji}\mathcal{F}_j + \frac{1}{2!}\sum_k \sum_j \mathcal{L}_{kji}\mathcal{F}_k\mathcal{F}_j + \ldots$$

Kinetic coefficients: $\mathcal{L}_{ji} = \left(\frac{\partial j_i^x}{\partial \mathcal{F}_j}\right)_{\mathcal{F}_{\ell \neq j}=0}$ (generalized conductivities)

Kinetic coefficients are functions only of the potentials:

$$\mathcal{L}_{ji} = \mathcal{L}_{ji}(\phi_0, \phi_1, \ldots \phi_i, \ldots)$$

The Onsager relation

$$\vec{\mathbf{j}}_i = \sum_j \overleftrightarrow{\mathcal{L}}_{i,j}\vec{\mathcal{F}}_j$$

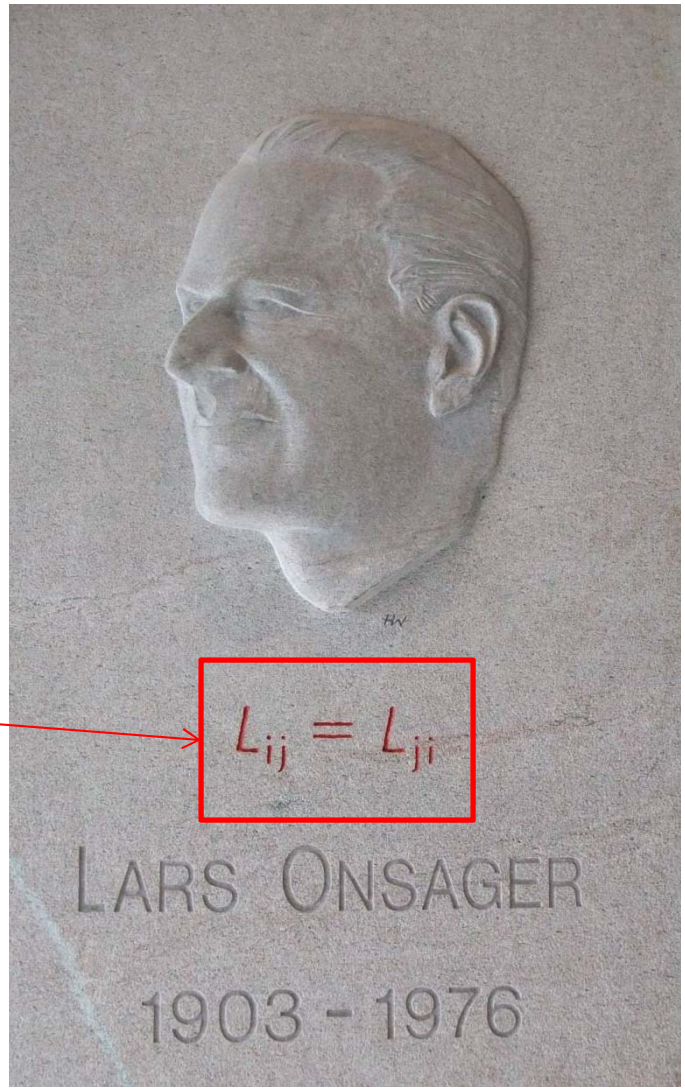
Linear transport: Onsager

Ohm's law, Fourier's law, Fick's law, ...

$$\vec{\mathbf{j}}_i = \sum_j \overleftrightarrow{\mathcal{L}}_{i,j} \vec{\mathcal{F}}_j$$

Dissipation: $\vec{\mathbf{j}} \bullet \vec{\mathcal{F}} = \dot{Q} = T\dot{S}$

Reciprocity:



Monument, NTNU, Trondheim

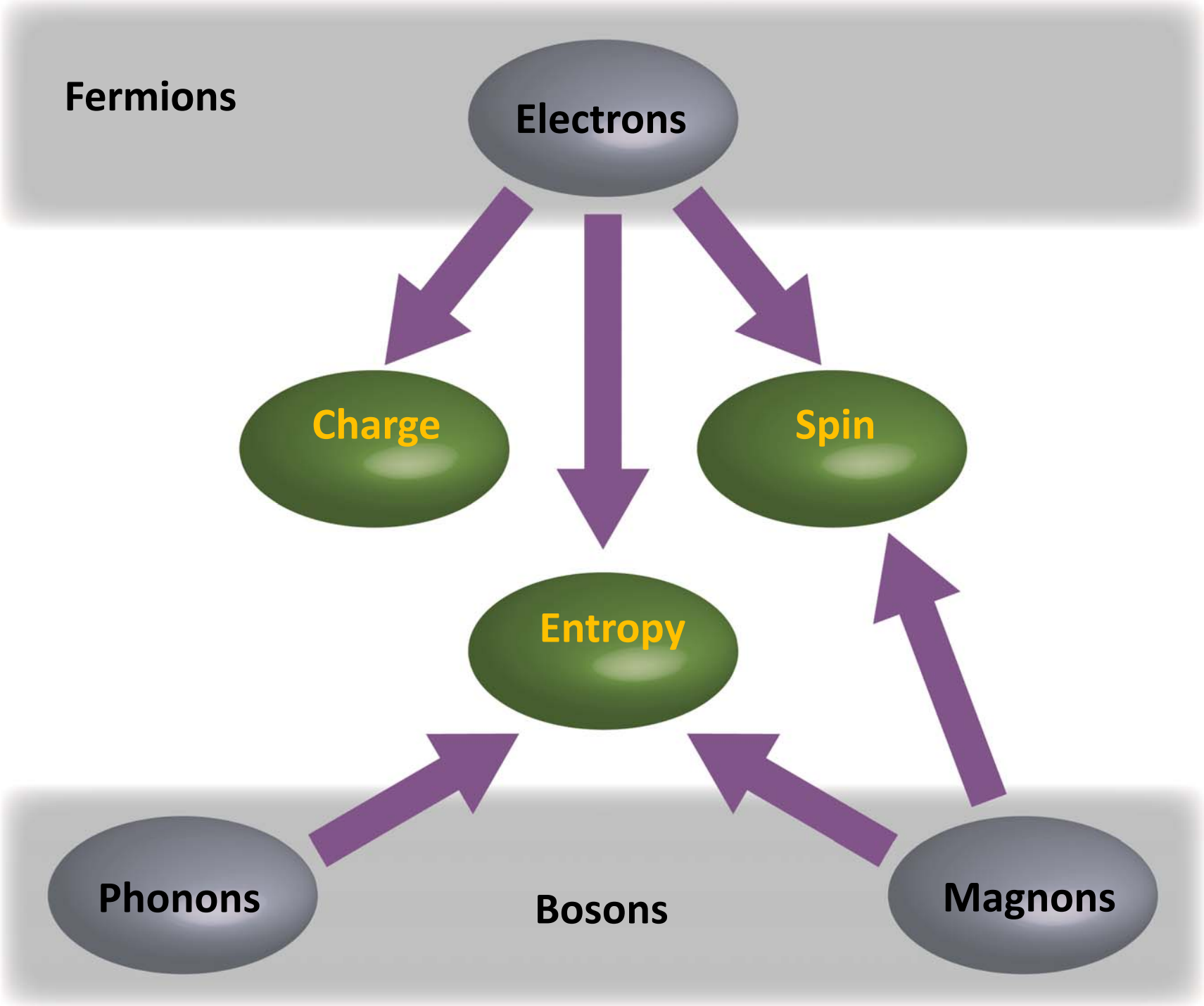
proofs

1. H. Callen, chap 15 and section 16.5

2. D. Kondepuri & I. Prigogine pp 355-358

3. L. Onsager, Phys. Rev. ***37*** *405 (1931)*

4. L. Onsager, Phys. Rev. ***38*** *2265 (1931)*


Fermions
Electrons
Charge
Spin
Entropy
Phonons
Bosons
Magnons

2. Delocalised electron transport

References:
J. M. Ziman, Electrons and Phonons, Oxford U. P. (1960)

A. Abrikosov, Fundamentals of the Theory of Metals, North Holland, Amsterdam (1988)

N. F. Mott and E. A. Davis, Electronic Processes in Non-crystalline Materials, Oxford , Clarendon Press, 2nd ed. (1979)

K. Behnia, Fundamentals of Thermoelectricity, Oxford U.P. (2015)

K. Behnia, On mobility of electrons in a shallow Fermi sea over a rough seafloor, in preparation, arXiv 1507.06084 (2015)

Types of electron transport

1. **Mean free path effects:**
    1. **Diffusive regime**: mean free path of the particles that carry heat, charge of spin is smaller than sample dimensions. Microscopic transport mechanisms governed by the **Boltzmann** equation.
        1. **The Fermi liquid**: electrons like a classic electron ideal gas
        2. **The band structure**: add periodic potential => **BAND TRANSPORT**
    2. **Hopping/tunneling regime**: mean free path too short compared to defects/traps
    3. **Ballistic regime**: mean free path limited by sample dimensions: Microscopic transport governed by **ray** equations.
2. **Quantum corrections to transport, electron wavefunction effects**:
    1. **Size-quantization**: particle wavefunction limited by sample dimensions
    2. **Weak Localization**: electron wavefunction interference w. impurities
    3. **Landau quantization**: electron wavefunction <= applied magnetic field
3. **Drag regimes** Phonon-electron Drag, magnon-electron drag

The four length scales for electron transport

1. The spatial extent of the electron wavefunction.
   - Electron (de Broglie) wavelength λ
   - Since transport is dominated by electrons at the Fermi level, the λ that matters is that at the Fermi wavevector value $k_F = 1/2\pi\lambda$
   - In a metal, it is related to the electron density $n = k_F^3/3\pi^2$

2. The electron mean free path ℓ
   - Mean distance between collisions
   - Sometimes it is important to distinguish between collisions that transfer energy (inelastic collisions) and those that transfer momentum only.
   - Often measured by the mobility, but this implies knowledge of 1: $\mu = \frac{e}{\hbar}\frac{\ell}{k_F}$

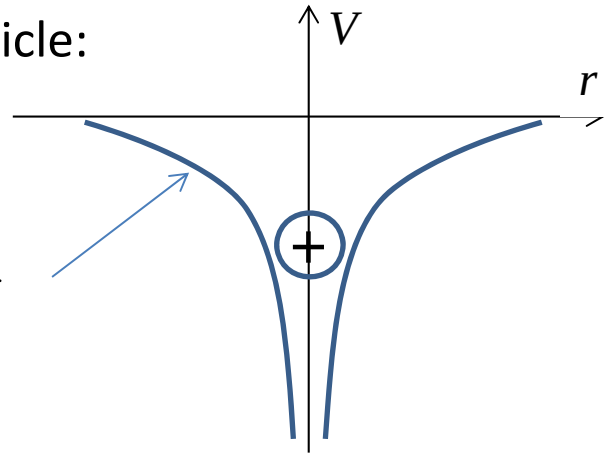
3. The effective Bohr radius a_B^*
   - Takes into account Coulombic interactions between electrons $a_B^* = \frac{\varepsilon}{\varepsilon_0}\frac{m_e}{m^*}a_B$

4. Thomas-Fermi screening length r_{TF}
   - Takes into account electrostatic screening
   - 3b, 3 and 1 are related by $r_{TF} = \frac{\pi a_B^*}{4k_F}$

The Thomas-Fermi screening length r_{TF}

Spatial potential distribution around a charged particle:

$$V(r) = e\frac{e^{-r/r_{TF}}}{4\pi\varepsilon r}$$



- In a metal with electrons following a Fermi-Dirac distribution, this locally perturbs the charge distribution.
- Ziman uses the Poisson equation with this as perturbative electric potential to obtain:

$$r_{TF} = \frac{\varepsilon_0}{e^2 \mathcal{D}(\mu_\phi)}$$

- In the Fermi liquid picture:

$$r_{TF} = \frac{\pi a_B^*}{4k_F}$$

J. M. Ziman, Principles of the Theory of Solids, Cambridge University Press, Cambridge (1960)

Criteria

1. The **Anderson (Ioffe-Regel) limit** based on **Quantum Mechanics**
   For electrons to develop a band structure, the electron wavevectors must exceed the mean free path

$$k_F \ell > 1$$

1b. The **minimum metallic conductivity** is a macroscopic expression of Anderson
   At T =0, this is the smallest non-zero value that the electrical conductivity can have:

$$\sigma > \sigma_{\min} = \frac{\pi^2}{z}\frac{e^2}{h}\frac{1}{a}$$

$$\sigma_{\min} = \frac{610\ \Omega^{-1}\mathrm{cm}^{-1}}{a(\text{Å})}$$

(octahedral bonds, z=6)

a = interatomic distance (Å); Z = atom coordination number

2. The **Mott criterion for metal-insulator transitions** based on **Electrodynamics**
   For electrons to conduct freely in a solid, the screened wavefunctions of the free electrons must overlap each-other.

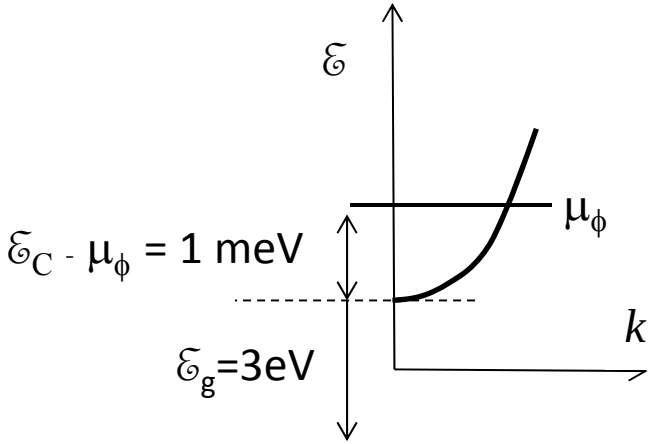
   In 3-dimensions:

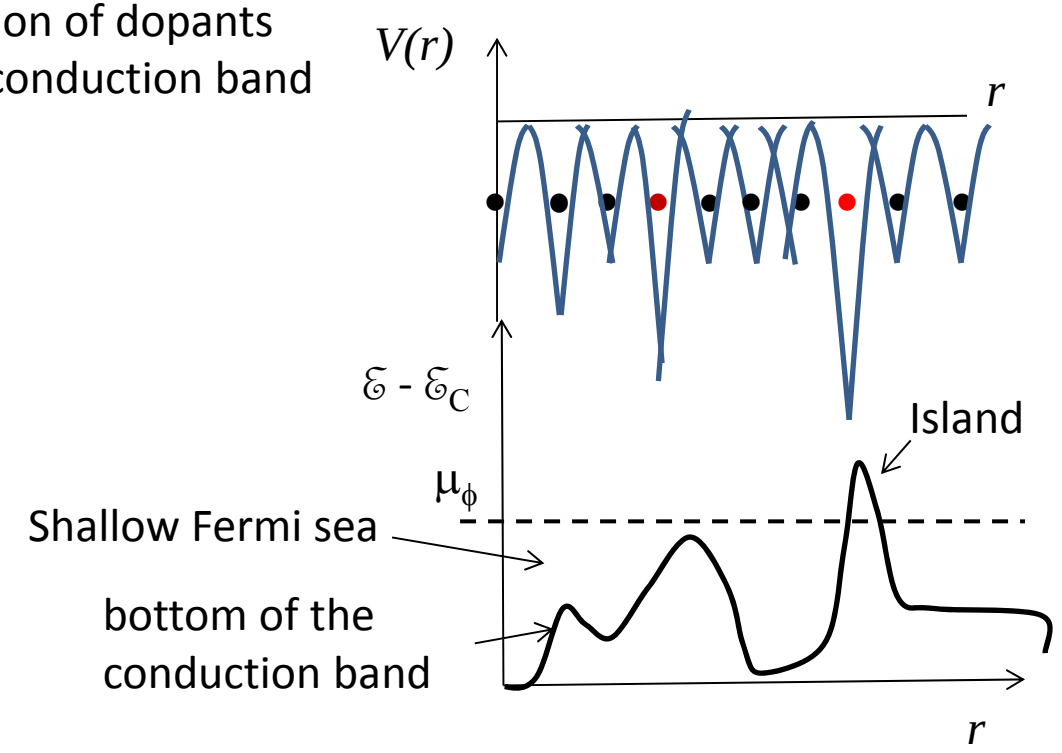
$$\frac{\left(a_B^*\right)^3}{n} \geq \frac{1}{2^6}\frac{\pi}{3}$$

The metal-insulator transition (Mott)

Consider a degenerately-doped semiconductors, with the Fermi energy near the band edge

Consider local variations of the composition of the sample
(*r* = spatial variable), stochastic distribution of dopants
=> local variations of the bottom of the conduction band





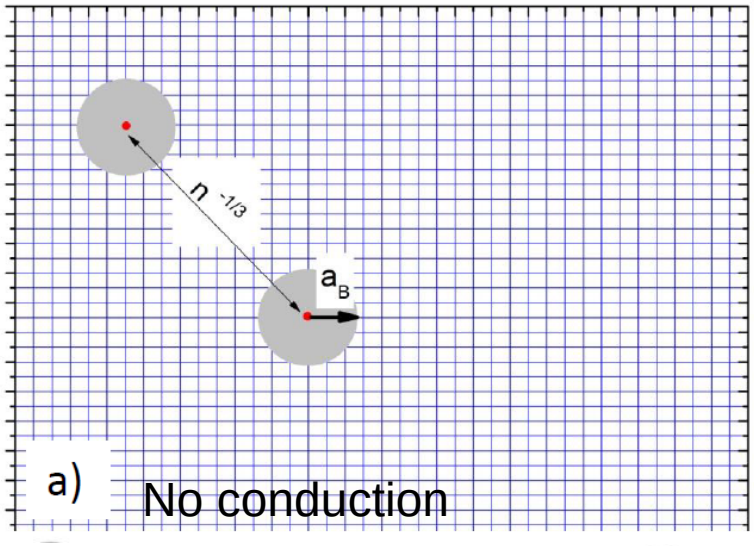
In the 1-dimensional picture and at *T=0*, one single island will block conduction, **unless** the island is screened electrostatically, i.e. if the effective Bohr radius is larger than the screening length around the island:

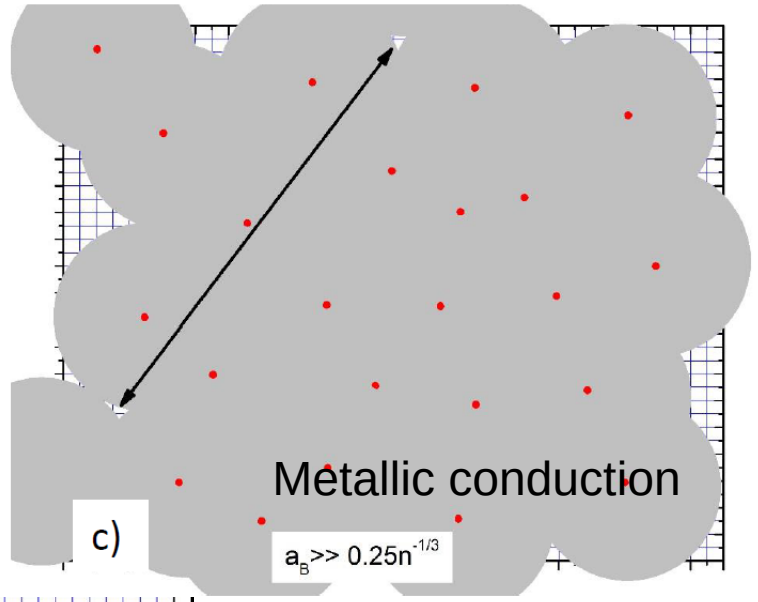
Band conduction if: $a_B^* > r_{TF}$

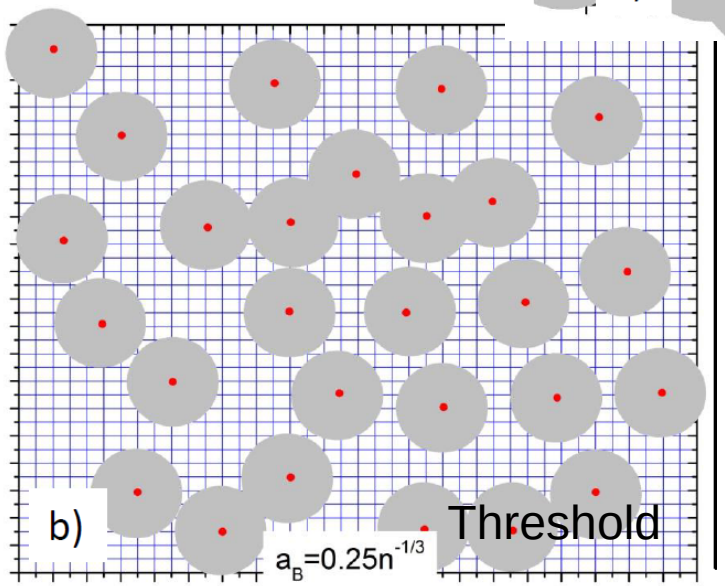
The Mott metal-insulator transition

$a_B^* > r_{TF}$ Substitute the variables: If $a_B^* n^{1/3} > \frac{1}{4}\left(\frac{\pi}{3}\right)^{1/3} \approx 0.253$ => **Band conduction**

If $a_B^* n^{1/3} < \frac{1}{4}\left(\frac{\pi}{3}\right)^{1/3} \approx 0.253$ => **Freeze-out** at low T





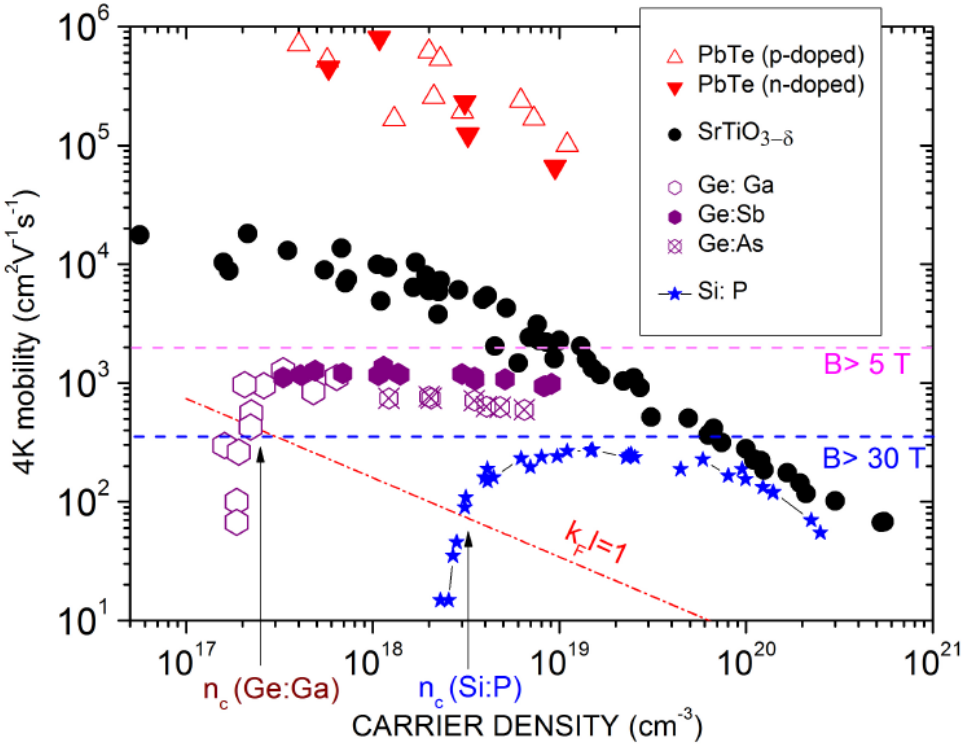


The Mott metal-insulator transition

If $a_B^* n^{1/3} > \frac{1}{4}\left(\frac{\pi}{3}\right)^{1/3} \approx 0.253 \Rightarrow \boxed{n > n_{CRIT} = 0.016/\left(a_B^*\right)^3}$ => **Band conduction**

If $n < n_{CRIT}$ => **Freeze-out** at low temperatures

Relation to mobility $\ell = \tau v_F \quad => \quad \mu = \frac{e}{\hbar}\frac{\ell}{k_F}$



At low temperature, it is the stochastic distribution of impurities that scatters.

SYSTEM	ϵ/ϵ_0	m^*/m_e	a_B^* (nm)	n_{CRIT}(cm^-3)
Si	12.5	0.45	1.5	4x10^18
Ge	16	0.24	3.5	3x10^17
$SrTiO_3$	20000	1.8	600	7x10^10
PbTe	1000	0.07	800	3x10^10

Conclusions:

1. Better mobility from higher dielectric constant
2. Better mobility from lower effective mass
3. You cannot freeze-out narrow-gap semiconductors

Band Transport

Dispersion relation: $\mathcal{E}(\vec{k}); \vec{v} = \frac{1}{\hbar}\frac{\partial \mathcal{E}(\vec{k})}{\partial \vec{k}}$

At thermodynamic equilibrium the particles have a statistical distribution function f^0 (Bose-Einstein or Fermi-Dirac). Under the forces, the probability that a particle have a certain position and momentum value $(\vec{k},\vec{r})$ becomes $f(\vec{k},\vec{r}) \neq f^0$

The flow of particles carried by an electron of momentum and position is the probability to find that electron times its velocity and charge: $j_{\mathrm{N},\vec{k},\vec{r}} = \vec{v} f(\vec{k},\vec{r})$

The flux of particles is the integral over all momenta of all electrons $\vec{j}_N = \iiint_{\vec{k}} \vec{v} f(\vec{k},\vec{r}) d\vec{k}$

The flux of electrical current is $\vec{j}_C = e\vec{j}_N$

The flux of energy is the integral over all momenta of all electrons: $\vec{j}_{\mathrm{U}} = \iiint_{\vec{k}} \mathcal{E}\vec{v} f(\vec{k},\vec{r}) d\vec{k}$

The flux of heat is $\vec{j}_Q = \vec{j}_U - \mu_\phi \vec{j}_N \quad \vec{j}_{\mathrm{Q}} = \iiint_{\vec{k}} (\mathcal{E} - \mu_\phi)\vec{v} f(\vec{k},\vec{r}) d\vec{k}$

The Boltzmann equation

The effects of the thermodynamic forces arises from the difference between f^0 and $f(\vec{k},\vec{r})$

Apply a "thermodynamic acceleration" $\vec{a} = \vec{\mathcal{F}} / m$

After a time interval δt the position and velocity of the particle have changed:

$$\vec{v} \to \vec{v} + m^{-1}\vec{\mathcal{F}}\delta t; \vec{k} \to \vec{k} + \hbar^{-1}\vec{\mathcal{F}}\delta t$$

$$\vec{r} \to \vec{r} + \vec{v}\delta t$$

$$f(\vec{k},\vec{r},t) \to f(\vec{k} + \hbar^{-1}\vec{\mathcal{F}}\delta t, \vec{r} + \vec{v}\delta t, t + \delta t)$$

Assume that under the forces, the deviation from thermal equilibrium is linear.
Differential with time: $df(\vec{k},\vec{r}) \Big/ dt$

$$df = f(\vec{k} + \hbar^{-1}\vec{F}\delta t, \vec{r} + \vec{v}\delta t) - f(\vec{k},\vec{r}) = \hbar^{-1}\vec{\mathcal{F}} \cdot \frac{\partial f}{\partial \vec{k}} dt + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} dt$$

For small deviations from f^0

$$\frac{df(\vec{k},\vec{r})}{dt} = \hbar^{-1}\vec{\mathcal{F}} \cdot \frac{\partial f^0}{\partial \vec{k}} + \vec{v} \cdot \frac{\partial f^0}{\partial \vec{r}}$$

Electric force

$$\left.\frac{\partial f(\vec{k},\vec{r})}{\partial t}\right|_{E} = \vec{v}\bullet e\vec{E}\,\frac{\partial f^{0}}{\partial \mathcal{E}}$$

Thermal equivalent "force"

$$\left.\frac{\partial f(\vec{k},\vec{r})}{\partial t}\right|_{TEMPEATURE} = \vec{v}\bullet\nabla T\,\frac{\partial f^{0}}{\partial T}$$

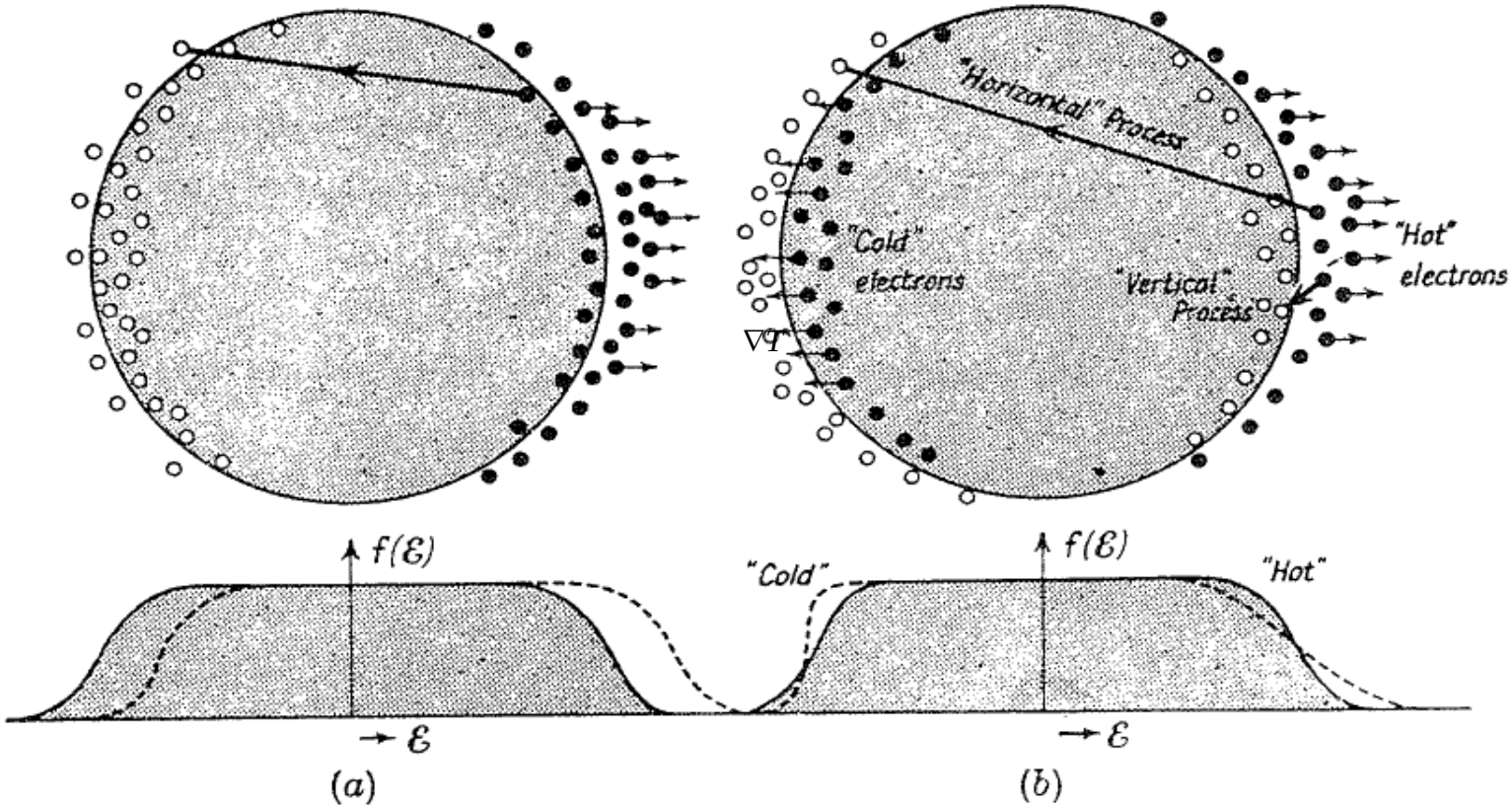


FIG. 122. The Fermi surface and distribution functions: (*a*) in electrical conduction; (*b*) in thermal conduction.

● extra electron ——— equilibrium distribution.
○ electron deficiency ---------- steady state transport distribution.

The Boltzmann equation for diffuse transport

The effects of the thermodynamic forces arises from the difference between f^0 and $f(\vec{k},\vec{r})$

The relaxation time approximation: under the effect of scattering, each the distribution function of each particle is brought back to thermal equilibrium after one relaxation time τ

$$\left.\frac{df(\vec{k},\vec{r},t)}{dt}\right|_{SCATTERING} = \frac{f(\vec{k},\vec{r}) - f^0}{\tau}$$

$$\vec{v}\bullet\vec{\mathcal{F}}\frac{\partial f^0}{\partial \mathcal{E}} + \vec{v}\bullet\nabla T\frac{\partial f^0}{\partial T} = -\frac{f(\vec{k},\vec{r}) - f^0}{\tau}$$

External Force Thermal Gradient Scattering

In diffuse transport, the applied forces are balanced by scattering at a rate τ

Diffuse transport of electrons

For diffuse transport only, j_C for **electrons** only

The particle flux is the integral over all momenta of all electrons

$$\vec{j}_N = \iiint_{\vec{k}} \vec{v} f(\vec{k},\vec{r}) d\vec{k}$$

The flux of heat is $$\vec{j}_Q = \iiint_{\vec{k}} (\mathcal{E} - \mu_\phi) \vec{v} f(\vec{k},\vec{r}) d\vec{k}$$

Substitute $$f(\vec{k},\vec{r}) = f^0 - \tau \vec{v} \bullet \left(\frac{\partial f^0}{\partial \mathcal{E}} \vec{\mathcal{F}} + \frac{\partial f^0}{\partial T} \nabla T \right)$$

$$\vec{j}_N = \iiint_{\vec{k}} \vec{v} f^0 d\vec{k} - \iiint_{\vec{k}} \tau \vec{v} \bullet \vec{v} \left(\frac{\partial f^0}{\partial \mathcal{E}} \right) d\vec{k} \vec{\mathcal{F}} - \iiint_{\vec{k}} \tau \vec{v} \bullet \vec{v} \left(\frac{\partial f^0}{\partial T} \right) d\vec{k} \nabla T$$

$\iiint_{\vec{k}} \vec{v} f^0 d\vec{k} = 0$

The average $\vec{v}$ over all directions is zero; there is no flux at thermal equilibrium

$\iiint_{\vec{k}} (\mathcal{E} - \mu_\phi) \vec{v} f^0 d\vec{k} = 0$

$$\vec{j}_Q = \iiint_{\vec{k}} (\mathcal{E} - \mu_\phi) \vec{v} f^0 d\vec{k} - \iiint_{\vec{k}} \tau (\mathcal{E} - \mu_\phi) \vec{v} \bullet \vec{v} \left(\frac{\partial f^0}{\partial \mathcal{E}} \right) d\vec{k} \vec{\mathcal{F}} - \iiint_{\vec{k}} \tau (\mathcal{E} - \mu_\phi) \vec{v} \bullet \vec{v} \left(\frac{\partial f^0}{\partial T} \right) d\vec{k} \nabla T$$

Diffuse transport

Map this onto the Onsager formalism

$$\begin{bmatrix} \vec{j}_N \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{NN} & \overleftrightarrow{L}_{NT} \\ \overleftrightarrow{L}_{TN} & \overleftrightarrow{L}_{TT} \end{bmatrix} \begin{bmatrix} \vec{\mathcal{F}} \\ -\nabla T \end{bmatrix}$$

Calculate energy and T-derivatives of distribution function, and replace integrals over **k**-space by the Density of States (transformation of variables):

$$\mathcal{D}(\mathcal{E}) = \iint_{A(\mathcal{E})} g \frac{dA}{(2\pi)^{DIM}} \frac{1}{\nabla_{\vec{k}} \mathcal{E}(\vec{k})}$$

End result are the **TRANSPORT INTEGRALS**

$$\overleftrightarrow{L}_{NN} = \int_{\mathcal{E}} \tau \vec{v} \bullet \vec{v} \mathcal{D}(\mathcal{E}) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

$$\overleftrightarrow{L}_{TN} = \int_{\mathcal{E}} \tau (\mathcal{E} - \mu_\phi) \vec{v} \bullet \vec{v} \mathcal{D}(\mathcal{E}) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

$$\overleftrightarrow{L}_{NT} = \frac{1}{T} \int_{\mathcal{E}} \tau \vec{v} \bullet \vec{v} \mathcal{D}(\mathcal{E}) (\mathcal{E} - \mu_\phi) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

$$\overleftrightarrow{L}_{TT} = \frac{1}{T} \int_{\mathcal{E}} \tau (\mathcal{E} - \mu_\phi)^2 \vec{v} \bullet \vec{v} \mathcal{D}(\mathcal{E}) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

Thermoelectricity

$$\begin{bmatrix} \vec{j}_C \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{EE} & \overleftrightarrow{L}_{ET} \\ \overleftrightarrow{L}_{TE} & \overleftrightarrow{L}_{TT} \end{bmatrix} \begin{bmatrix} \vec{E} \\ -\nabla T \end{bmatrix}$$

End result are the **TRANSPORT INTEGRALS**

$$\vec{\mathcal{F}} = e\vec{E};\ \vec{j}_C = e\vec{j}_N$$

$$\overleftrightarrow{L}_{EE} = e^2 \int_{\mathcal{E}} \tau \vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E}) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

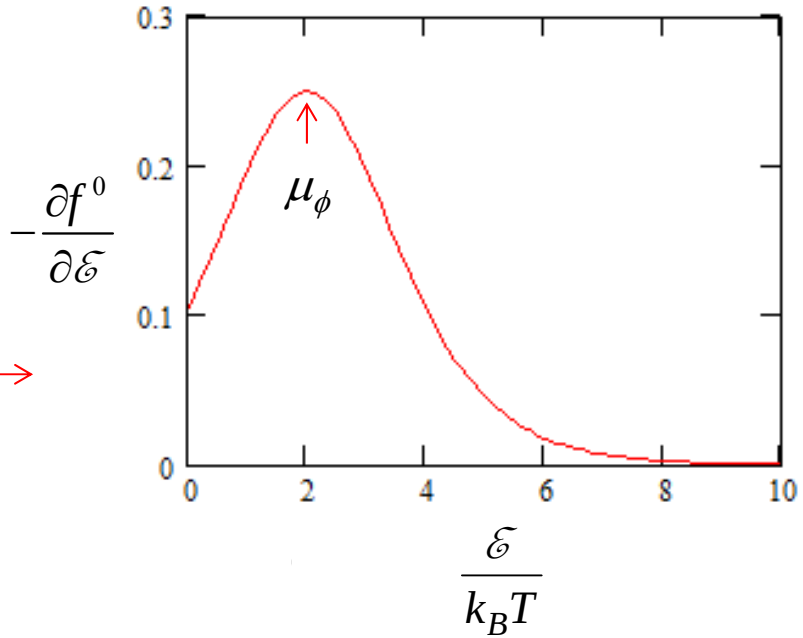
$$\overleftrightarrow{L}_{TE} = e \int_{\mathcal{E}} \tau(\mathcal{E} - \mu_\phi) \vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E}) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

$$\overleftrightarrow{L}_{ET} = \frac{e}{T} \int_{\mathcal{E}} \tau \vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E}) (\mathcal{E} - \mu_\phi) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

$$\overleftrightarrow{L}_{TT} = \frac{1}{T} \int_{\mathcal{E}} \tau(\mathcal{E} - \mu_\phi)^2 \vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E}) \left(-\frac{\partial f^0}{\partial \mathcal{E}} \right) d\mathcal{E}$$

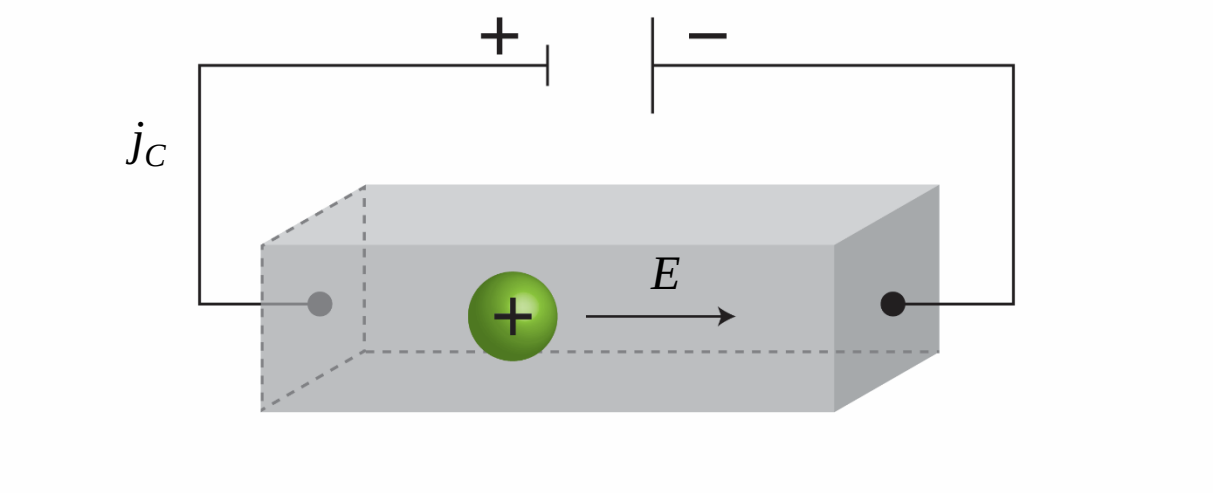
The integrals only matter within a few $k_B T$ around the electrochemical potential

$$-\frac{\partial f^0}{\partial \mathcal{E}} = e^{\frac{\mathcal{E}-\mu_\phi}{k_B T}} \Big/ \left(e^{\frac{\mathcal{E}-\mu_\phi}{k_B T}} + 1 \right)^2 \longrightarrow$$

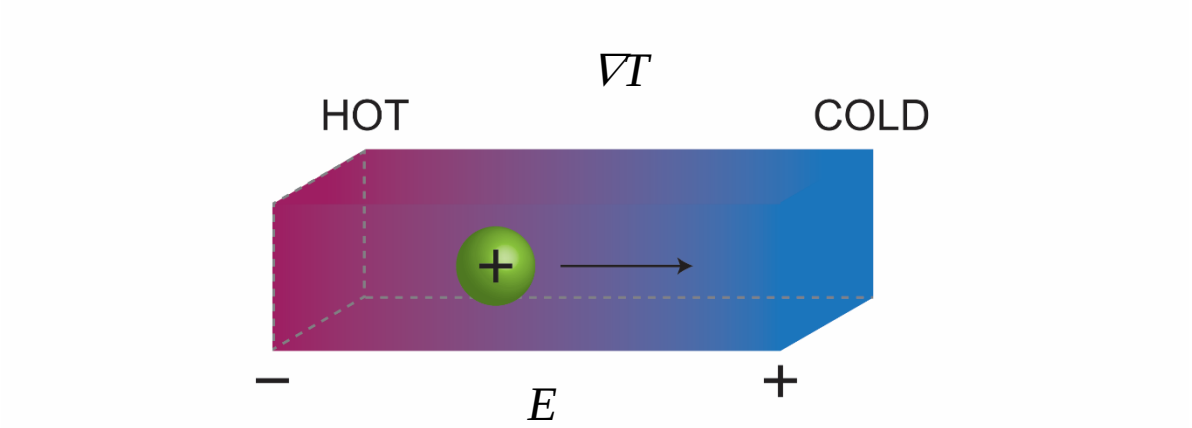


Electrical conductivity

$$j_C = \sigma E$$

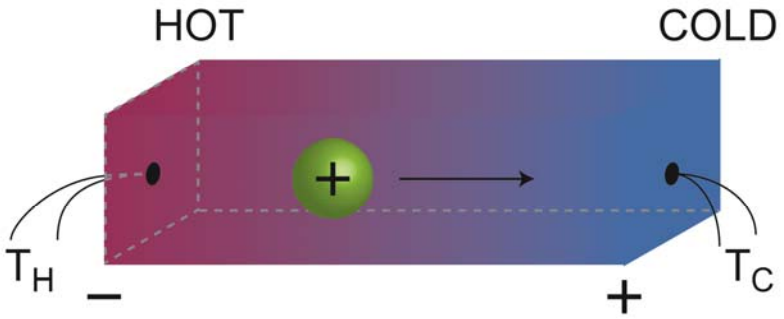


Thermopower – Seebeck coefficient



$$\alpha = \left.\frac{E}{\nabla T}\right|_{j_C=0}$$

Thermal conductivity



$$j_Q = -\kappa \nabla T\Big|_{j_C=0}$$

Relation between L and measured transport coefficients

$$\begin{bmatrix} \vec{j}_C \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{EE} & \overleftrightarrow{L}_{ET} \\ \overleftrightarrow{L}_{TE} & \overleftrightarrow{L}_{TT} \end{bmatrix} \begin{bmatrix} \vec{E} \\ -\nabla T \end{bmatrix}$$

1. Electrical conductivity when ∇T=0: $\overleftrightarrow{\sigma} = \overleftrightarrow{L}_{EE}$

2. Thermopower is defined as: $\overleftrightarrow{\alpha} \equiv \left[\vec{E} \ (\nabla T)^{-1} \right]_{j_C=0}$

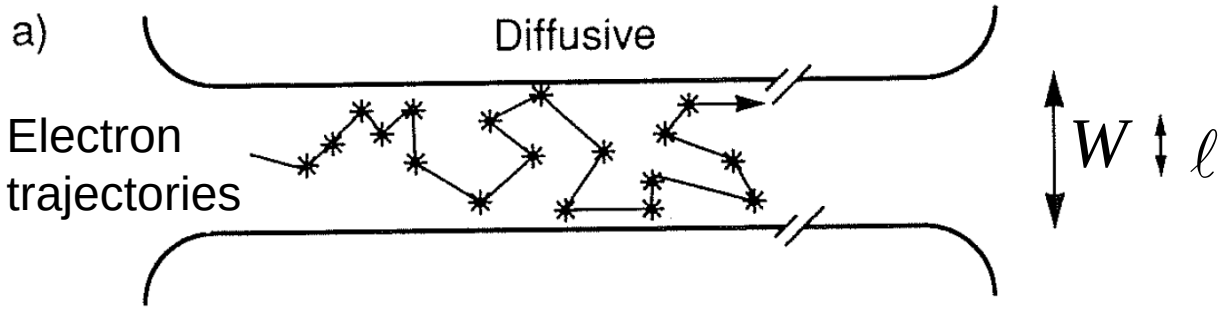
Solve for j_C=0 => Thermopower is $\overleftrightarrow{\alpha} = \overleftrightarrow{L}_{ET} \overleftrightarrow{L}_{EE}^{-1}$

3. Thermal conductivity defined as: $\overleftrightarrow{\kappa} \equiv \left[\vec{j}_Q \left(-\nabla T \right)^{-1} \right]_{\vec{j}_C=0}$

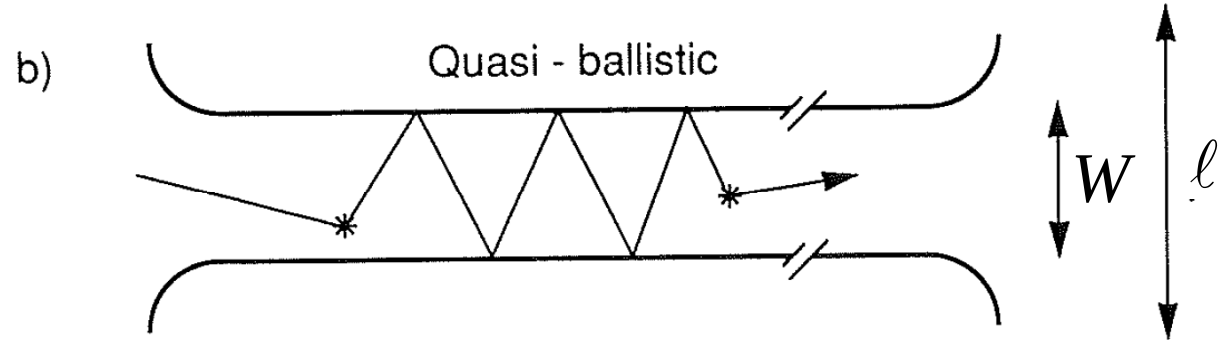
Solve top line for j_C=0 , *derive value of E and substitute into bottom line =>* $\overleftrightarrow{\kappa} = -\overleftrightarrow{L}_{ET} \overleftrightarrow{L}_{TE} \overleftrightarrow{L}_{EE}^{-1} + \overleftrightarrow{L}_{TT}$

We now generalize this approach to cover cases other than the diffusive transport.

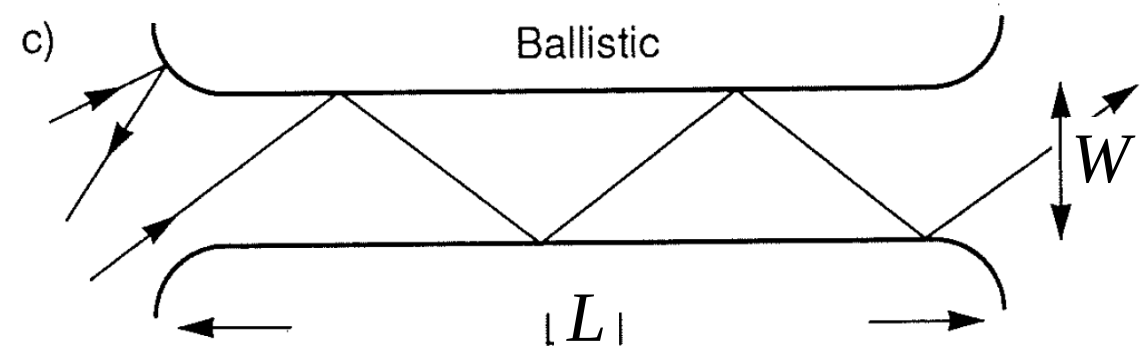
Progression from diffusive to ballistic transport



Diffusive:
mfp ℓ< Width W &
length L of sample
* denotes collision that would also happen in bulk



Quasi-ballistic
Width W < mfp ℓ<
length L



Ballistic
Width W < length L < mfp ℓ

Ultimately, electrons will go through the constriction one at a time: 1 “channel”

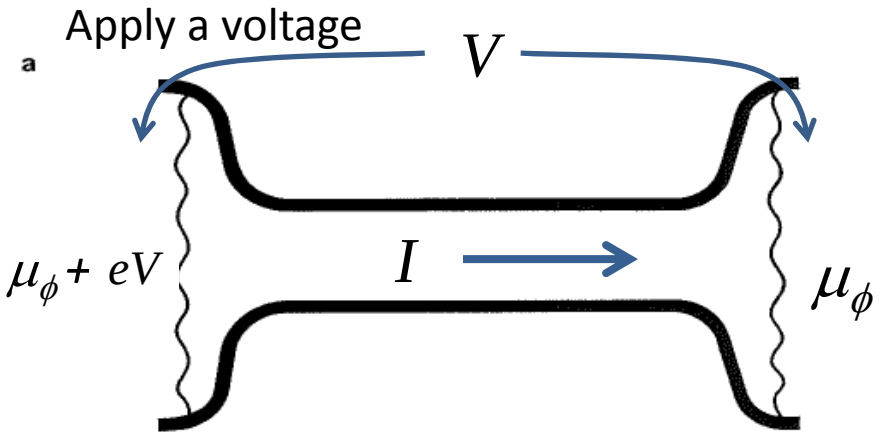
H. Van Houten & al., Physics and Technology of submicron structures, Springer, Berlin 1988

Landauer: conductance as transmission problem

Narrow channel connects two electron gas "reservoirs", one at electrochemical potential μ_ϕ, the other at $\mu_\phi + \delta\mu$

$$I = GV$$

$$G = G_0 Tr$$

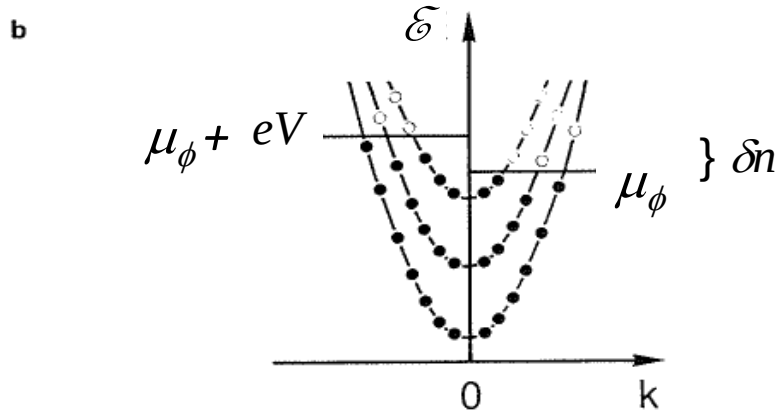


N = number of channels

i = 1..N index of each channel

Each channel has a transmission function Tr_i

Here, 1 or 0



2 = spin

$$G = 2\frac{e^2}{h}\sum_{i=1}^{N} Tr_i$$

Natural quantum of conductance

The Landauer-Büttiker formalism

Landauer formalism approaches Boltzmann formalism, but is more universal.

Define an **electron transmission coefficient** $\mathcal{T}(\mathcal{E})$

$\mathcal{T}(\mathcal{E})$ is the probability that a wave-packet with energy $\mathcal{E}$ be transmitted across the constriction being measured.

Advantages:

1. No longer beholden to diffusive transport or to the use of a relaxation time
2. No longer beholden to the definition of a reciprocal lattice and dispersion relation; will work with just a density of states as function of energy
3. Valid for constrictions, low-dimensional structures,…
4. Valid for transport across interfaces or tunneling
5. Valid for localization, hopping, disordered solids

R. Landauer, IBM J. Res. Dev. ***1*** *223 (1957)* *M. Büttiker, Phys. Rev. Lett.* ***57*** *1761 (1986)*

The Landauer-Büttiker formalism

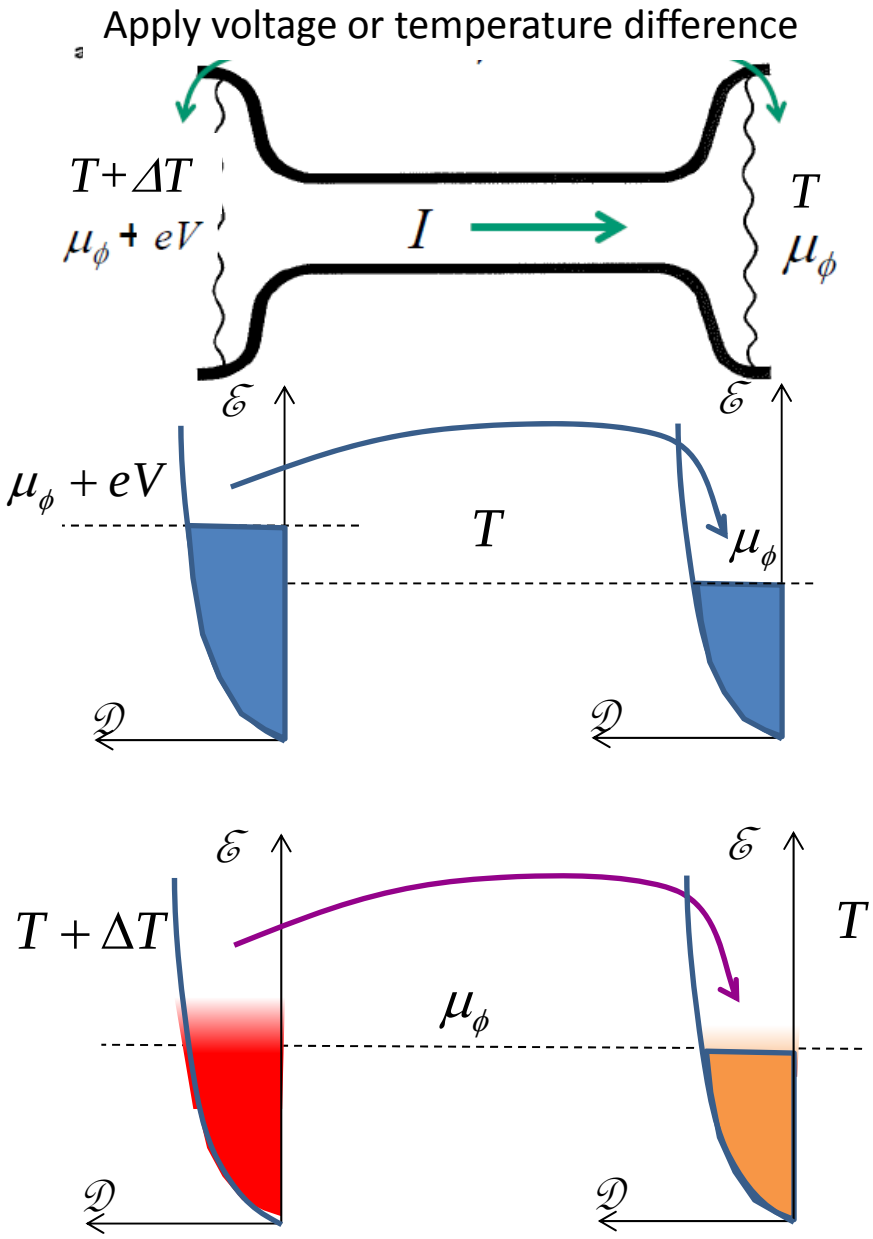
Particle flow: $$I_N = \frac{2}{h}\int_{\mathscr{E}} f(T,\mathscr{E})\mathfrak{I}(\mathscr{E})d\mathscr{E}$$

Current: $$I_C = 2\frac{e}{h}\int_{\mathscr{E}} f(T,\mathscr{E})\mathfrak{I}(\mathscr{E})d\mathscr{E}$$

Internal energy flow: $$I_U = \frac{2}{h}\int_{\mathscr{E}} \mathscr{E}\, f(T,\mathscr{E})\mathfrak{I}(\mathscr{E})d\mathscr{E}$$

Heat flow: $$I_Q = \frac{2}{h}\int_{\mathscr{E}} (\mathscr{E}-\mu_\phi)\, f(T,\mathscr{E})\mathfrak{I}(\mathscr{E})d\mathscr{E}$$

The transport integrals in Landauer formalism



The difference in distribution function between the two reservoirs comes from either:

1. the change in energy level due to the voltage $\mu_\phi \Rightarrow \mu_\phi + eV$
2. the change in temperature $T \Rightarrow T + \Delta T$

First-order expansion:

$$f(T,\mathcal{E}) = f^0 + \left(eV \frac{\partial f^0}{\partial \mathcal{E}} + \Delta T \frac{\partial f^0}{\partial T} \right)$$

$$f(T,\mathcal{E}) = f^0 + \frac{\partial f^0}{\partial \mathcal{E}} \left(eV - \frac{\mathcal{E} - \mu_\phi}{k_B T} \Delta T \right)$$

Transport integrals in Landauer formalism

- Same process as with Boltzmann.
- Map currents onto Onsager.
- Solve transport integrals.

$$\begin{pmatrix} I_C \\ I_Q \end{pmatrix} = \begin{pmatrix} G & L \\ LT & K \end{pmatrix} \begin{pmatrix} V \\ \Delta T \end{pmatrix}$$

$$G = -2\frac{e^2}{h}\int_{\mathcal{E}}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)\mathcal{T}(\mathcal{E})d\mathcal{E}$$

$$L = 2\frac{e^2}{h}\frac{k_B}{e}\int_{\mathcal{E}}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)\left(\frac{\mathcal{E}-\mu_\phi}{k_B T}\right)\mathcal{T}(\mathcal{E})d\mathcal{E}$$

$$K = 2\frac{e^2}{h}\left(\frac{k_B}{e}\right)^2 T\int_{\mathcal{E}}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)\left(\frac{\mathcal{E}-\mu_\phi}{k_B T}\right)^2\mathcal{T}(\mathcal{E})d\mathcal{E}$$

The thermopower is:

$$\alpha \equiv V/\Delta T = -L/G$$

Transport	Kinetic coeff	Natural unit	Constants	Value	Units
Electrical Conductance	G	G_0	e^2/h	$3.87\ 10^{-5}$	$1/\Omega$
Thermopower	L	L/G_0	k_B/e	$86\ 10^{-6}$	V / K
Entropy conductance	K/T	$G_0(k_B/e)^2$	$(k_B/e)^2$	$2.87\ 10^{-13}$	W / K^2

Relation Landauer - Boltzmann

Sir Neville Mott defined the "Mott conductivity" $\sigma_{\mathscr{E}}(\mathscr{E})$ in 1930's:

Mott: " $\sigma_{\mathscr{E}}(\mathscr{E})$ represents the conductivity the system *would have* if the energy at the surface of the Fermi distribution were $\mathscr{E}$; its variation with $\mathscr{E}$ is important in the discussion of the thermoelectric phenomena."

The Mott conductivity is equivalent to the transmission coefficient

$$\sigma_{\mathscr{E}}(\mathscr{E}) = 2G_0\mathscr{T}(\mathscr{E})$$

=> Re-write the Landauer formalism for bulk conductivities

N. F. Mott and H. Jones, "The Theory of Properties of Metals and Alloys, Clarendon Press, Oxford (1936)

The Mott relation, general case

$$\sigma_{\mathcal{E}}(\mathcal{E}) = 2G_0\mathcal{J}(\mathcal{E})$$

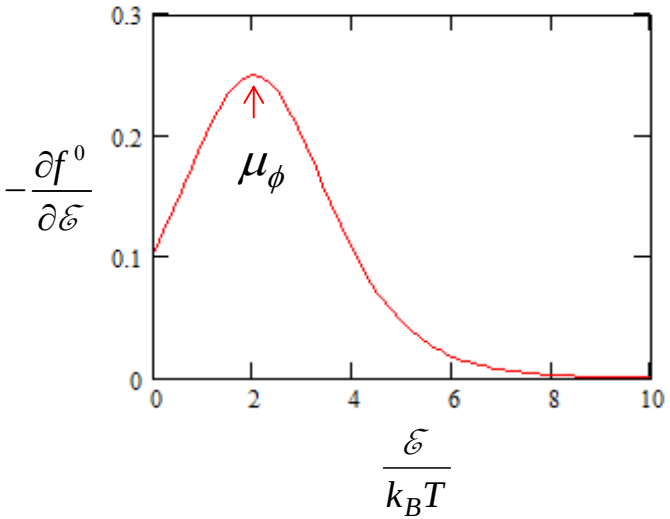
$$\sigma = 2G_0\int_{\mathcal{E}}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)\mathcal{J}(\mathcal{E})d\mathcal{E}$$

$$\alpha = \frac{L_{ET}}{\sigma} = \left(\frac{k_B}{e}\right)\frac{1}{k_BT}\left\{\frac{\int_{\mathcal{E}}\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\mathcal{E}\mathcal{J}(\mathcal{E})d\mathcal{E}}{\int_{\mathcal{E}}\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\mathcal{J}(\mathcal{E})d\mathcal{E}} - \mu_\phi\right\}$$

$$\kappa = 2G_0T\left(\frac{k_B}{e}\right)^2\int_{\mathcal{E}}\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\left(\frac{\mathcal{E}-\mu_\phi}{k_BT}\right)^2\mathcal{J}(\mathcal{E})d\mathcal{E}$$

General case

$$f^0 = \frac{1}{e^{(\mathcal{E}-\mu_\phi)/k_BT}+1}$$



Valid for all Fermions, as long as we know the transmission function

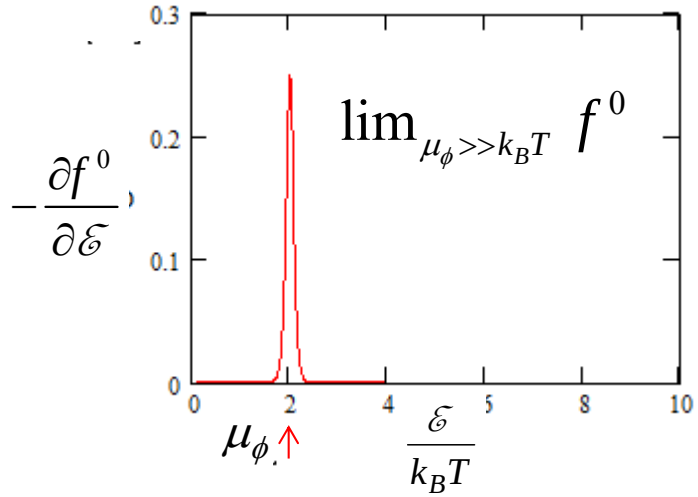
*Mott & Wiedemann-Franz, **Fermions** with degenerate stats.*

Bethe-Sommerfeld expansion, 2nd order

$$\sigma \approx \sigma_{\mathcal{E}}(\mu_\phi) = 2G_0 \mathcal{T}(\mu_\phi)$$

$$L_{ET} \approx \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)(k_B T)\sigma'_{\mathcal{E}}(\mu_\phi)$$

$$\kappa / T \approx \left(\frac{k_B}{e}\right)^2 \frac{\pi^2}{6} 2\sigma_{\mathcal{E}}(\mu_\phi)$$



The Mott relation: The thermopower is proportional to the energy derivative of the transmission coefficient or Mott conductivity

$$\alpha = \frac{L_{ET}}{\sigma}\mathcal{T}(\mu_\phi) = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)(k_B T)\frac{1}{\sigma}\frac{d\sigma_{\mathcal{E}}(\mathcal{E})}{d\mathcal{E}}\bigg|_{\mu_\phi} =$$

The Wiedemann-Franz-Lorenz relation: the electronic thermal conductivity is proportional to the electrical conductivity

The proportionality constant is the **Lorenz number** L_0

$$\kappa = L_0 \sigma T \;;\; L_0 = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 = 2.45\times 10^{-8}[\mathrm{V^2K^2}]$$

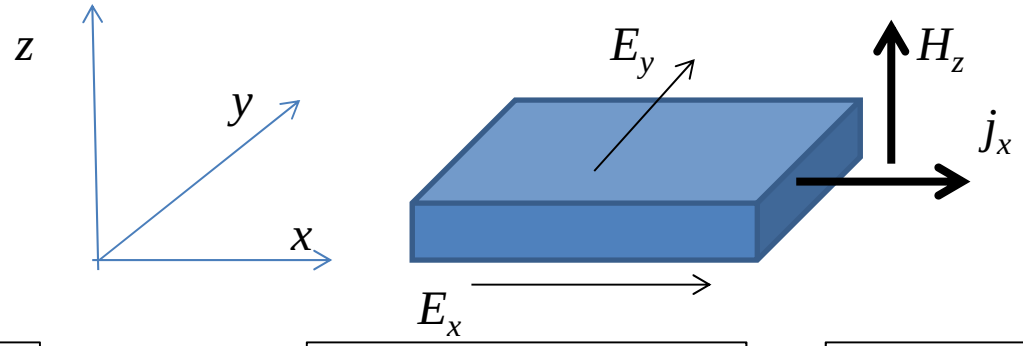
Add an external magnetic field

$$\begin{bmatrix} \vec{j}_C \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{EE} & \overleftrightarrow{L}_{ET} \\ \overleftrightarrow{L}_{TE} & \overleftrightarrow{L}_{TT} \end{bmatrix} \begin{bmatrix} \vec{E} \\ -\nabla T \end{bmatrix}$$

The transport integrals are solved as before (see specialized course)

$$\vec{\mathcal{F}} = e\vec{E} + \vec{v} \times \vec{H}\,;\; \vec{j}_C = e\vec{j}_N$$

Example: for the case



=> Magnetoconductivity

=> Hall

=> MagnetoSeebeck

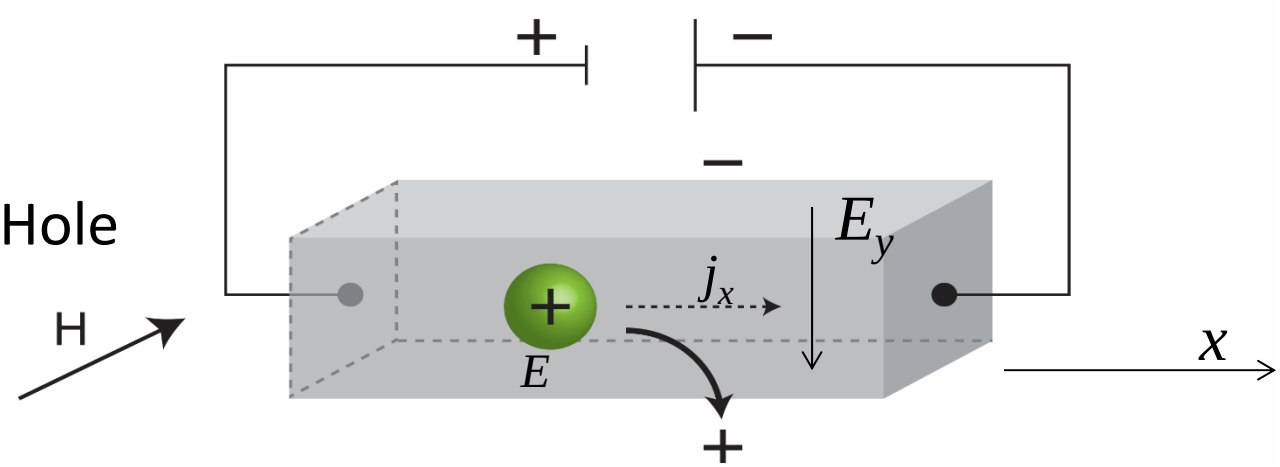
=> Nernst

$$\begin{pmatrix} j_{Cx} \\ j_{Cy} \\ j_{Qx} \\ j_{Qy} \end{pmatrix} = \begin{bmatrix} L_{EExx} = \sigma_{xx} & L_{EExy} = \sigma_{xy} & L_{ETxx} & L_{ETxy} \\ L_{EEyx} = \sigma_{yx} & L_{EEyy} = \sigma_{yy} & L_{ETyx} & L_{ETyy} \\ L_{TExx} & L_{TExy} & L_{TTxx} & L_{TTxy} \\ L_{TEyx} & L_{TEyy} & L_{TTyx} & L_{TTyy} \end{bmatrix} \begin{pmatrix} E_x \\ E_y \\ -\nabla_x T \\ -\nabla_y T \end{pmatrix} \begin{bmatrix} \vec{E} \\ -\nabla T \end{bmatrix}$$

=> Magnetothermal conductivity

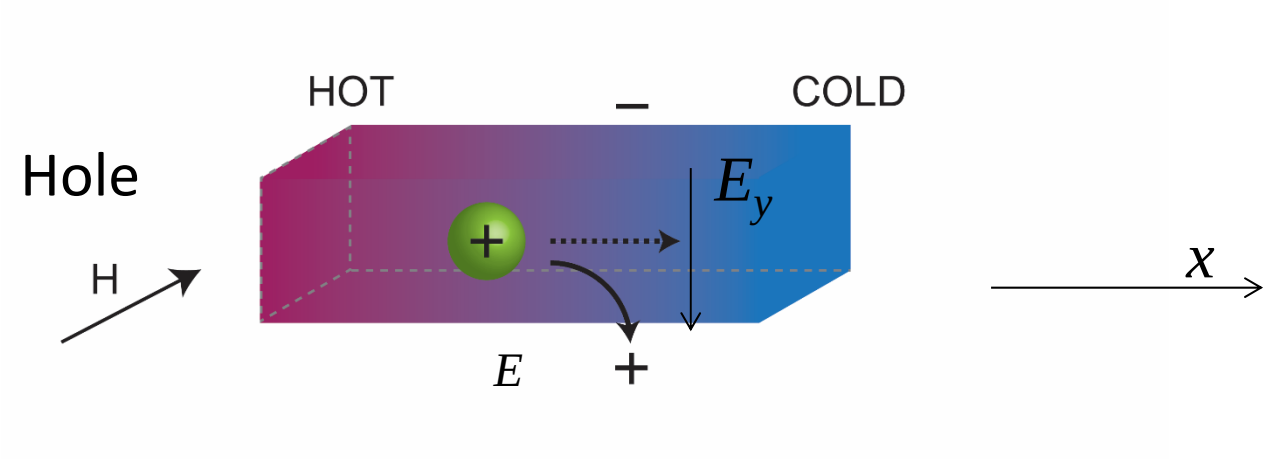
=> Magghi-Righi-Leduc

Hall effect



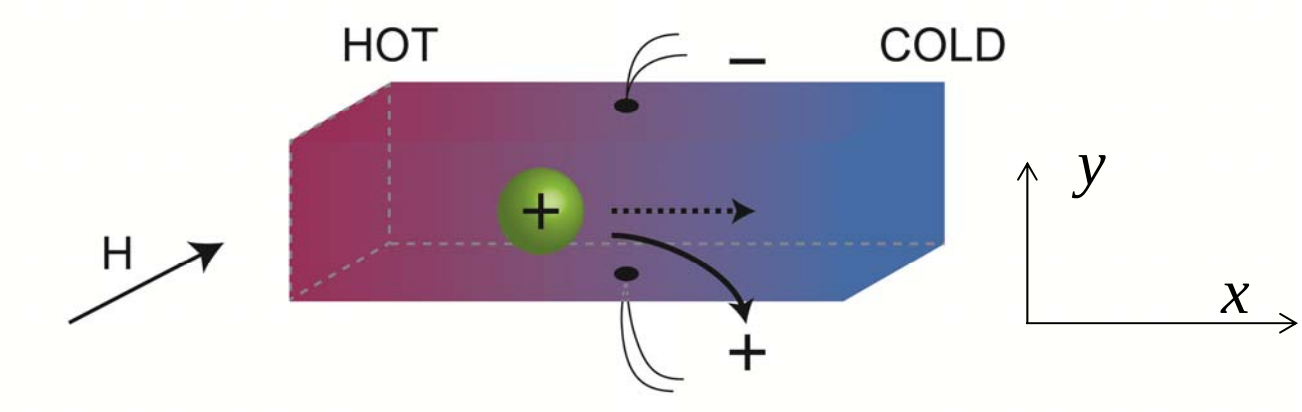
$$\rho_{xy} = E_y / j_x$$

The Nernst effect



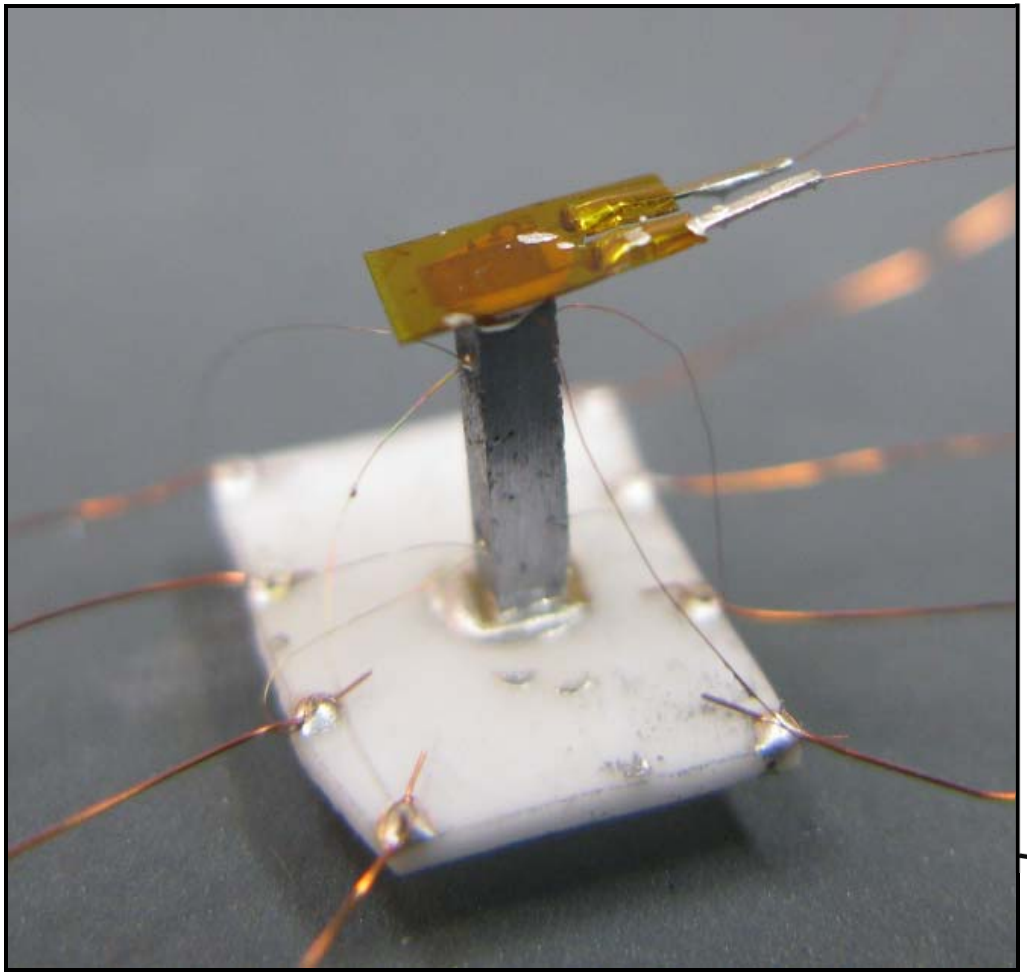
$$\alpha_{xy} = \left.\frac{E_y}{\nabla_x T}\right|_{j_C=0,\nabla_x T=0}$$

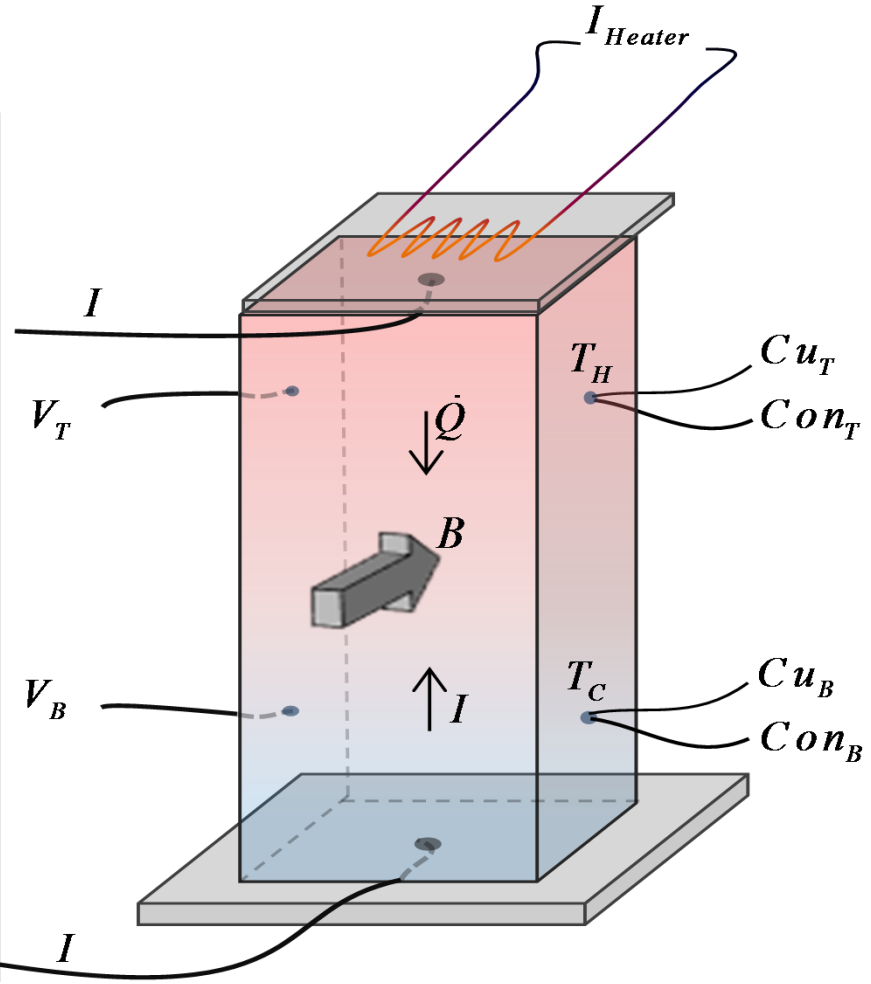
Magghi-Righi-Leduc effect



$$\kappa_{xy} = \left. \frac{\nabla_y T}{\nabla_x T} \right|_{j_C = 0}$$

Measurements





Multicarrier transport

1. Several different pockets to the Fermi surface
- Si, Ge, ...

2. Electrons and holes:
- Semimetals, Weyl semimetals, Dirac systems
- Semiconductors in the intrinsic regime

3. Spin polarized electrons
- Spin-mixing models

Multicarrier transport

SIMPLEST SOLUTION:

- Assume the different particles do not interact: each has it's own L-tensor
- Add the fluxes
- Two cases:
  - Particles have different charge: careful with polarity
  - Particles have different spin: spin currents vs charge currents
- Example for electrons and holes:

$$\begin{bmatrix} \vec{j}_C = \vec{j}_{Ce} + \vec{j}_{Ch} \\ \vec{j}_Q = \vec{j}_{Qe} + \vec{j}_{Qh} \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{EEe} + \overleftrightarrow{L}_{EEh} & \overleftrightarrow{L}_{ETe} + \overleftrightarrow{L}_{ETh} \\ \overleftrightarrow{L}_{TEe} + \overleftrightarrow{L}_{TEh} & \overleftrightarrow{L}_{YTe} + \overleftrightarrow{L}_{TTh} \end{bmatrix} \begin{bmatrix} \vec{E} \\ -\nabla T \end{bmatrix}$$

Algebra becomes messy very quickly

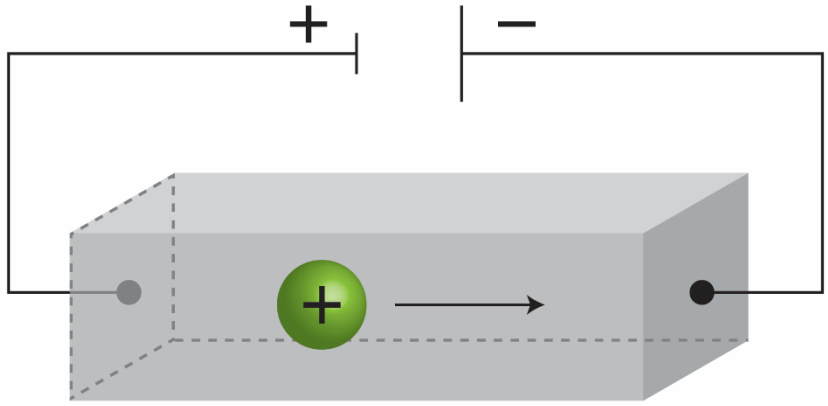
At low field

electrical conductivity	σ	$\sigma_1 + \sigma_2$
Hall constant	R	$\dfrac{R_1\sigma_1^2 + R_2\sigma_2^2}{(\sigma_1 + \sigma_2)^2}$
Seebeck	Θ	$\dfrac{\Theta_1\sigma_1 + \Theta_2\sigma_2}{\sigma_1 + \sigma_2}$
Nernst	Q	$\dfrac{Q_1\sigma_1(\sigma_1+\sigma_2) + Q_2\sigma_2(\sigma_1+\sigma_2) + (\Theta_1 - \Theta_2)\sigma_1\sigma_2(R_1\sigma_1 - R_2\sigma_2)}{(\sigma_1 + \sigma_2)^2}$
Thermal conductivity	κ	$\kappa_L + \kappa_1 + \kappa_2 + T\dfrac{\sigma_1\sigma_2(\Theta_1 - \Theta_2)^2}{\sigma_1 + \sigma_2}$
Magghi-Righi-Leduc (i.e. Thermal Hall)	S	$S_1 + S_2 + \dfrac{T}{\kappa} \times \dfrac{2\sigma_1\sigma_2(\sigma_1+\sigma_2)(\Theta_1-\Theta_2)(Q_1-Q_2) + \sigma_1^2\sigma_2^2(R_1+R_2)(\Theta_1-\Theta_2)^2}{(\sigma_1 + \sigma_2)^2}$

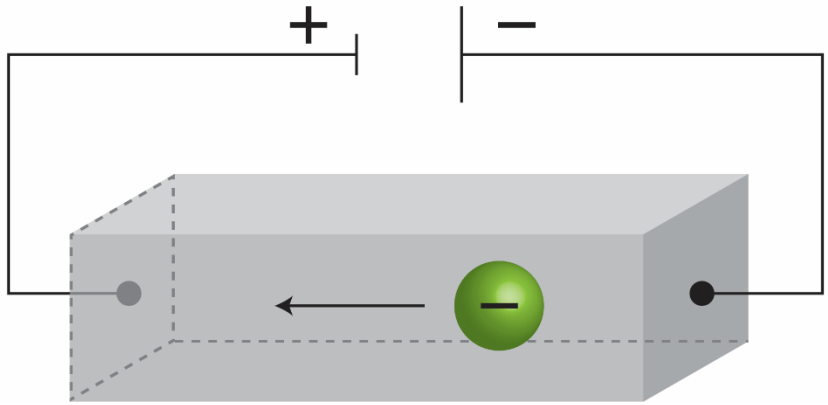
Ambipolar terms usually dominate in semimetals

Electrical conductivity

Resistivity = EVEN function of polarity

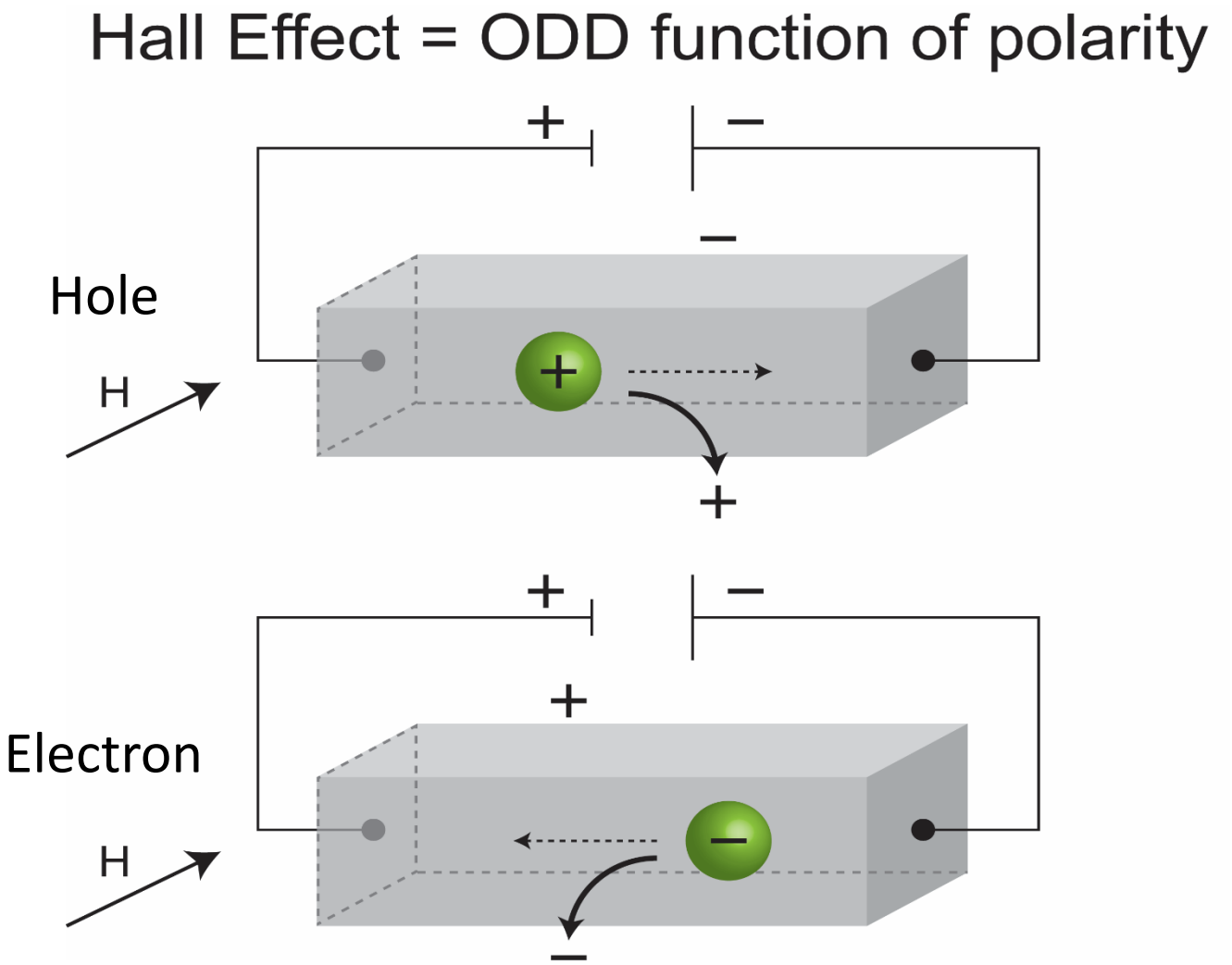


Hole



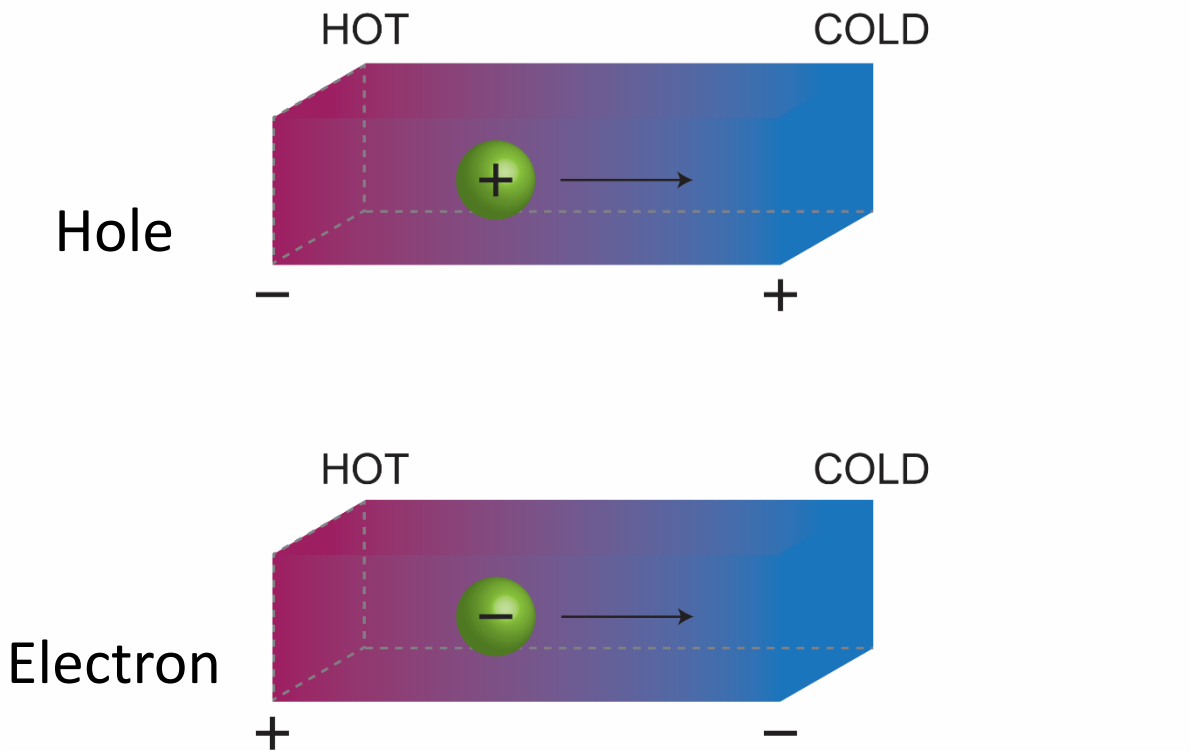
Electron

Hall effect



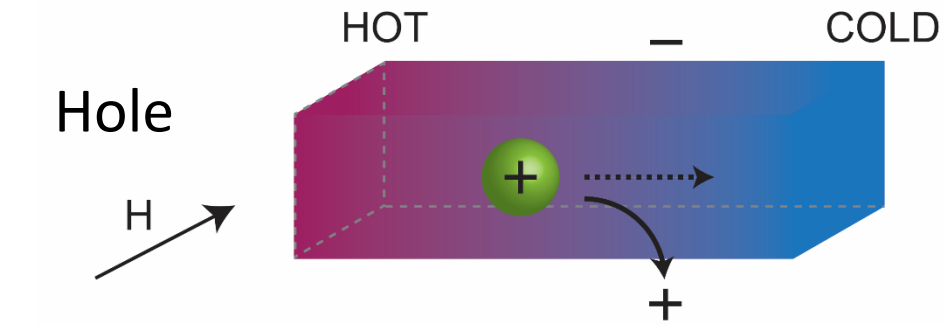
Thermopower – Seebeck coefficient

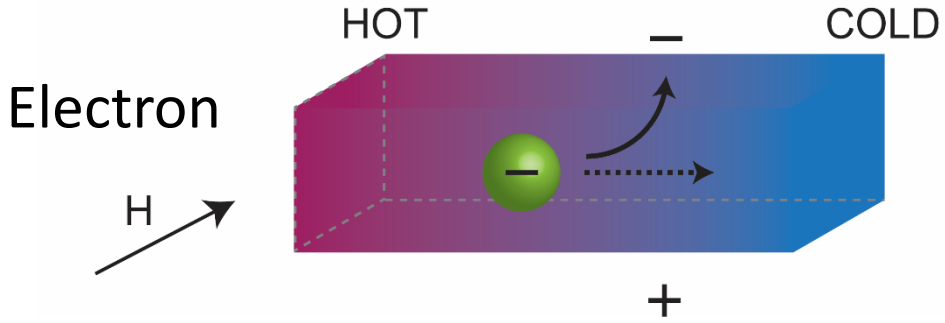
Seebeck Effect = ODD function of polarity



The Nernst effect

Nernst Effect = EVEN function of polarity

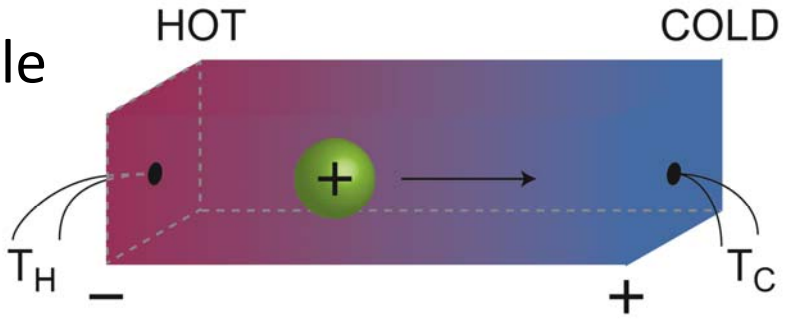




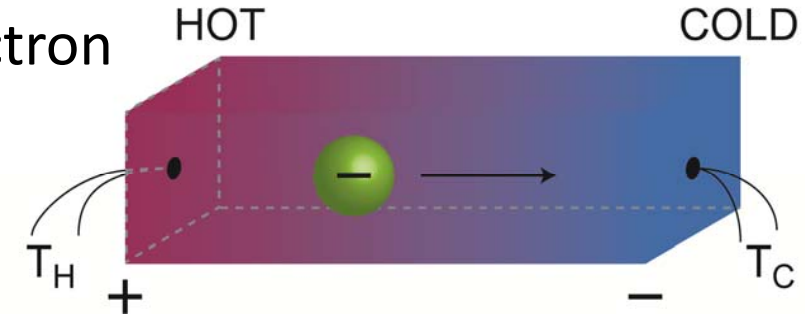
Thermal conductivity

Thermal Conductivity =
EVEN function of polarity

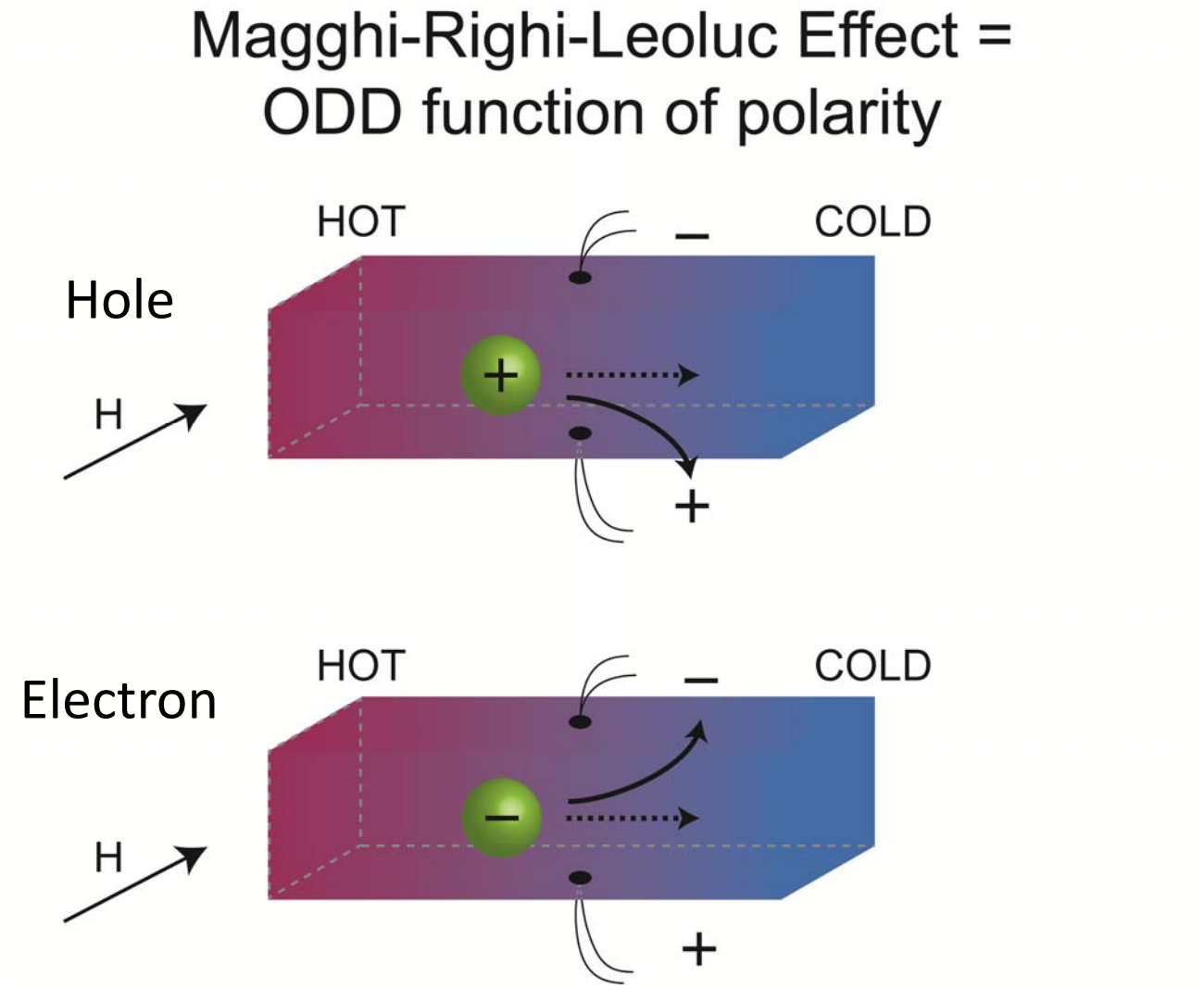
Hole



Electron



Magghi-Righi-Leduc effect



Advertisement for CEM research on Weyl semimetals

1. Solve both the electron and the hole part of the Dirac dispersion together (Tim McCormick, N. Trivedi) =>

2. Nernst effect is entirely ambipolar (Watzman & McCormick et al., arXiv 2017)

3. Thermal conductivity in-plane (no arcs) is entirely ambipolar
(U. Stockert et al, Watzman, Heremans, arXiv 2017, J. Phys. C. submitted)

4. Thermal conductivity along c-axis (i.e. perpendicular to the arcs) has conveyer-belt transport (McCormick , Watzman & al., arXiv 2017) => strong magnetothermal conductivity

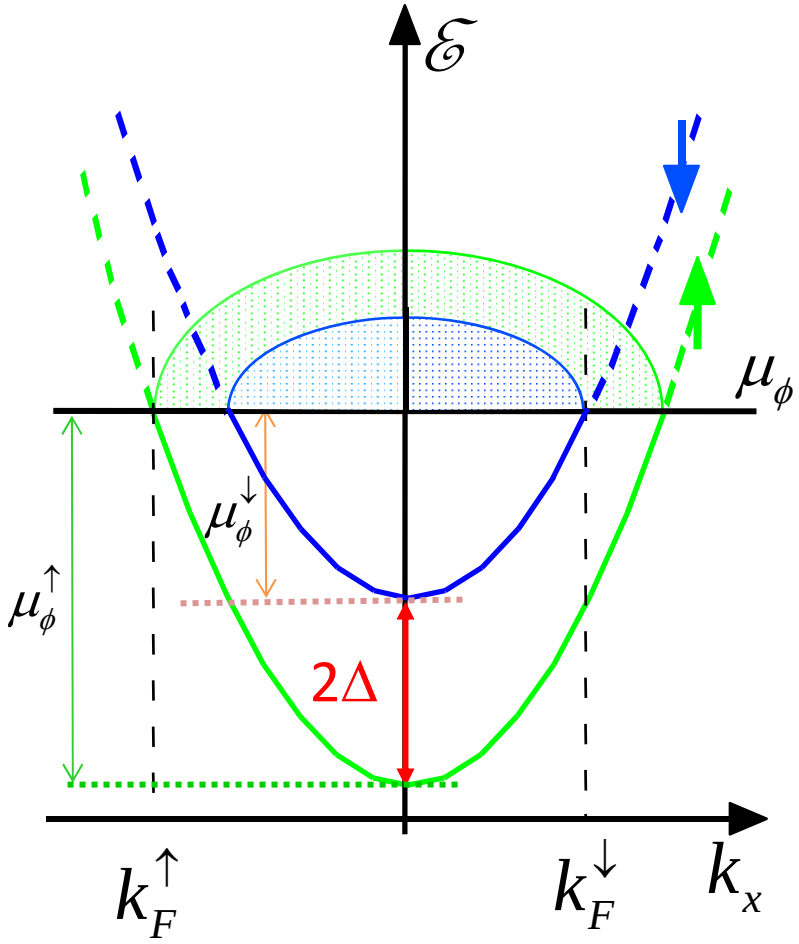
Normally $\vec{\vec{\kappa}} \equiv \left[\vec{j}_Q \left(-\nabla T \right)^{-1} \right]_{\vec{j}_C = 0}$

With arcs $\vec{\vec{\kappa}} \equiv \left[\vec{j}_Q \left(-\nabla T \right)^{-1} \right]_{\vec{j}_C \neq 0}$

$$\begin{bmatrix} \vec{j}_C \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \vec{\vec{L}}_{EE} & \vec{\vec{L}}_{ET} \\ \vec{\vec{L}}_{TE} & \vec{\vec{L}}_{TT} \end{bmatrix} \begin{bmatrix} \vec{E} \\ -\nabla T \end{bmatrix}$$

Spins on conduction electrons: Stoner model

Two bands, spin-up and spin-down



Carrier concentrations $n_\uparrow, n_\downarrow$

Electrochemical potentials $\mu_{\phi\uparrow}, \mu_{\phi\downarrow}$

Density of states $\mathcal{D}_\uparrow, \mathcal{D}_\downarrow$

Carrier mobilities $\mu_\uparrow, \mu_\downarrow$

Current carried $j_{C\uparrow}, j_{C\downarrow}$

Spin carried $j_{S\uparrow}, j_{S\downarrow}$

Partial electrical conductivity $\sigma_\uparrow, \sigma_\downarrow$

Partial thermopower $\alpha_\uparrow, \alpha_\downarrow$

Spin and charge fluxes

Careful: the charge is conserved, but the spin polarization NOT ALWAYS! (LATER)

Everywhere in an FM, but only microscopically at any given point in an NM:

Charge flux: $j_C = j_{C\uparrow} + j_{C\downarrow}$

Spin flux: $j_S = j_{S\uparrow} - j_{S\downarrow} = \frac{\hbar}{e}\left(j_{C\uparrow} - j_{C\downarrow}\right)$

Heat flux: $j_Q = j_{Q\uparrow} + j_{Q\downarrow} = \frac{k_B T}{e}\left(j_{C\uparrow} + j_{C\downarrow}\right)$

Onsager, applied electric field only: $\begin{bmatrix} j_{C\uparrow} \\ j_{C\downarrow} \end{bmatrix} = \begin{bmatrix} G_\uparrow & 0 \\ 0 & G_\downarrow \end{bmatrix} \begin{bmatrix} \nabla\mu_\phi^\uparrow \\ \nabla\mu_\phi^\downarrow \end{bmatrix}$

Onsager: spin dependent conductance

Transformation of variables

$$j_C \equiv j_{c\uparrow} + j_{c\downarrow}$$ Charge current

$$j_S \equiv \frac{\hbar}{e}\left(j_{C\uparrow} - j_{\downarrow C} \right)$$ Spin current

$$\nabla \mu_\phi = \frac{1}{2}\frac{\partial\left(\mu_\phi^\uparrow + \mu_\phi^\downarrow\right)}{\partial x}$$ electrochemical potential

$$\nabla \mu_S = \frac{\partial\left(\mu_\phi^\uparrow - \mu_\phi^\downarrow\right)}{\partial x}$$ *spin accumulation potential*

$$G \equiv G_\uparrow + G_\downarrow$$ charge conductivity

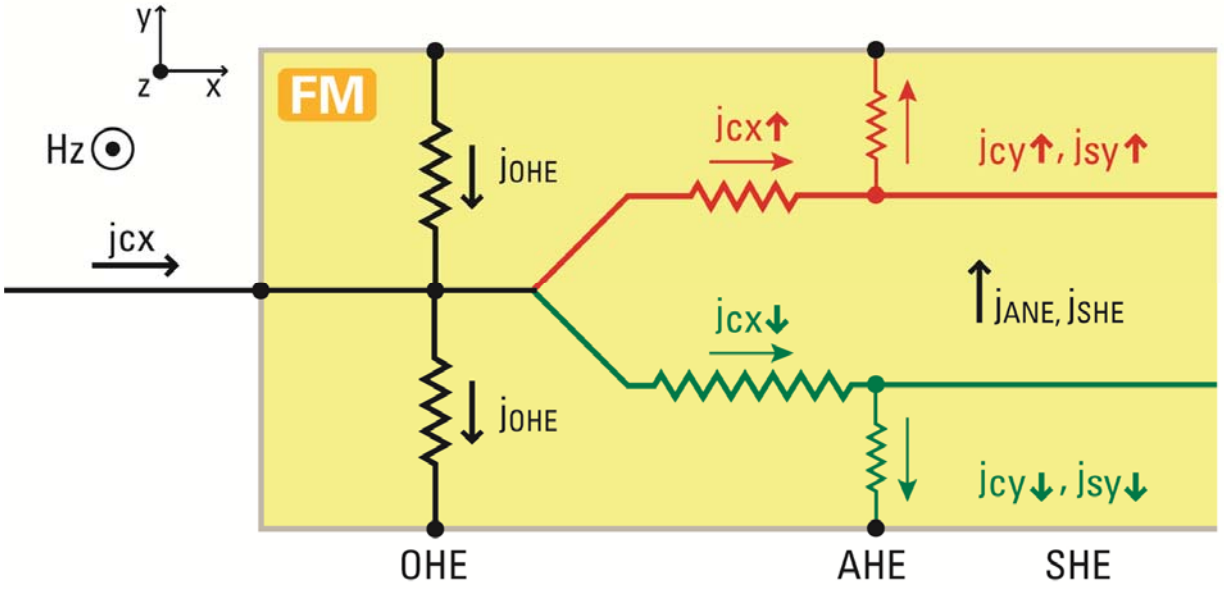
$$G_S \equiv G_\uparrow - G_\downarrow$$ *spin mixing conductivity*

$$\begin{bmatrix} j_C \\ j_S \, e/\hbar \end{bmatrix} = \begin{bmatrix} G & G_S \\ G_S & G \end{bmatrix} \begin{bmatrix} \nabla \mu_\phi \\ \frac{1}{2}\nabla \mu_S \end{bmatrix}$$

Electrical transport only

1. Spins also move under the magnetic force $F = \nabla(\vec{M} \bullet \vec{B})$
2. Temperature gradients
3. This is only local and microscopic, and subject to finite spin lifetime

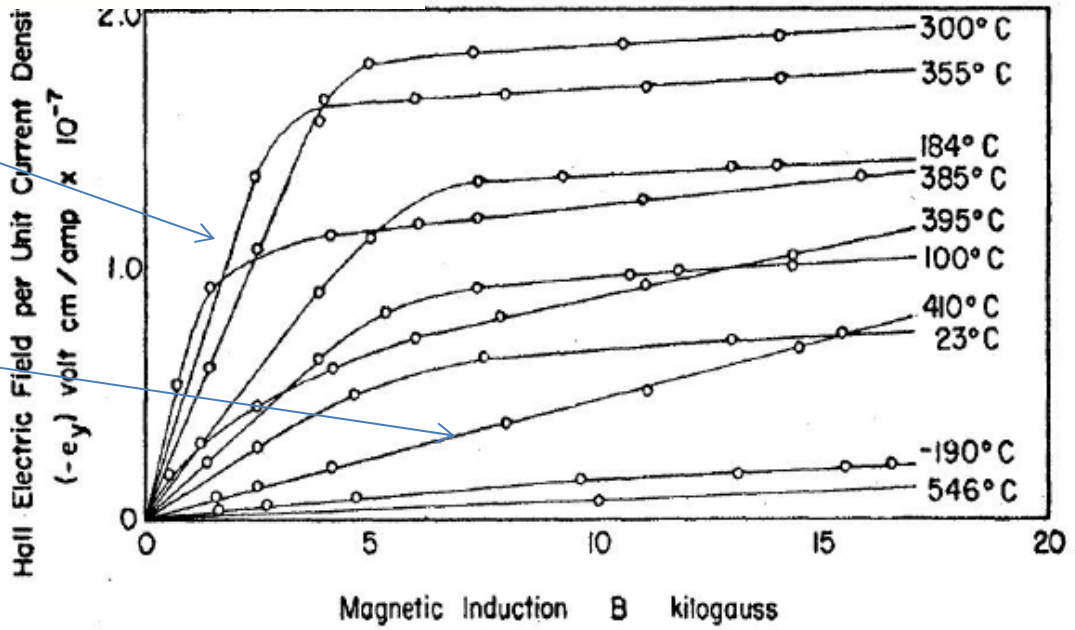
Anomalous Hall effect and Spin Hall Effect



Hall effect measurements on Ni

Anomalous Hall Effect (AHE)

Ordinary Hall Effect (OHE)



Nagaosa,& al. Rev. Mod. Phys. ***82****, 1539 2010*

When does this apply?

1. Ferromagnetic metals: spin-up and spin down bands are different

=> Spin polarization is always present

=> AHE and SHE are always present.

AHE IS NOT THE SAME AS AN ORDINARY HALL EFFECT WITH THE INTERNAL MAGNEITZATION INDUCTION (i.e. $B=M+\mu_0 H$)

2. Normal metals with low spin-orbit interactions

=> Spin flux injection results in spin polarization for a finite spin lifetime.

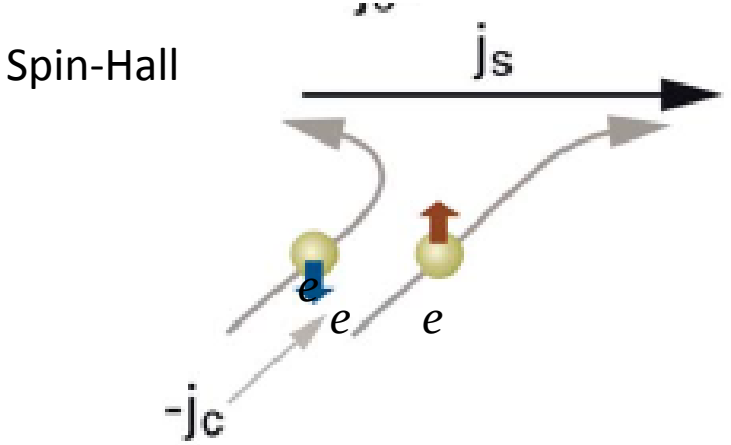
3. Normal metals with strong spin-orbit interactions

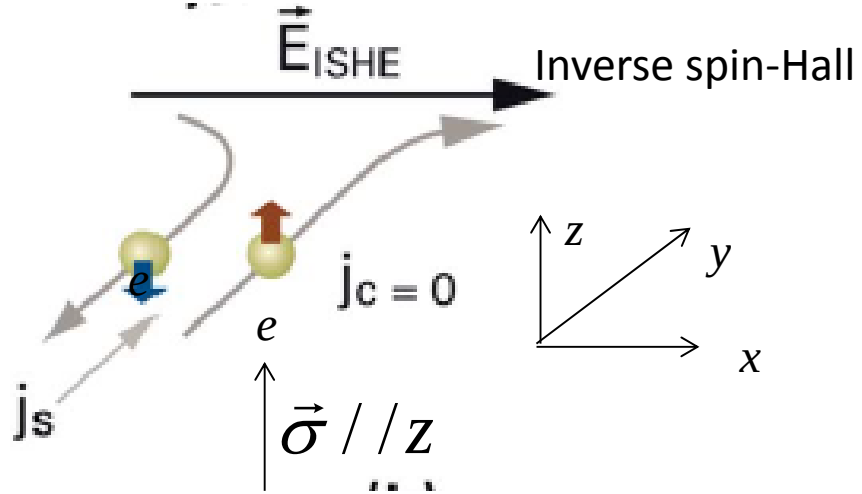
=> Charge current injection results in spin currents (spin-Hall effect)

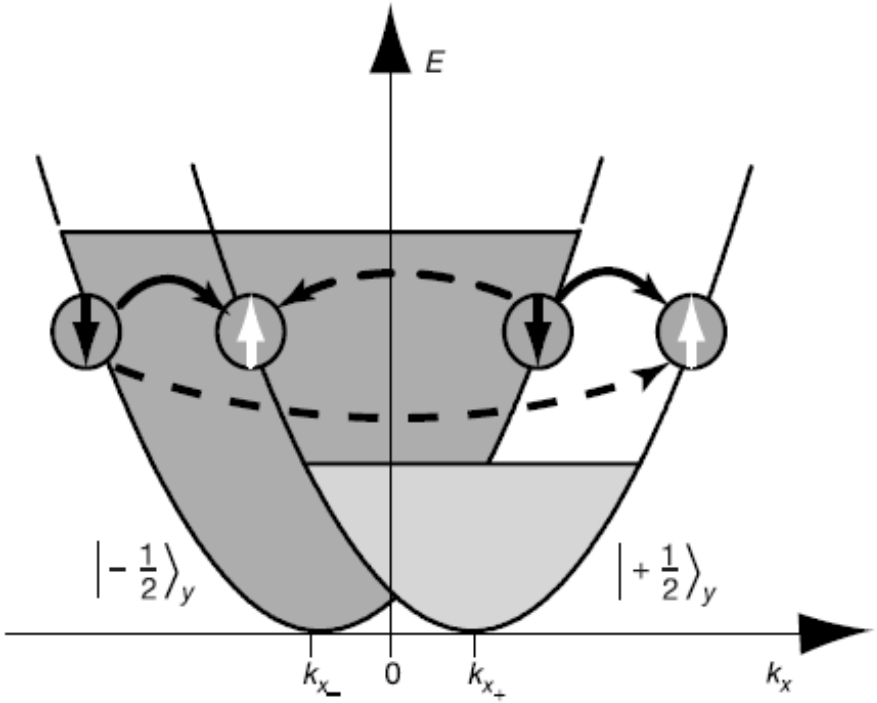
=> Spin current injection results in charge currents (inverse spin-Hall effect)

=> Both last only for a finite spin lifetime.

(Inverse) Spin Hall Effect (intrinsic only)







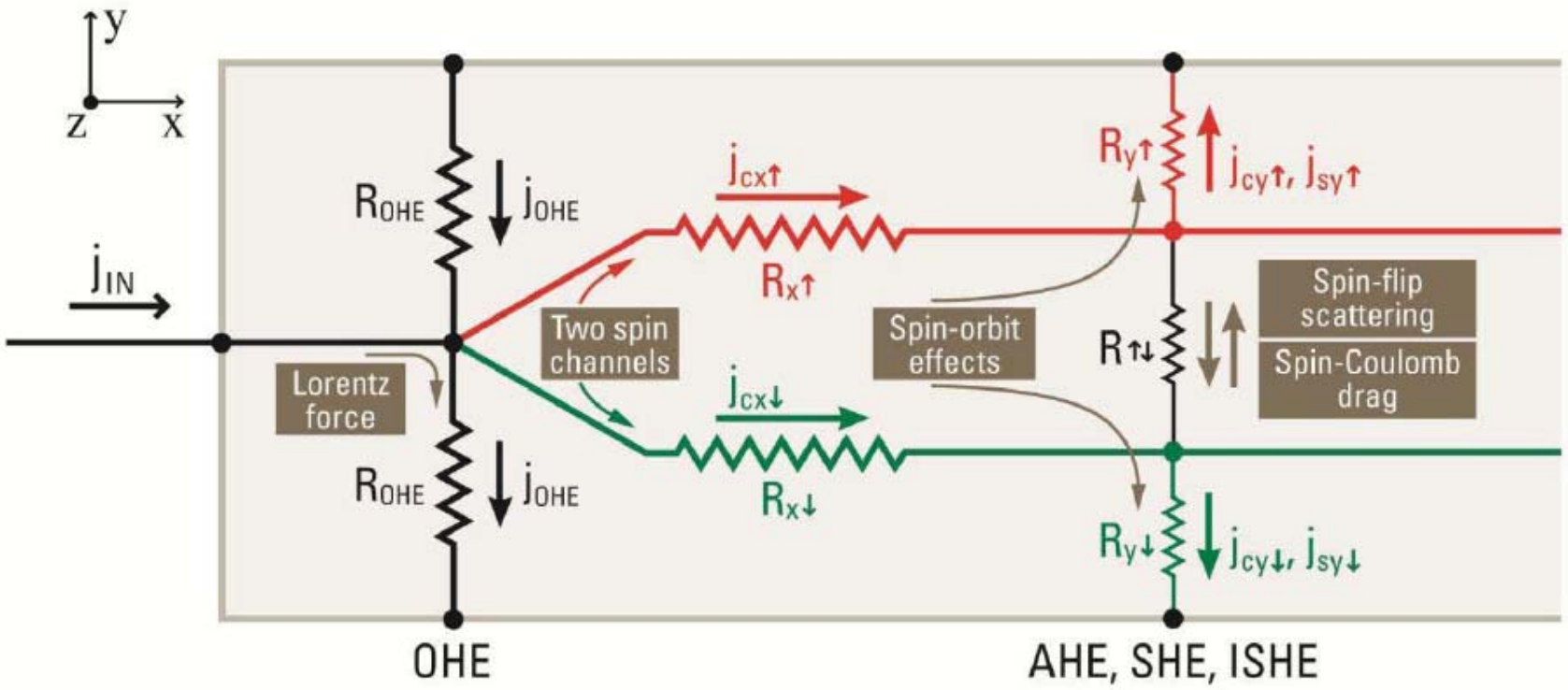
Sinova et al., Rev. Mod. Phys. ***87*** *1213 2015*

E_{ISHE} : If one spin subband is preferentially occupied by spin injection, asymmetric spin-flip scattering results in a current in the x direction. The rate of spinflip scattering depends on the value of the initial and final k-vectors. There are four distinct spin-flip scattering events possible.

$$\vec{E}_{ISHE} = D_{ISHE}(\vec{j}_S \times \vec{\sigma})$$

$$\mathbf{j}_c = \alpha_{\mathrm{SH}} \frac{2e}{\hbar} \mathbf{j}_s \times \boldsymbol{\sigma}$$

There is a connection between the two spin channels



Spin is not conserved => the two spin channels recombine with a **spin lifetime** τ_s

=> DRIFT-DIFFUSION EQUATION

Drift-diffusion

1. Continuity equation

$$\frac{\partial n}{\partial t} = \dot{G}_n - \frac{n(t) - n_0}{\tau_S} + \nabla \bullet \vec{j}_n$$

Generation rate; equilibrium population; lifetime; flux

2. Onsager

$$\vec{j}_n = \sigma \vec{\mathcal{F}} + D_n \nabla n$$

conductivity; force; Diffusion constant

3. Einstein (ideal gas):

$$D_n = k_B T \mu_{n,mob}$$

mobility

Notes

1. Never mix lifetime (τ_S) and scattering time (in mobility)
2. The diffusion constant is also a transport property, for classical parabolic bands:

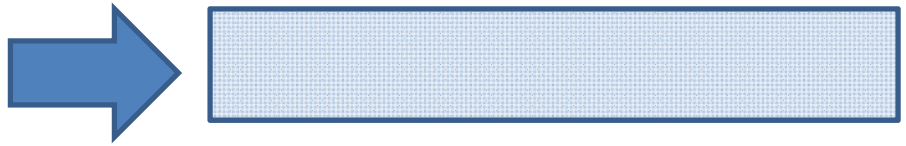
$$D_n = 2 k_B T \mu_{n,mob} \frac{F_{1/2}(\frac{\mu}{k_B T})}{F_{-1/2}(\frac{\mu}{k_B T})}$$

Electrochemical potential vis-a-vis band edge

Drift-diffusion

- Put this all together => one second-order differential equation (1-D).
- Assume STEADY STATE
- Assume all generation to take place at one surface

Spin pumping localized to x=0



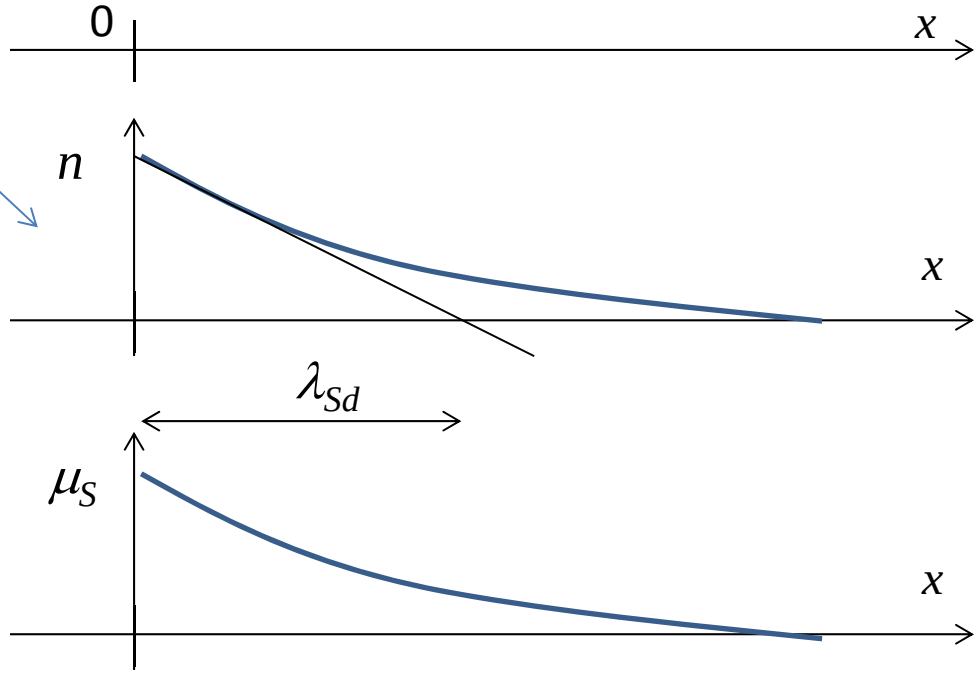
$$n(x) = n(0)\exp(-\frac{x}{\lambda_{Sd}})$$

Spin Diffusion Length

$$\lambda_{Sd} = \sqrt{D_n \tau_S}$$

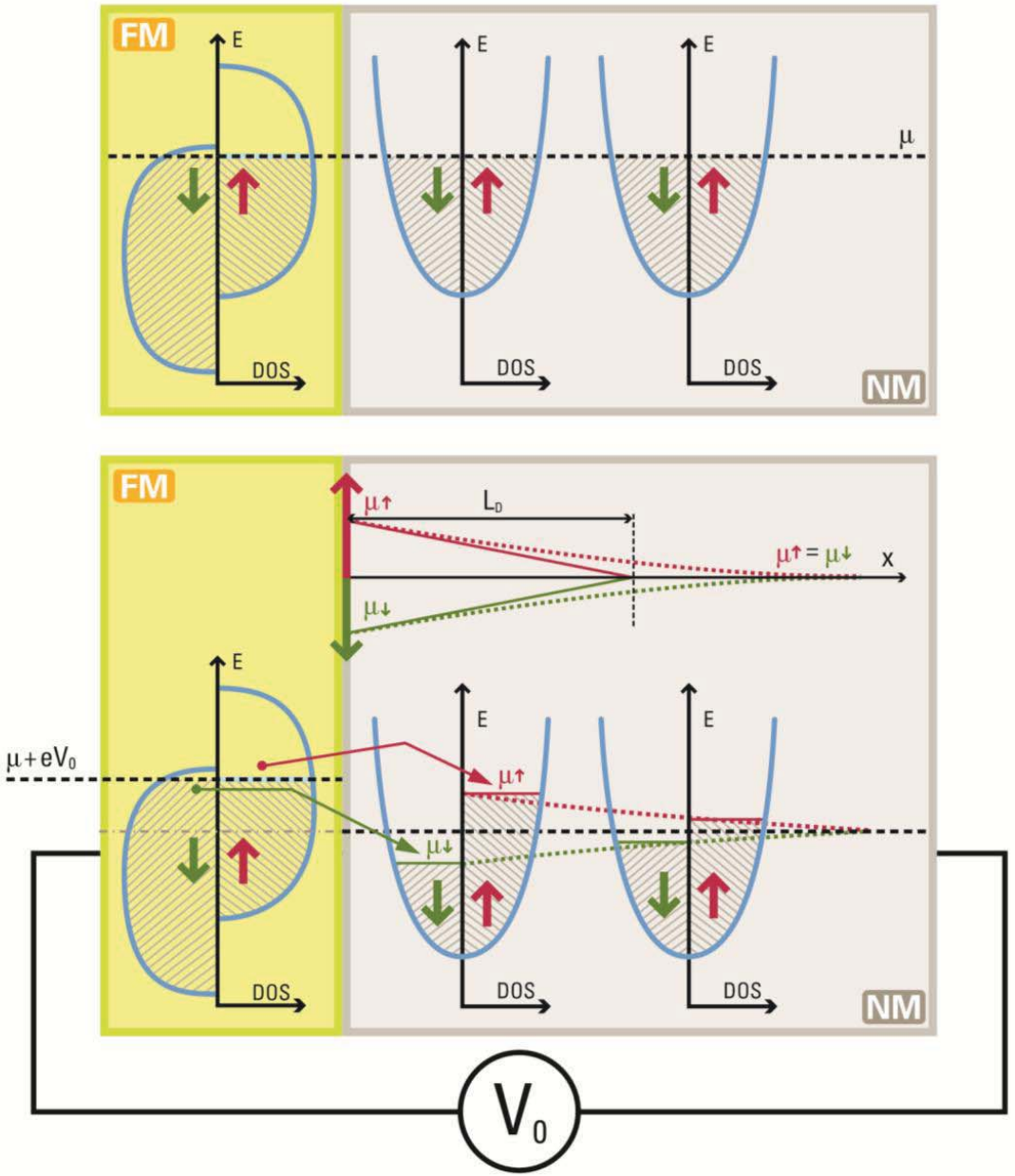
Electron diffusion constant, contains mobility and thus scattering time $D_n = k_B T \mu_{n,mob}$

Spin lifetime



Spin accumulation potential also decays

Example: Electrical spin injection across FM/NM metal interfaces



Johnson & Silsbee
Phys. Rev. B
1980's

Spin-Hall angle and spin diffusion length

are usually counter-indicated

TABLE I. Experimental spin Hall angles and effective spin-orbit-coupling parameters, $k_F^2\lambda_{e-so}$. The values marked measured but taken from the literature. The Fermi momenta are taken to be $k_F = 1.75 \times 10^8$ cm^{-1} (Al), $1.21 \times 1($ 10^8 cm^{-1} (Nb), and 1.0×10^8 cm^{-1} (Mo, Pd, Ta, Pt). Here, $k_F l = (3\pi/2)\sigma/k_F(h/e^2)$. References: (1) Valenzuela and T (2) Seki *et al.* (2008); (3) Mosendz *et al.* (2010b); (4) Niimi *et al.* (2011); (5) Morota *et al.* (2009); (6) Morota *et al.* (2011 (2010); (8) Kimura *et al.* (2007); (9) Vila, Kimura, and Otani (2007); (10) Ando *et al.* (2008); and (11) Liu *et al.* (2

	λ_{sd} (nm)	$k_F l$	$k_F^2\lambda_{e-so}$	α_{SH} (%)	$\lvert\alpha_{SH}^{sj}/\alpha_{SH}\rvert$
Al (4.2 K)	455 ± 15	73	0.0079	0.032 ± 0.006	0.67
Al (4.2 K)	705 ± 30	118	0.0083	0.016 ± 0.004	0.88
Au (295 K)	86 ± 10	371	0.3	11.3	0.014
Au (295 K)	$35 \pm 3^*$	253	0.52	0.35 ± 0.03	1.17
CuIr (10 K)	5–30			2.1 ± 0.6	
Mo (10 K)	10	36.8	0.32	−0.20	8.7
Mo (10 K)	10	8.11	0.07	−0.075	23
Mo (10 K)	8.6 ± 1.3	34.1	0.34	$-(0.8 \pm 0.18)$	2.5
Mo (295 K)	$35 \pm 3^*$	56.7	0.14	$-(0.05 \pm 0.01)$	9.9
Nb (10 K)	5.9 ± 0.3	11.3	0.14	$-(0.87 \pm 0.20)$	2.9
Pd (295 K)	9^*	24.0	0.23	1.0	1.9
Pd (10 K)	13 ± 2	26.8	0.18	1.2 ± 0.4	1.1
Pd (295 K)	$15 \pm 4^*$	48.6	0.28	0.64 ± 0.10	1.8
Pt (295 K)		77.9	0.74	0.37	5.1
Pt (5 K)	14	97.3	0.61	0.44	2.9
Pt (295 K)	10	67.6	0.58	0.9	1.9
Pt (10 K)	11 ± 2	98.5	0.77	2.1 ± 0.5	0.74
Pt (295 K)	7^*	77.8	0.97	8.0	0.31
Pt (295 K)	3–6	60.8	0.88–1.75	$7.6^{+8.4}_{-2.0}$	0.57
Pt (295 K)	$10 \pm 2^*$	29.2	0.25	1.3 ± 0.2	1.31
Ta (10 K)	2.7 ± 0.4	3.90	0.17	$-(0.37 \pm 0.11)$	24

Sinova et al., Rev. Mod. Phys. ***87*** *1213 2015*

Spin-dependent Seebeck

$$\begin{bmatrix} j_{C\uparrow} \\ j_{C\downarrow} \\ j_{Q\uparrow} \\ j_{Q\downarrow} \end{bmatrix} = \begin{bmatrix} G_{\uparrow} & 0 & L_{ET\uparrow} & 0 \\ 0 & G_{\downarrow} & 0 & L_{ET\downarrow} \\ L_{TE\uparrow} & 0 & L_{TT\downarrow} & 0 \\ 0 & L_{TE\downarrow} & 0 & L_{TT\downarrow} \end{bmatrix} \begin{bmatrix} \nabla \mu_{\phi}^{\uparrow} \\ \nabla \mu_{\phi}^{\downarrow} \\ \nabla T \\ \nabla T \end{bmatrix}$$

Partial Seebecks

$$\alpha_{\uparrow} = \frac{L_{ET\uparrow}}{G_{\uparrow}}$$

Total Thermopower: $\alpha = \dfrac{\alpha_{\uparrow} G_{\uparrow} + \alpha_{\downarrow} G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}}$

=> Thermally-driven accumulation due to Seebeck effect carries with it a spin accumulation:
=> **Spin-dependent Seebeck**

=> Onsager reciprocal: Spin-dependent Peltier

This has all been observed by Bart van Wees' group.

Spins on delocalized conduction electrons:

Part 3: Spins on localized electrons in FM metals OR insulators

MAGNON TRANSPORT

Here: only for ferromagnets

Magnons, Heisenberg ferromagnet

Spins = classical vectors of magnitude S

Energy: $U = -2J\sum_{p=1}^{N}\mathbf{S}_p \cdot \mathbf{S}_{p+1}$

exchange energy

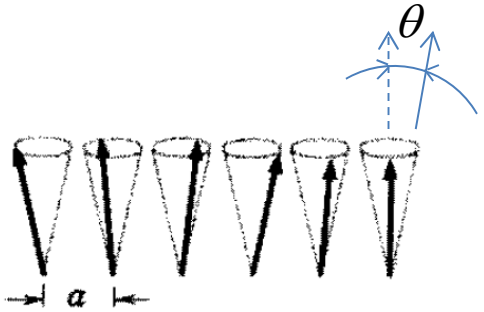
The **ferromagnetic ground state** has all spins parallel.

$\hbar\mathbf{S}_p$ = angular momentum of spin at site *p*

Ground state energy: $U_0 = -2NJS^2$

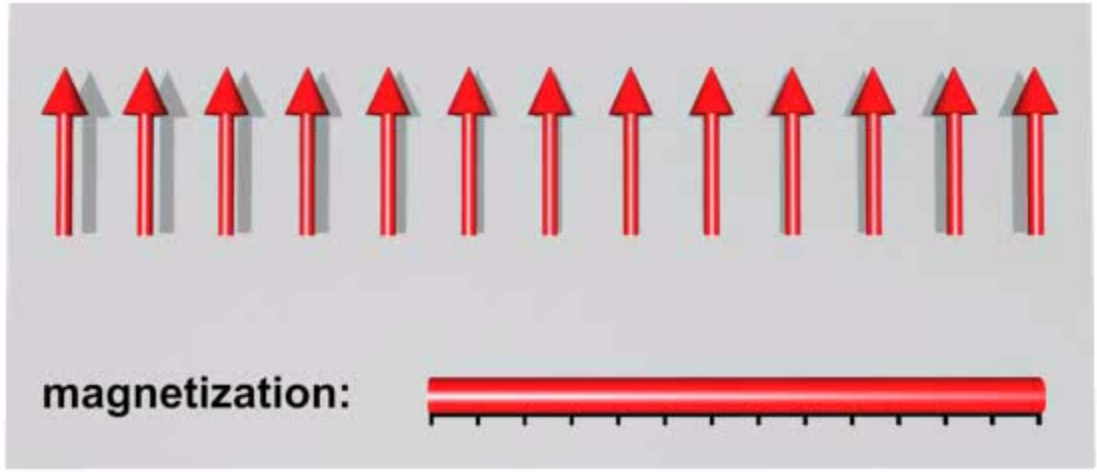
Excited states: all atoms share a little bit of thermally-driven spin reversal

=> spins precess



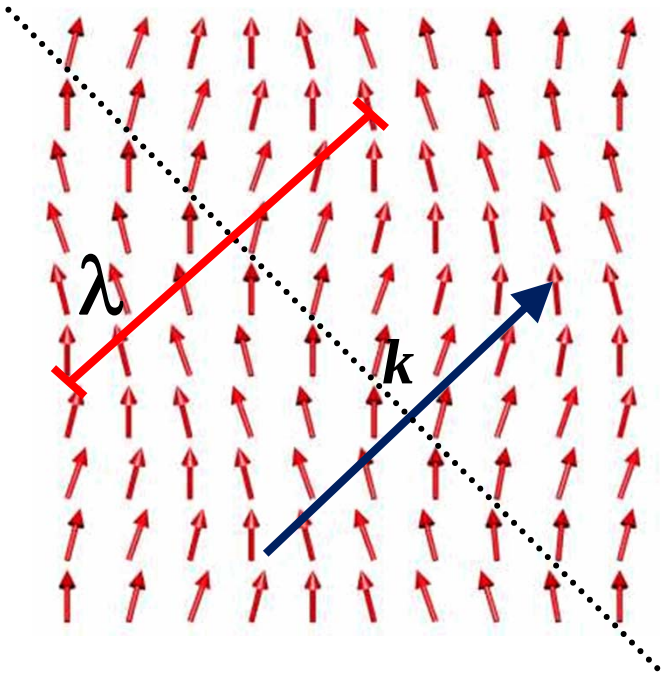
Magnons = propagating waves of the precession $\theta = \theta_0 e^{i(\omega t - kx)}$

Ground state => excited state



Slide adapted from Burkard Hillebrands, U. Kaiserslautern

Magnon wave equation



$$\theta = \theta_0 e^{i(\omega t - kx)}$$

Magnons have dispersion relations $\omega(k)$ just like phonons

Magnon dispersion relation

For a 1-dimensional chain:

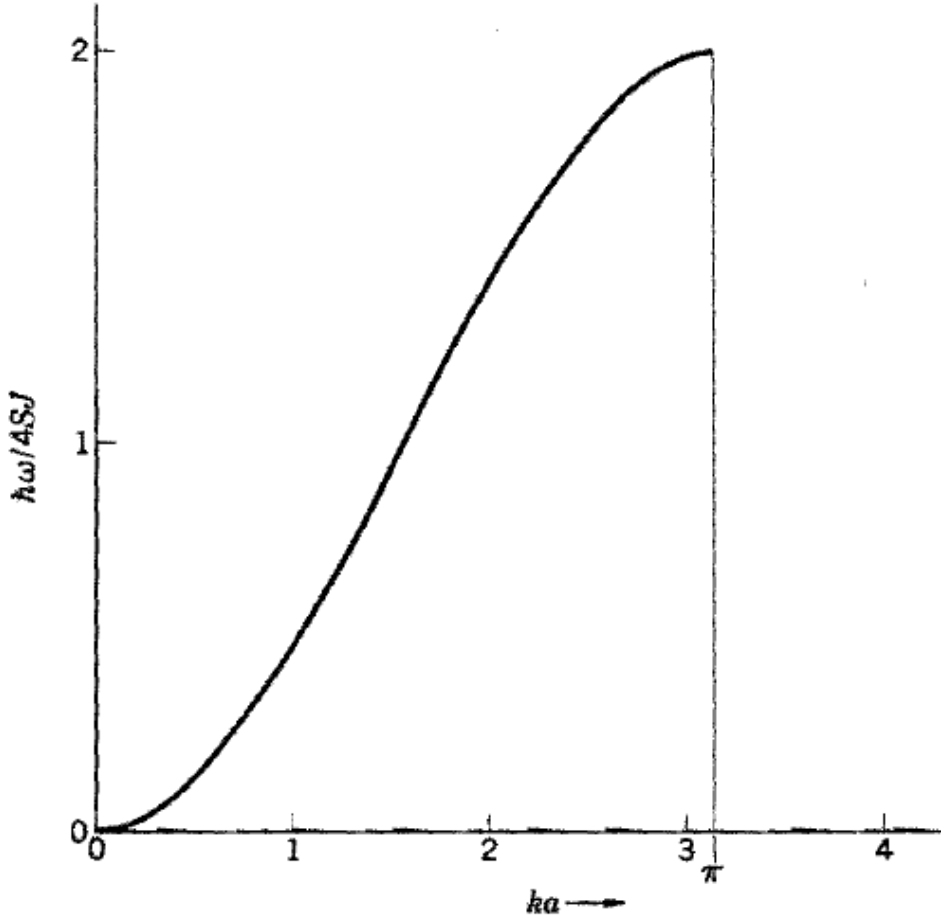
$$\hbar\omega = 4JS(1 - \cos ka)$$

At low k-values near zone center:

$$\hbar\omega \cong (2JS)a^2k^2 = Dk^2a^2$$

D is called the magnon "stiffness", closely related to J and to the Curie temperature T_C

Parabolic dispersion like electrons



Add an external field or an anisotropy field

C. Kittel, Quantum theory of solids, 2th. Ed., John Wiley, 1987

Hamiltonian considering nearest-neighbors, and Zeeman splitting

Zeeman energy term

$$\mathcal{H} = -J\sum_{p,\mathbf{a}} \mathbf{S}_p \cdot \mathbf{S}_{p+\mathbf{a}} - 2\left(\frac{\mu_B g}{2}\right) H_z \sum_p S_{p,z}$$

Index of the atom

Intensity of static magnetic field along z

Vector connecting atom p to it's neighbor

Zeeman term gives a gap at k=0.

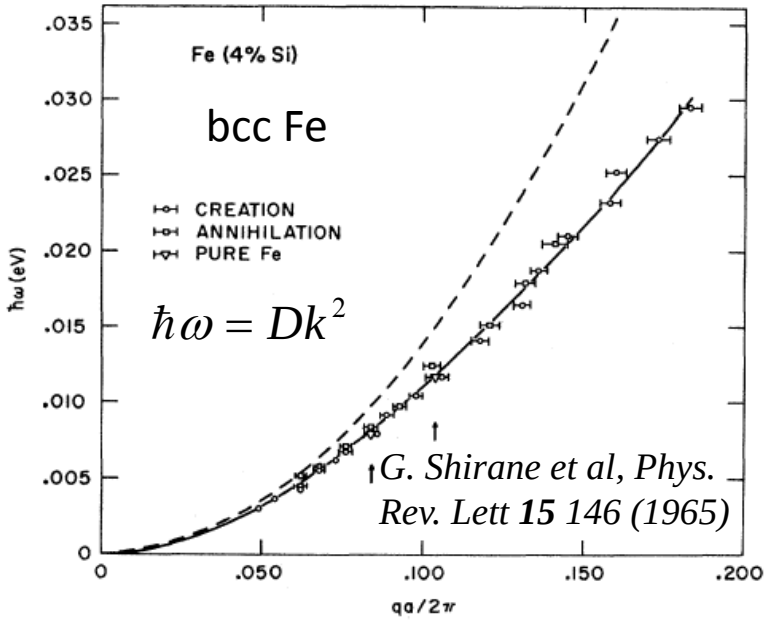
$$\hbar\omega_k = \mu_B g H_z + 2JSa^2k^2$$

The anisotropy field gives the same effect as the external magnetic field

Examples

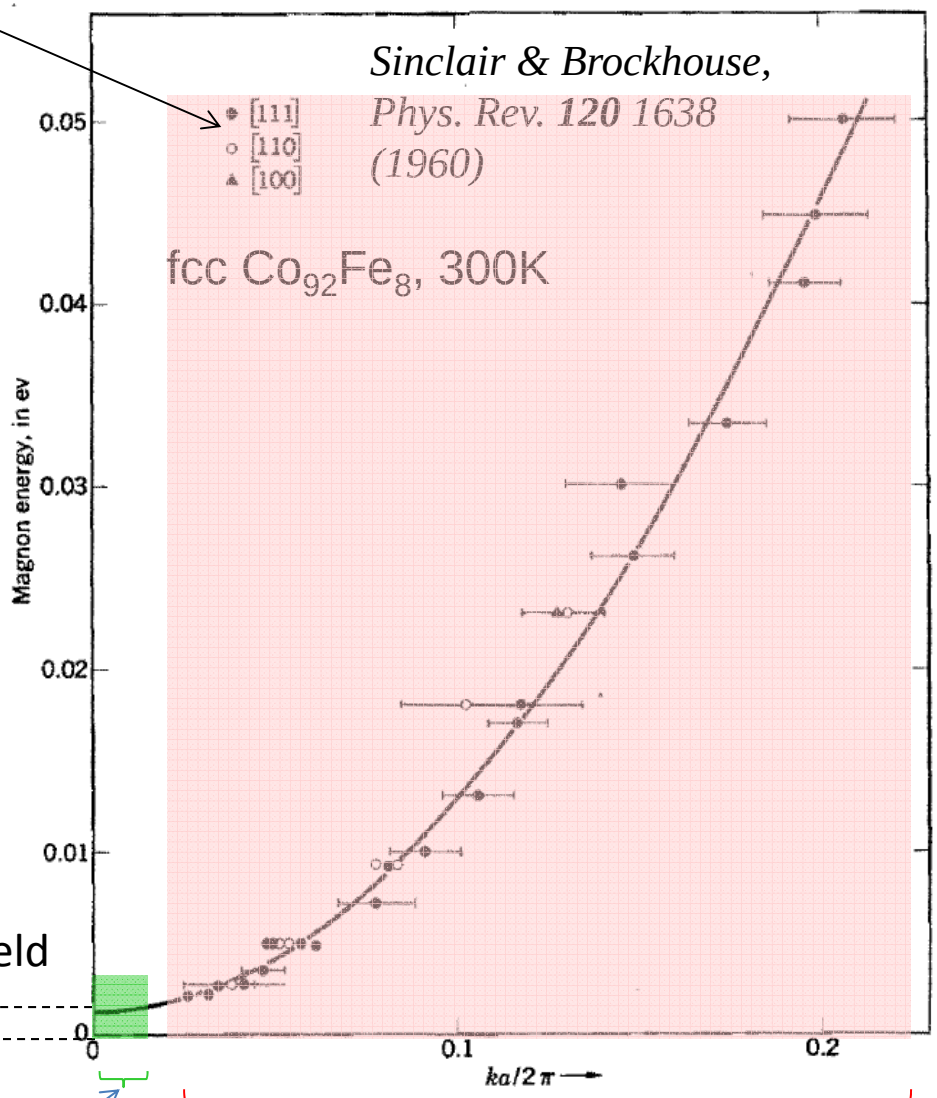
$$\hbar\omega_k = \mu_B g H_z + 2JSa^2k^2$$

Dispersion itself very isotropic



G. Shirane et al, Phys. Rev. Lett ***15*** *146 (1965)*

FIG. 2. Magnon dispersion relation for iron, containing 4% Si. The arrows call attention to the two points measured for pure iron. The dashed curve is the function $\hbar\omega = 286q^2$, while the smooth curve is a least-squares fit through the experimental points as explained in the text.



Sinclair & Brockhouse, Phys. Rev. ***120*** *1638 (1960)*

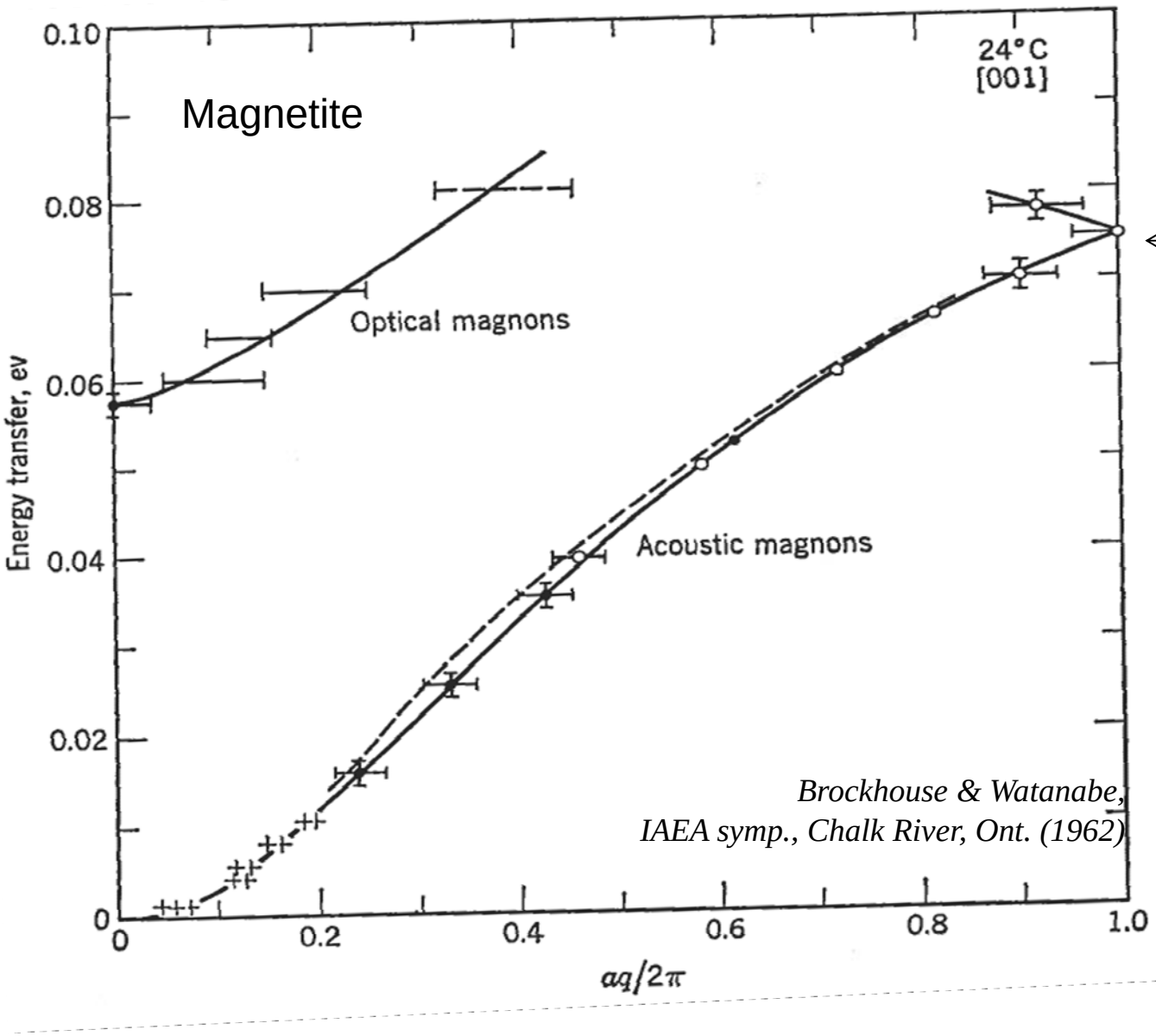
Anisotropy field

$g\mu_B H_{ANIS}$

Dipole-coupled magnons

Exchange-coupled magnons

Magnon dispersions, multi-atom ferromagnets



Brockhouse & Watanabe, IAEA symp., Chalk River, Ont. (1962)

$\mathcal{E}_{MAX}$ = 0.075 meV
= k_B x 870 K

Directly related to the Curie temperature

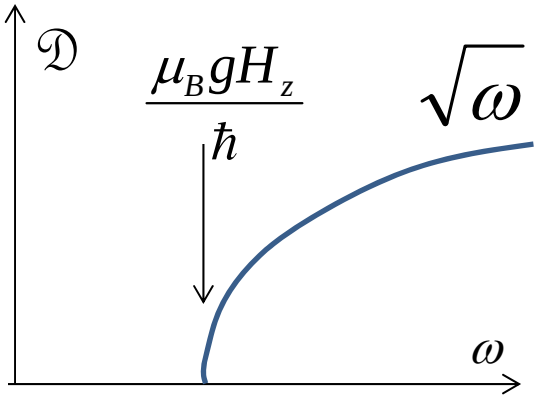
Density of states (3-dimensional) $\mathcal{D}(\omega)$ (ferromagnets)

Magnons have only a single polarization for each value of *k*

Number of modes of wavevector less than *k* in unit volume: $(1/2\pi)^3(4\pi k^3/3)$

Number of magnons of frequency between ω and ω+$d\omega$ in unit volume of crystal

$$\mathcal{D}(\omega)d\omega = \left(\frac{1}{2\pi}\right)^3 4\pi k^2 \frac{dk}{d\omega} d\omega$$



$$\hbar\omega_k = \mu_B g H_z + 2JSa^2k^2$$

$$\frac{d\omega}{dk} = 2\left(\frac{2JSa^2}{\hbar}\right)\sqrt{\omega}$$

$$\mathcal{D}(\omega) = \begin{cases} 0 & \text{if } \omega < \mu_B g H_z/\hbar \\ \frac{1}{4\pi^2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\sqrt{\omega} & \text{if } \omega > \mu_B g H_z/\hbar \end{cases}$$

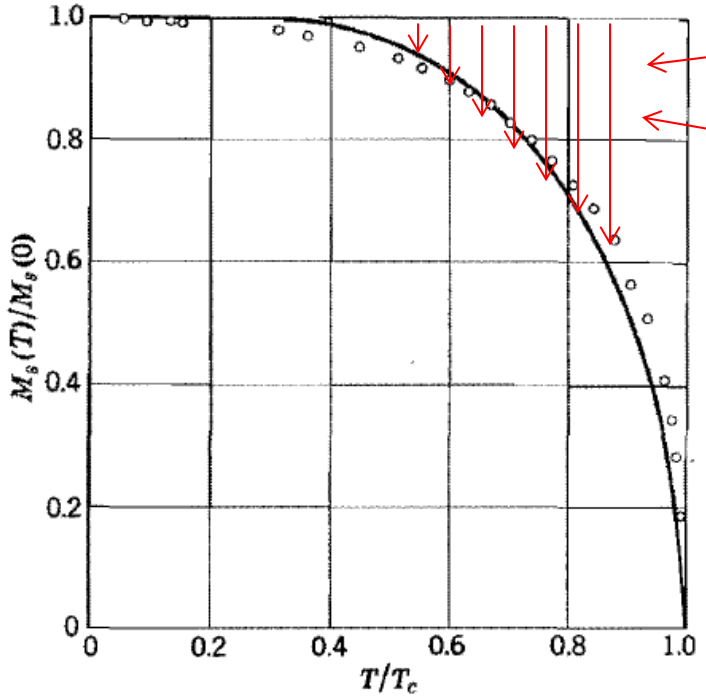
Temperature-dependence of magnetization

Magnons follow Bose-Einstein statistics $f_0 = \left(\exp(\frac{\hbar\omega}{k_B T}) - 1 \right)^{-1}$

Number density of magnons at $T\ (H=0)$:

$$n(T) = \int_0^\infty \mathcal{D}(\omega)\, f_0(\omega) d\omega \approx \frac{\zeta(\frac{3}{2})}{8\pi^{3/2}} \left(\frac{k_B T}{2JSa^2} \right)^{3/2}$$

Loss of magnetization with increasing temperature:



$$\frac{\Delta M_S(T)}{M_S(T=0)} = \frac{n(T)}{NS}$$

$$\frac{\Delta M_S(T)}{M_S(T=0)} = \frac{0.0578}{SQ} \left(\frac{k_B T}{2JS} \right)^{3/2}$$

The "Bloch $T^{3/2}$ law"

Number of atoms per unit volume=Q/a^3, Q=1 (sc), 2 (bcc), 3 (fcc)

Experimentally verified, $T < T_C$ / *(5 to 10)*

Felix Bloch, Z. Physik ***61*** *206 (1931)*

Magnon specific heat (ferromagnets)

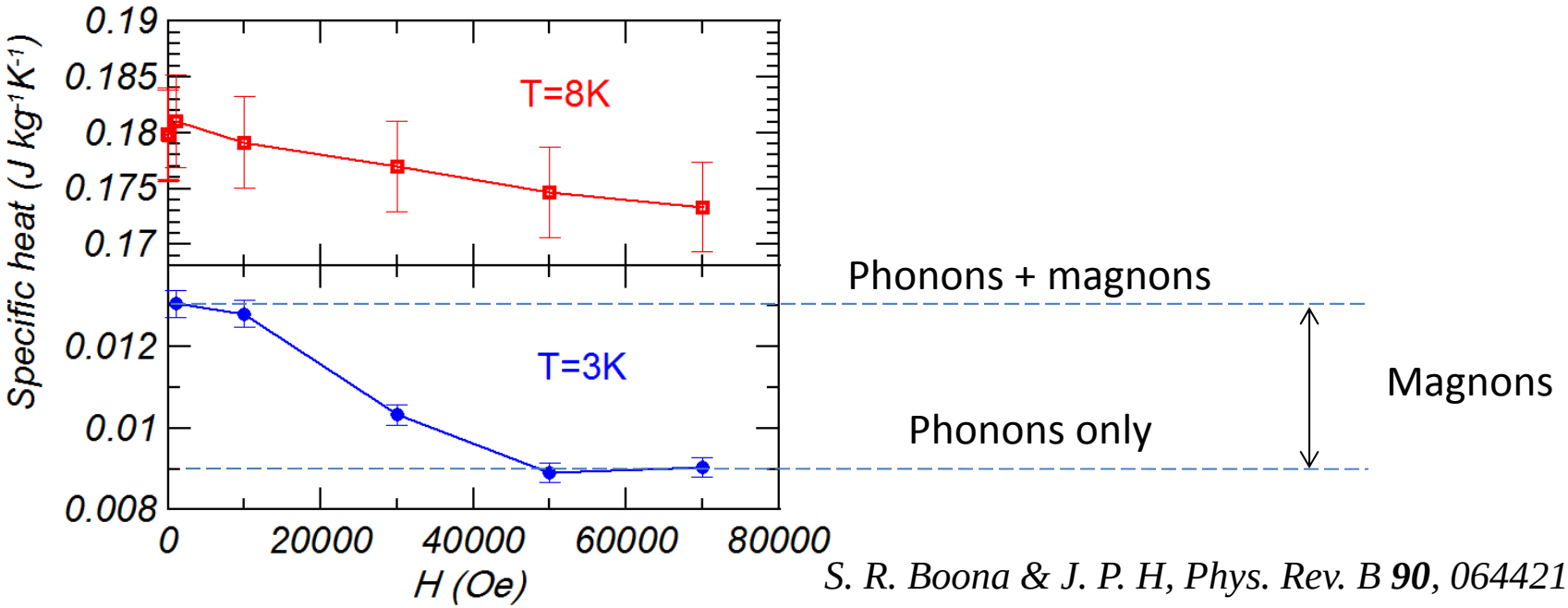
$H=0$

$$U(T) = \int_0^\infty \hbar\omega \mathcal{D}(\omega) f_0(\omega) d\omega$$

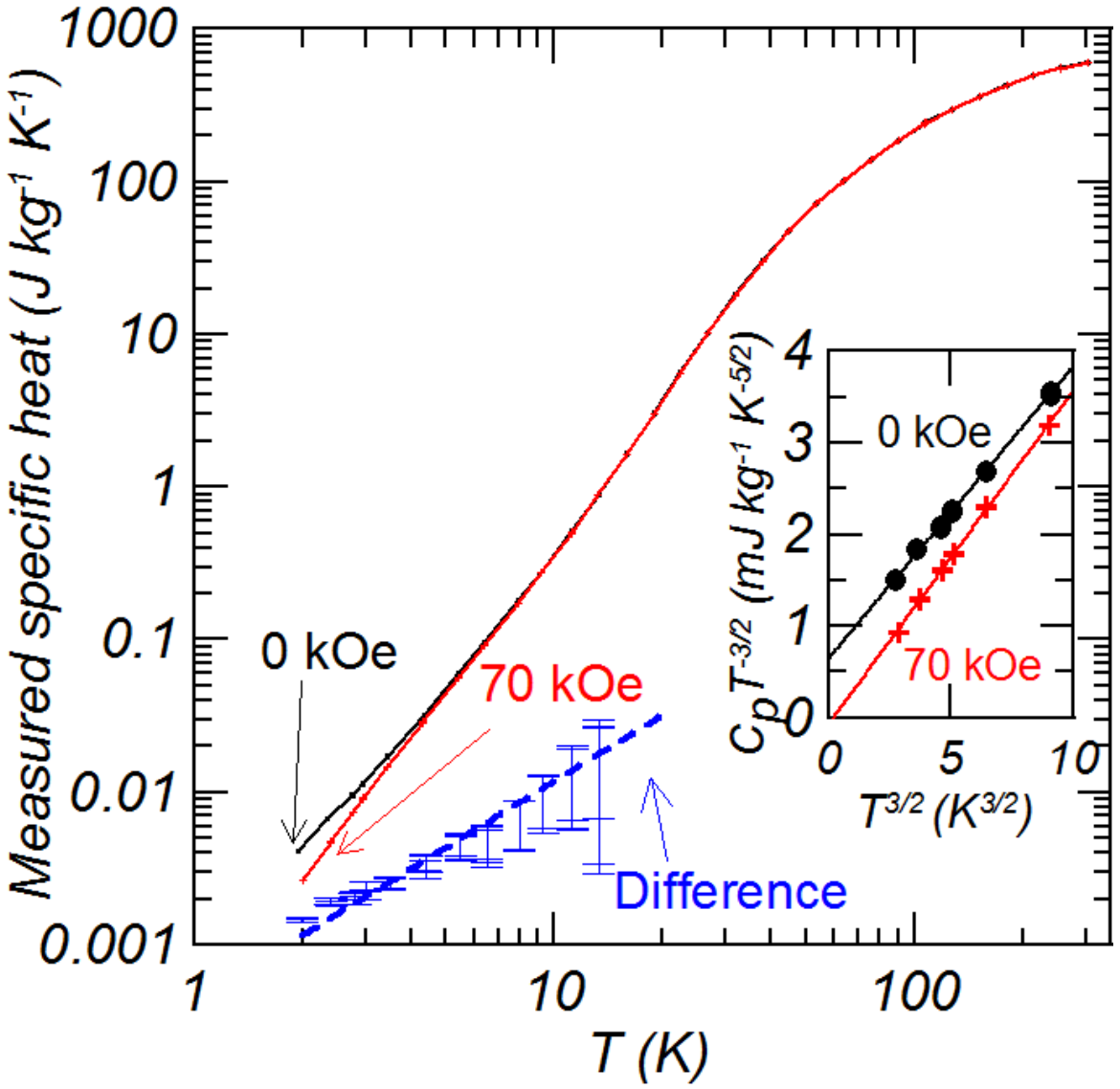
$$C(T) \equiv \frac{dU}{dT} = 0.113 \left(\frac{k_B T}{2JSa^2} \right)^{3/2}$$

Add a magnetic field, and the integral doesn't start at zero but at $-g\ \mu_B B$

$$C(T) \equiv \frac{dU}{dT} = 0.113 \left(\frac{k_B T}{2JSa^2} \right)^{3/2} f(\mu_B g H_z / k_B T)$$



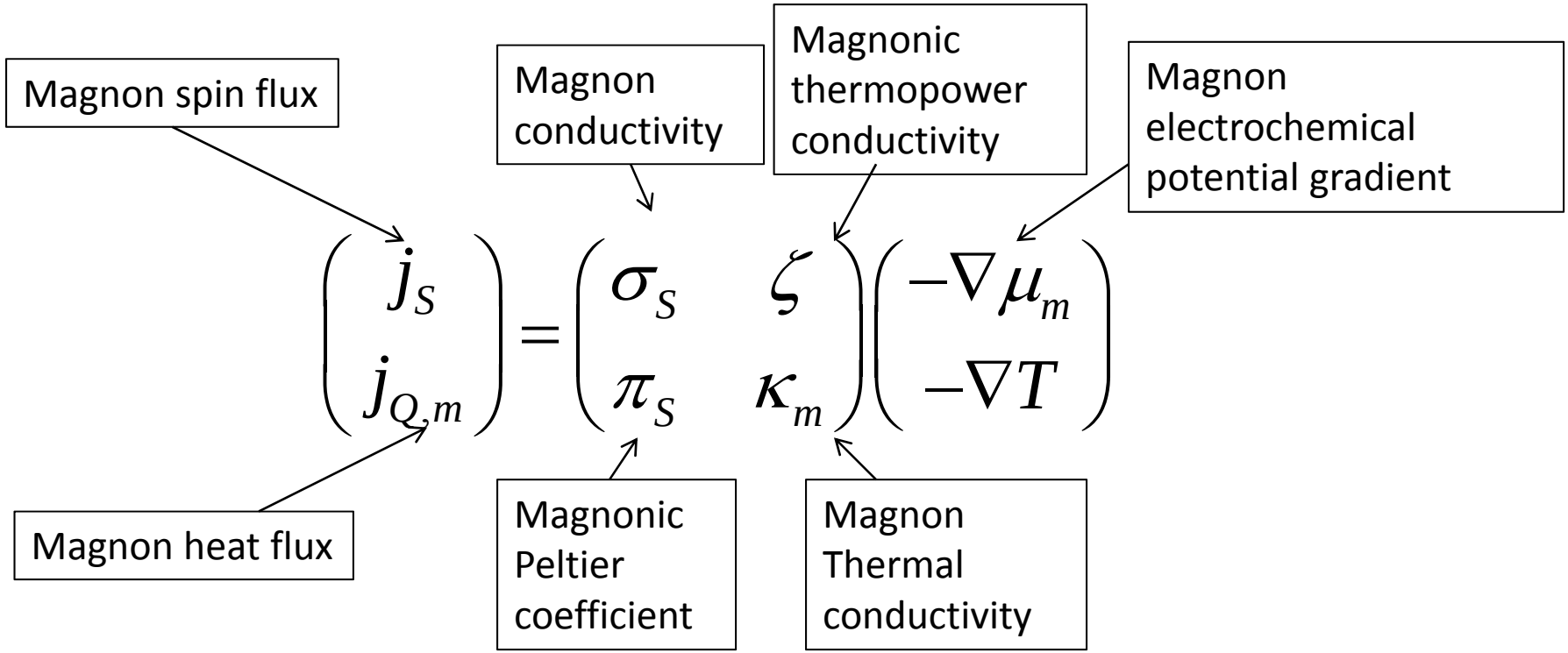
Magnon Specific Heat



S. R. Boona & J. P. H, Phys. Rev. B ***90****, 064421 (2014).*

Transport: Onsager for Magnons

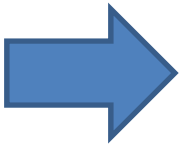
Linear response theory: a number of **very new concepts** in transport:



Flebus, Bender, Tserkovnyak and Duine, arXiv 1510.05316v2, 30 Oct 2015
Review: Vandaele, Watzman, Flebus, Prakash, Zheng, Heremans..,
Materials Today Physics, Accepted (2017)

Magnon chemical potential

Active magnon pumping



Ferromagnetic insulator

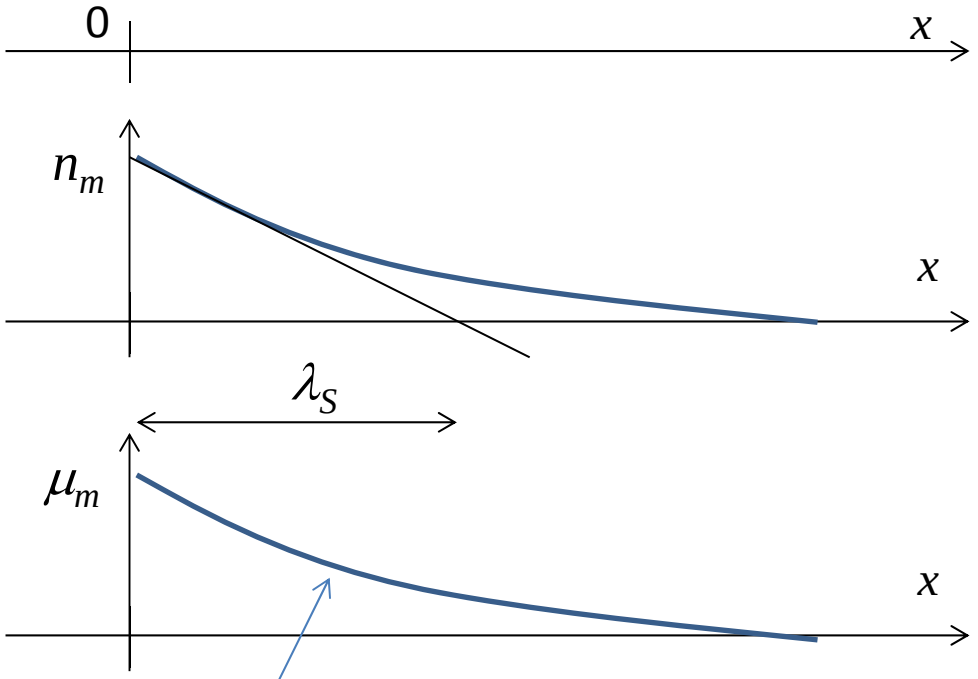
$$n(x) = n(0)\exp(-\frac{x}{\lambda_{Sd}})$$

Spin Diffusion Length

$$\lambda_S = \sqrt{D_m \tau_S}$$

Magnon diffusion constant, contains mobility and thus scattering time $D_m = k_B T \mu_{m,mob}$

Spin lifetime

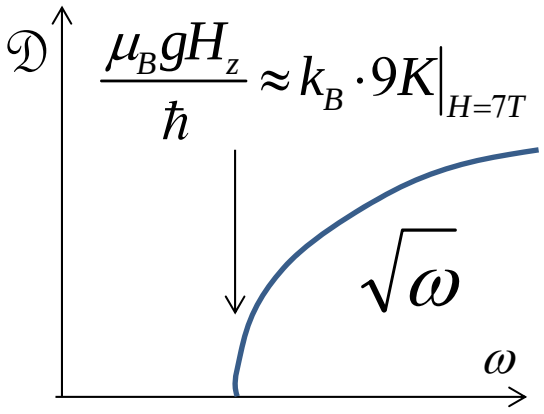


In the region where there is pumping, the excess magnons are represented in the distribution function

$$f = \left(\exp(\frac{\hbar\omega - \mu_m}{k_B T}) - 1 \right)^{-1}$$

Far from the pumping: Thermodynamic equilibrium => μ_m=0

$$f_0 = \left(\exp(\frac{\hbar\omega}{k_B T}) - 1 \right)^{-1}$$

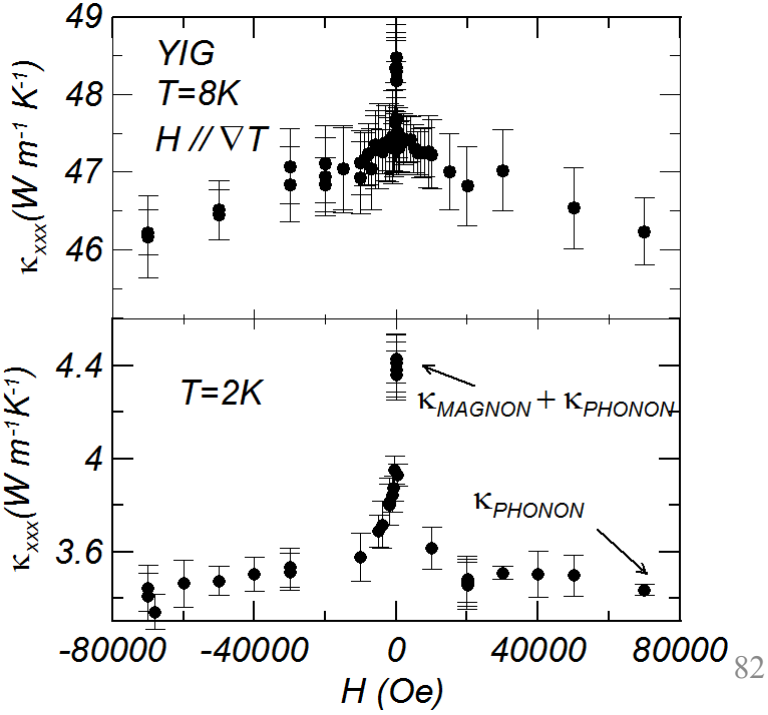


Magnonic thermal conductivity

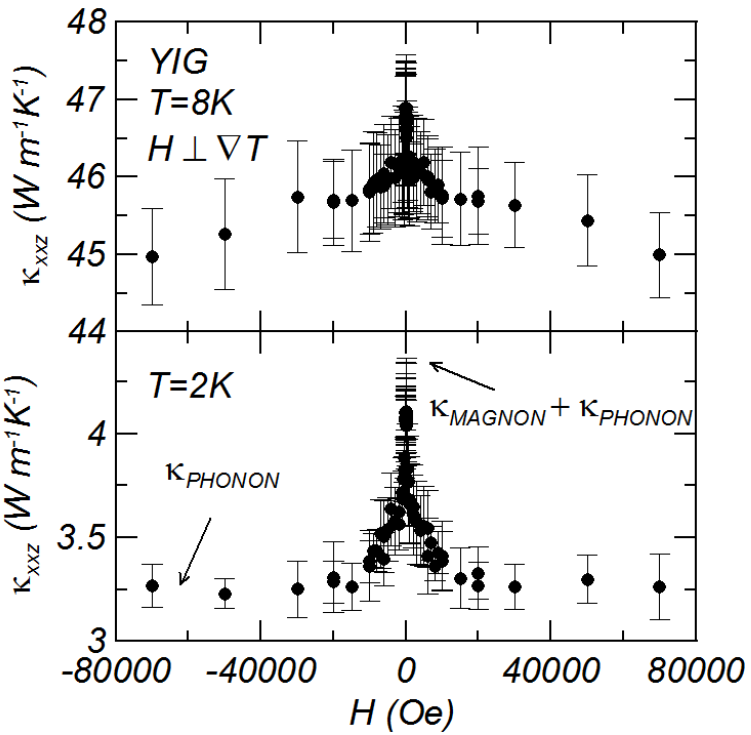
Like for specific heat, magnetic fields can freeze out magnons,
~ 10^{-4}eV/T or 1.3 K / T

The field direction vis-a-vis the heat flux does not matter
Alignment of local moments always // field.

Thermal conductivity field // heat

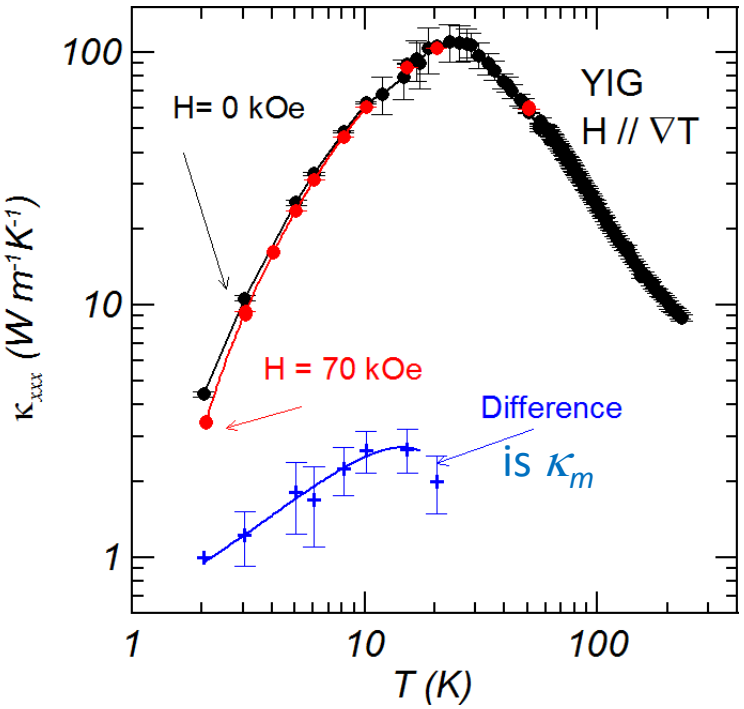


Thermal conductivity field ⊥ heat

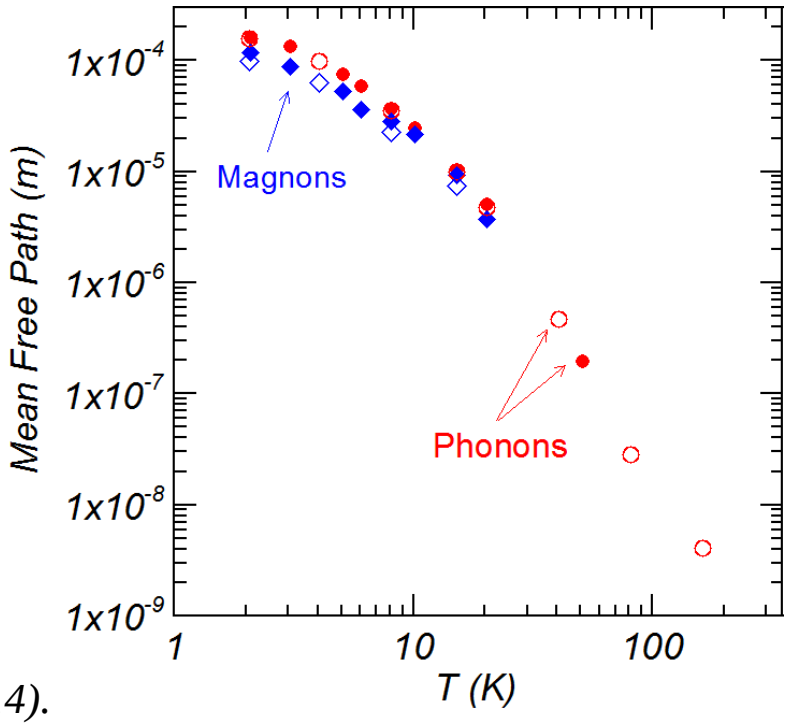


S. R. Boona & J. P. H, Phys. Rev. B ***90****, 064421 (2014).*

Magnonic thermal conductivity



Magnon energy mean free path ℓ



Treating magnons like an ideal gas =>

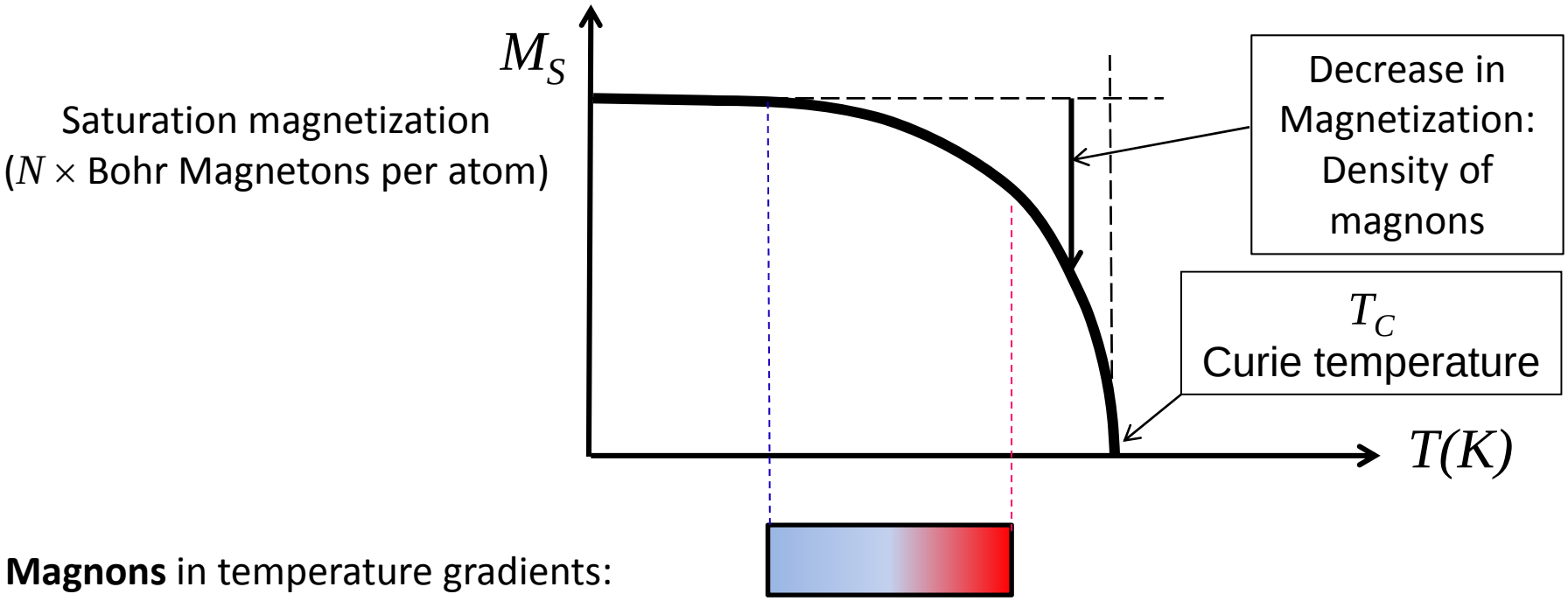
$$\kappa_{PHONON} = \tfrac{1}{3} C_{PHONON} v_{PHONON} \ell_{PHONON}$$

$$\kappa_{MAGNON} = \tfrac{1}{3} C_{MAGNON} v_{MAGNON} \ell_{MAGNON}$$

S. R. Boona & J. P. H, Phys. Rev. B ***90****, 064421 (2014).*

Magnonic thermal conductivity gives spin flux

Magnons are the reason magnets loose strength with increasing temperature:



Magnons in temperature gradients:

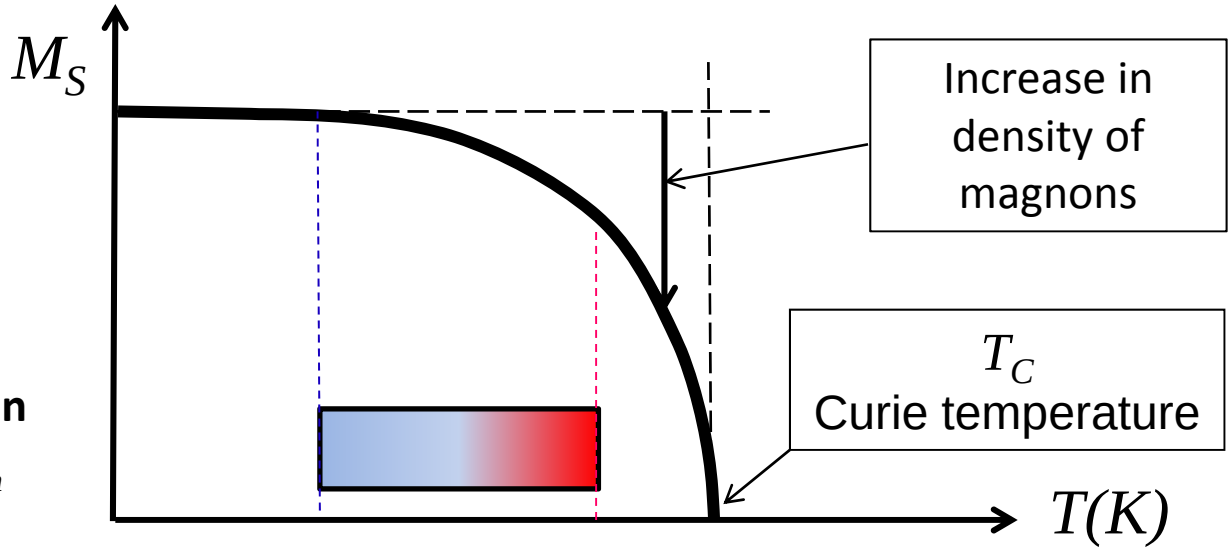
Gradient: $\nabla T \Rightarrow \nabla n_m$ & ∇M

Flux: $j_{Q,m} \Rightarrow j_{magnon\ density}$ & $j_{MAGNETIZATION}$

Magnonic heat flux is a spin flux => $j_s \approx \frac{\hbar}{k_B T} j_{Q,m} \approx \frac{\hbar}{k_B T} \kappa_m \nabla T$

Vandaele & al. Materials Today Physics, Accepted (2017)

Magnonic thermopower



In the presence of spin injection
=> Gradient: ∇T => ∇n_m & $\nabla \mu_m$

The ***magnonic thermopower*** is defined by considering $\begin{pmatrix} j_S \\ j_{Q,m} \end{pmatrix} = \begin{pmatrix} \sigma_S & \zeta \\ \pi_S & \kappa_m \end{pmatrix} \begin{pmatrix} -\nabla \mu_m \\ -\nabla T \end{pmatrix}$

under open-circuit conditions, i.e., solving for j_S=0

$$\alpha_m = -\frac{\nabla \mu_m}{\nabla T} = -\frac{\zeta}{\sigma_S}$$

Vandaele & al. Materials Today Physics, Accepted (2017)

Microscopic solution for magnonic thermopower

Treat magnons as a dilute "ideal" gas (i.e. no interactions):

Internal energy gradient $\nabla U = C_m \nabla T + n_m \nabla \mu_m$ exerts a force $\mathbf{F}$ that drives the magnon flow.

The force is the gradient in pressure, which is 2/3 ∇U

Newton's second law to an element of the magnon gas of volume δV

Magnon mass ↘ ↙ Magnon velocity

$$n_m M \, \delta V \frac{d\mathbf{v}_m}{dt} = \delta \mathbf{F}$$

Magnon acceleration $$\frac{d\mathbf{v}_m}{dt} = -\frac{2}{3 n_m M} C_m \nabla T - \frac{2}{3M} \nabla \mu$$

No current => net acceleration is zero =>

$$\alpha_m = -\frac{\nabla \mu}{\nabla T} = \frac{C_m}{n_m}$$

Vandaele & al. Materials Today Physics, Accepted (2017)

Conclusion

Fermions

Thermopower is the energy-derivative of the transmission function (or energy-dependent electrical conductivity)

$$\alpha_{\uparrow/\downarrow} = \frac{\pi^2}{3}\frac{k_B}{e}k_B T \frac{\left| d\sigma_{\uparrow/\downarrow}(E) \middle/ dE \right|_{E=\mu_e}}{\sigma_{\uparrow/\downarrow}(\mu)}$$

The more electrons there are the lower the thermopower

$$\alpha \propto -\ln\left(n_e\right)$$

Bosons

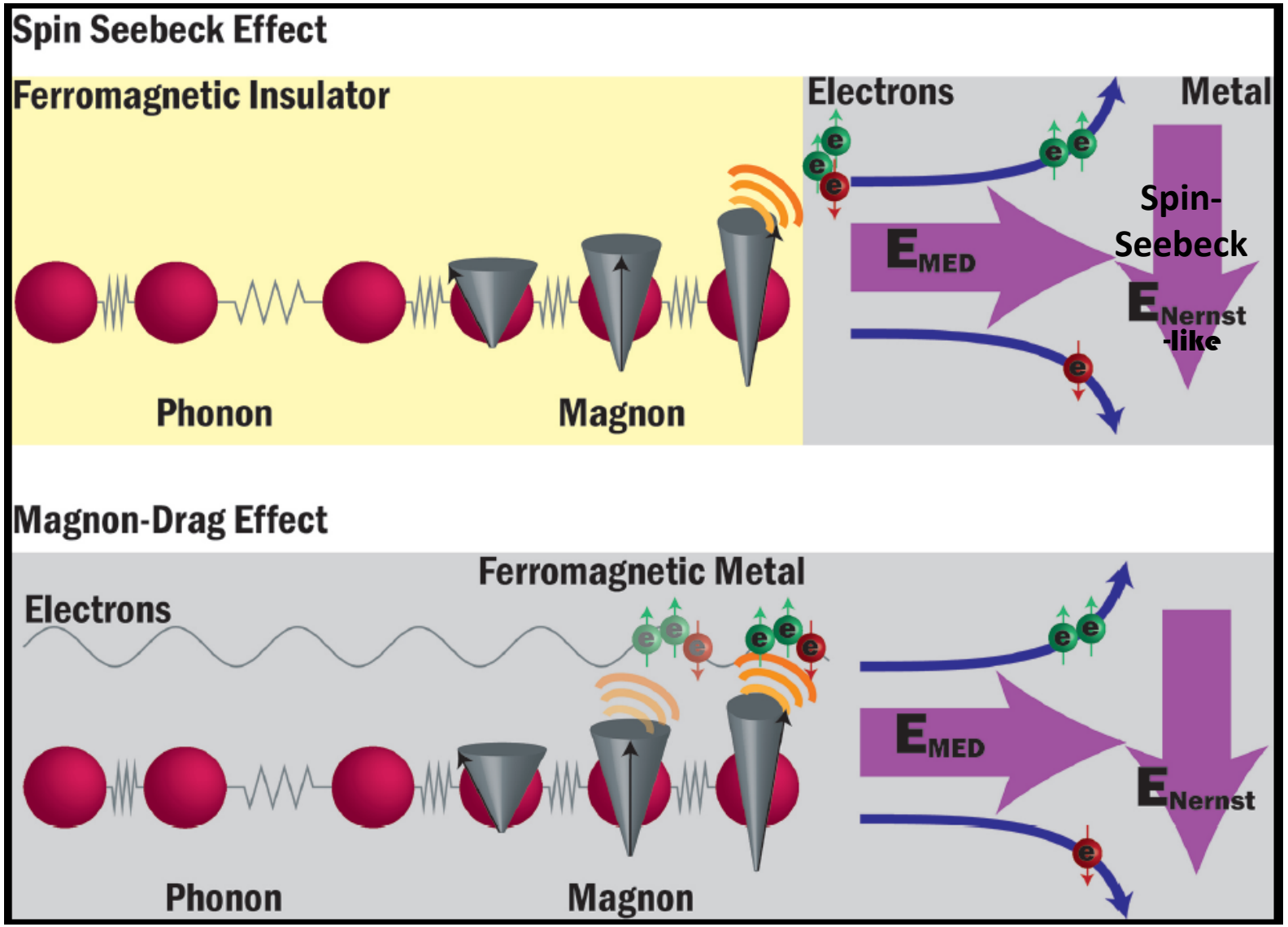
Thermopower is the specific heat per particle

$$\alpha_m = \frac{C_m}{n_m}$$

Thermopower less dependent on density

=> it is better to use a temperature gradient to drive magnons and make magnons drive electrons: ADVECTIVE TRANSPORT

Advective transport: spin-Seebeck effect & magnon drag



Boona...JPH, APL Materials ***4****, 104502 (2016)*

Spares

The potentials are intensive

Potentials:

$$T \equiv \left(\frac{\partial S}{\partial U} \right)_{X_i}^{-1} \qquad \phi_i \equiv -T^{-1} \left(\frac{\partial S}{\partial X_i} \right)_{X_{j \neq i}}$$

Are intensive because

$$T(\lambda \times system) = \left[\left(\frac{\partial S(\lambda U, \lambda X_i)}{\partial(\lambda U)} \right)_{X_i} \right]^{-1} = \left[\left(\frac{\lambda \partial S(U, X_i)}{\lambda \partial U} \right)_{X_i} \right]^{-1} = \left[\left(\frac{\partial S(U, X_i)}{\partial U} \right)_{X_i} \right]^{-1} = T(system)$$

$$\phi_i(\lambda \times system) = -T^{-1} \left(\frac{\partial S(\lambda U, \lambda X_i)}{\partial(\lambda X_i)} \right)_{X_{j \neq i}} = -T^{-1} \left(\frac{\lambda \partial S(U, X_i)}{\lambda \partial(X_i)} \right)_{X_{j \neq i}} = -T^{-1} \left(\frac{\lambda \partial S(U, X_i)}{\lambda \partial(X_i)} \right)_{X_{j \neq i}} = \phi_i(system)$$

Potentials pair up with their extensives:

Pressure -⇔ volume Stress ⇔ strain

Electrochemical potential⇔ Electrical charge and with Number of Particles

Magnetic field ⇔ magnetization

Mathematically, temperature is a potential, even though entropy is different from the other extensives (equation of state): Temperature⇔ entropy

The forces

The fluxes are driven by $$\frac{df(\vec{k},\vec{r})}{dt} = \hbar^{-1}\vec{\mathcal{F}}\cdot\frac{\partial f^0}{\partial \vec{k}} + \vec{v}\cdot\frac{\partial f^0}{\partial \vec{r}}$$

The direct forces, e.g. electric field $\vec{\mathcal{F}} = e\vec{E}$

$$\left.\frac{\partial f(\vec{k},\vec{r})}{\partial t}\right|_{FORCE} = \hbar^{-1}\vec{\mathcal{F}}\cdot\frac{\partial f^0}{\partial \vec{k}} = \hbar^{-1}\vec{\mathcal{F}}\cdot\frac{\partial f^0}{\partial \mathcal{E}}\frac{\partial \mathcal{E}}{\partial \vec{k}} = \vec{v}\bullet\vec{\mathcal{F}}\frac{\partial f^0}{\partial \mathcal{E}}$$

The temperature gradient working on the statistical distribution function

$$\left.\frac{\partial f(\vec{k},\vec{r})}{\partial t}\right|_{TEMPEATURE} = \vec{v}\cdot\frac{\partial f^0}{\partial \vec{r}} = \vec{v}\bullet\nabla T\frac{\partial f^0}{\partial T}$$

So temperature gradients work :

- Thermodynamically like all other forms of potential gradients.
- Microscopically they work via the statistical distribution function (valid for all distribution functions).

Distribution functions

Electrons follow Fermi-Dirac distribution function $f^0 = \dfrac{1}{e^{\frac{\mathcal{E}-\mu_\phi}{k_B T}}+1}$

Phonons and magnons follow Bose-Einstein distribution function $f^0 = \dfrac{1}{e^{\frac{\mathcal{E}-\mu_\phi}{k_B T}}-1}$

For both cases, we have: $\dfrac{\partial f^0}{\partial T} = -\dfrac{\mathcal{E}-\mu_\phi}{T}\dfrac{\partial f^0}{\partial \mathcal{E}}$

$$\begin{bmatrix} \vec{j}_N \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{NN} & \overleftrightarrow{L}_{NT} \\ \overleftrightarrow{L}_{TN} & \overleftrightarrow{L}_{TT} \end{bmatrix} \begin{bmatrix} \vec{\mathcal{F}} \\ \nabla T \end{bmatrix}$$

$$\overleftrightarrow{L}_{NN} = \iiint_{\vec{k}} \tau \vec{v}\bullet\vec{v}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\vec{k} \qquad \overleftrightarrow{L}_{TN} = \iiint_{\vec{k}} \tau(\mathcal{E}-\mu_\phi)\vec{v}\bullet\vec{v}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\vec{k}$$

$$\overleftrightarrow{L}_{NT} = -\frac{1}{T}\iiint_{\vec{k}} \tau \vec{v}\bullet\vec{v}\left(\mathcal{E}-\mu_\phi\right)\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\vec{k} \qquad \overleftrightarrow{L}_{TT} = -\frac{1}{T}\iiint_{\vec{k}} \tau(\mathcal{E}-\mu_\phi)^2\vec{v}\bullet\vec{v}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\vec{k}$$

Note that this obeys the reciprocity relation

Density of states to solve the k-space volume integrals

1. Know the dispersion relations $\mathcal{E}(\vec{k})$
2. Derive the group velocities $\vec{v} = \hbar^{-1}\nabla_{\vec{k}}\mathcal{E}(\vec{k})$

$$\begin{bmatrix} \vec{j}_N \\ \vec{j}_Q \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}_{NN} & \overleftrightarrow{L}_{NT} \\ \overleftrightarrow{L}_{TN} & \overleftrightarrow{L}_{TT} \end{bmatrix} \begin{bmatrix} \vec{\mathcal{F}} \\ \nabla T \end{bmatrix}$$

3. Substitute this into the transport integrals

4. Express the proper force that is applied to the particle, and the proper flux to be measured

5. Transform the integrals over k-space into integrals over energy. To do that, use the concept of density of states DOS $\mathcal{D}$:

$$\mathcal{D}(\mathcal{E}) = \iint_{S(\mathcal{E})} g \frac{dS}{(2\pi)^{DIM}} \frac{1}{\nabla_{\vec{k}}\mathcal{E}(\vec{k})}$$

S = surface of equal energy $\mathcal{E}$

g = degeneracy of the state

$$\overleftrightarrow{L}_{NN} = \int_{\mathcal{E}} \tau \vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E})\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\mathcal{E} \qquad \overleftrightarrow{L}_{TN} = \int_{\mathcal{E}} \tau(\mathcal{E}-\mu_\phi)\vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E})\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\mathcal{E}$$

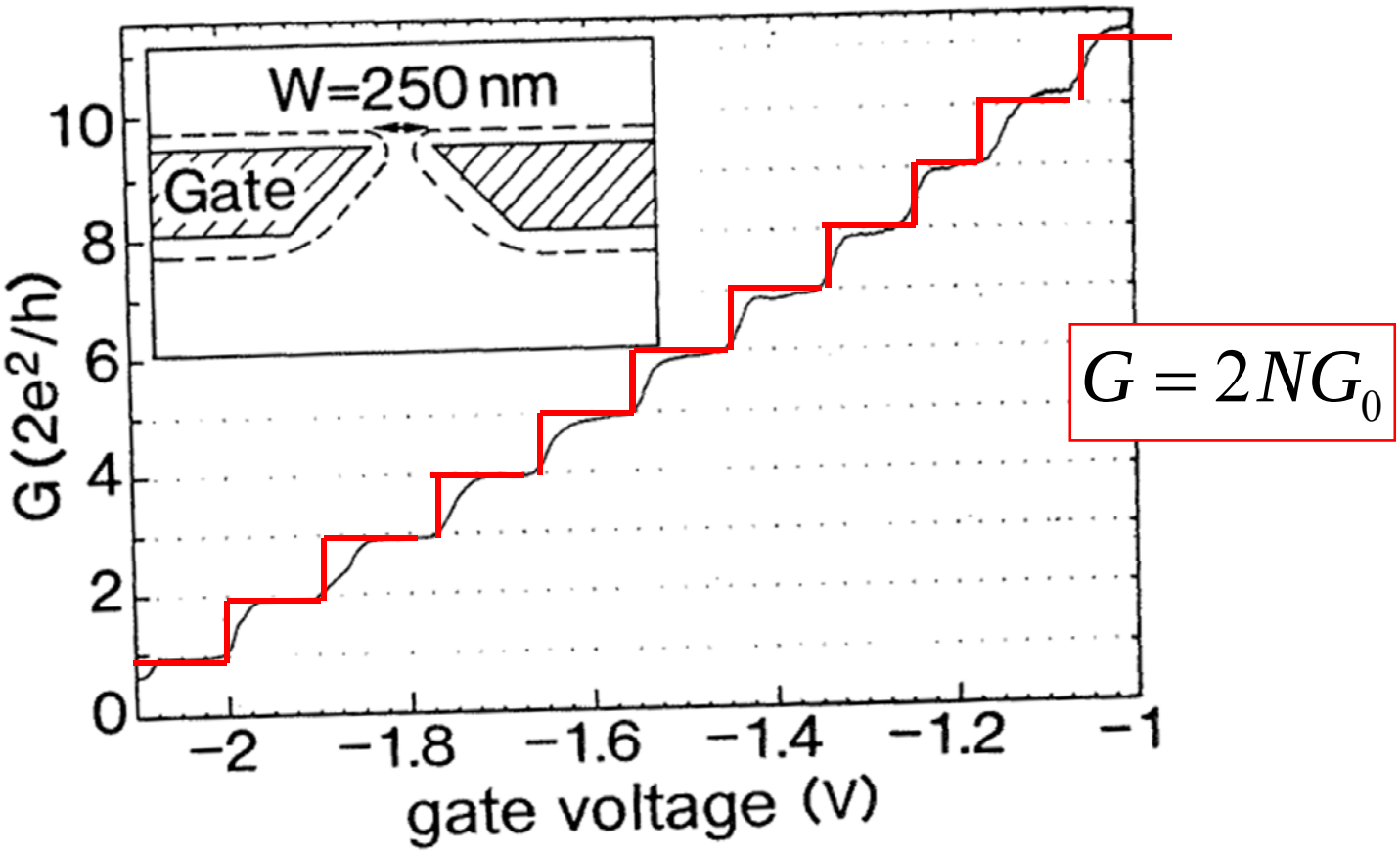
$$\overleftrightarrow{L}_{NT} = -\frac{1}{T}\int_{\mathcal{E}} \tau \vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E})\left(\mathcal{E}-\mu_\phi\right)\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\mathcal{E} \qquad \overleftrightarrow{L}_{TT} = -\frac{1}{T}\int_{\mathcal{E}} \tau(\mathcal{E}-\mu_\phi)^2\vec{v}\bullet\vec{v}\mathcal{D}(\mathcal{E})\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right)d\mathcal{E}$$

This will be done for electrons, phonons and magnons on a case by case basis

Conductance quantization: the other extreme

Gate voltage changes the width of the constriction => the number of channels N

$$G_{N=1} = \lim_{L\to 0}(\sigma_{1D}) = \lim_{L<<\ell}(G_0 4\ell) = 2G_0$$



$$G = 2NG_0$$

FIG. 44. Point contact conductance as a function of gate voltage at 0.6 K, demonstrating the conductance quantization in units of $2e^2/h$. The data are obtained from the two-terminal resistance after subtraction of a background resistance. The constriction width increases with increasing voltage on the gate (see inset). Taken from B. J. van Wees *et al.*, *Phys. Rev. Lett.* **60**, 848

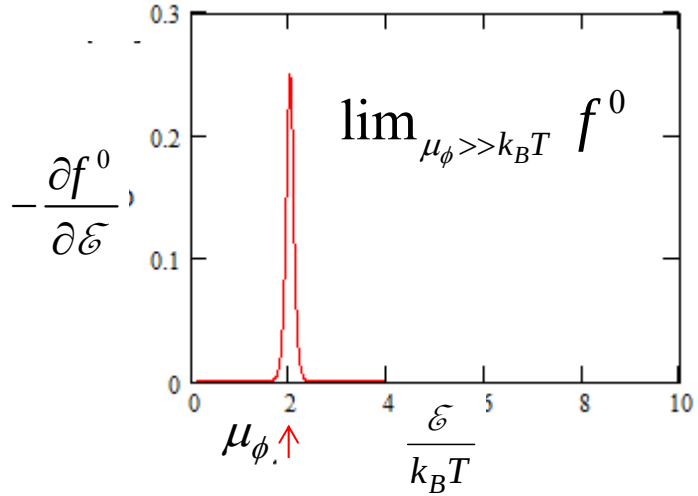
Metals and degenerately-doped semiconductors

Bethe-Sommerfeld expansion, 2nd order

$$\sigma = \int_{\mathscr{E}} \left(-\frac{\partial f^0}{\partial \mathscr{E}} \right) \sigma_{\mathscr{E}}(\mathscr{E}) d\mathscr{E} \qquad \alpha = \frac{L_{ET}}{\sigma}$$

$$L_{ET} = \left(\frac{k_B}{e} \right) \int_{\mathscr{E}} \left(\frac{\partial f^0}{\partial \mathscr{E}} \right) \left(\frac{\mathscr{E} - \mu_\phi}{k_B T} \right) \sigma_{\mathscr{E}}(\mathscr{E}) d\mathscr{E}$$

$$\kappa / T = \left(\frac{k_B}{e} \right)^2 \int_{\mathscr{E}} \left(\frac{\partial f^0}{\partial \mathscr{E}} \right) \left(\frac{\mathscr{E} - \mu_\phi}{k_B T} \right)^2 \sigma_{\mathscr{E}}(\mathscr{E}) d\mathscr{E}$$



$$x \equiv \left(\mathscr{E} - \mu_\phi \right) / (k_B T); \varsigma \equiv \mu_\phi / (k_B T)$$

See appendix

$$L = \int_{x=-\varsigma}^{\infty} \left(-\frac{\partial f^0}{\partial x} \right) F(x) dx \approx F(0) + \frac{\pi^2}{6} \frac{d^2 F(x)}{dx^2}\bigg|_{x=0} + \ldots$$

Notice that all the integrands have the form of: $F_i = x^i \sigma_{\mathscr{E}}(k_B T x)$

$x=0$

$$L_{i=0} = \sigma_{\mathscr{E}}(0); L_{i=1} = \pi^2/6 \left(2\sigma'_{\mathscr{E}}(0) + x\sigma''_{\mathscr{E}}(0) \right)$$

$$L_{i=2} = \pi^2/6 \left(2\sigma_{\mathscr{E}}(0) + 4x\sigma'_{\mathscr{E}}(0) + x^2\sigma''_{\mathscr{E}}(0) \right)$$

6.4 Physical meaning

$$\alpha = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)(k_B T)\left.\frac{d\ln(\sigma_{\mathscr{E}}(\mathscr{E}))}{d\mathscr{E}}\right|_{\mu_\phi}$$

$$\kappa = L\sigma T \;;\; L_0 = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 = 2.45\times10^{-8}[\mathrm{V^2K^2}]$$

$$\sigma_{\mathscr{E}}(\mathscr{E}) = 2G_0\mathscr{T}(\mathscr{E})$$

The Mott formalism for thermopower and the Wiedemann-Franz law have the same advantages as the Landauer formalism:

1. No longer beholden to diffusive transport or to the use of a relaxation time
2. No longer beholden to the definition of a reciprocal lattice and dispersion relation; will work with just a density of states as function of energy
3. Valid for constrictions, low-dimensional structures,…
4. Valid for localization, hopping, disordered solids

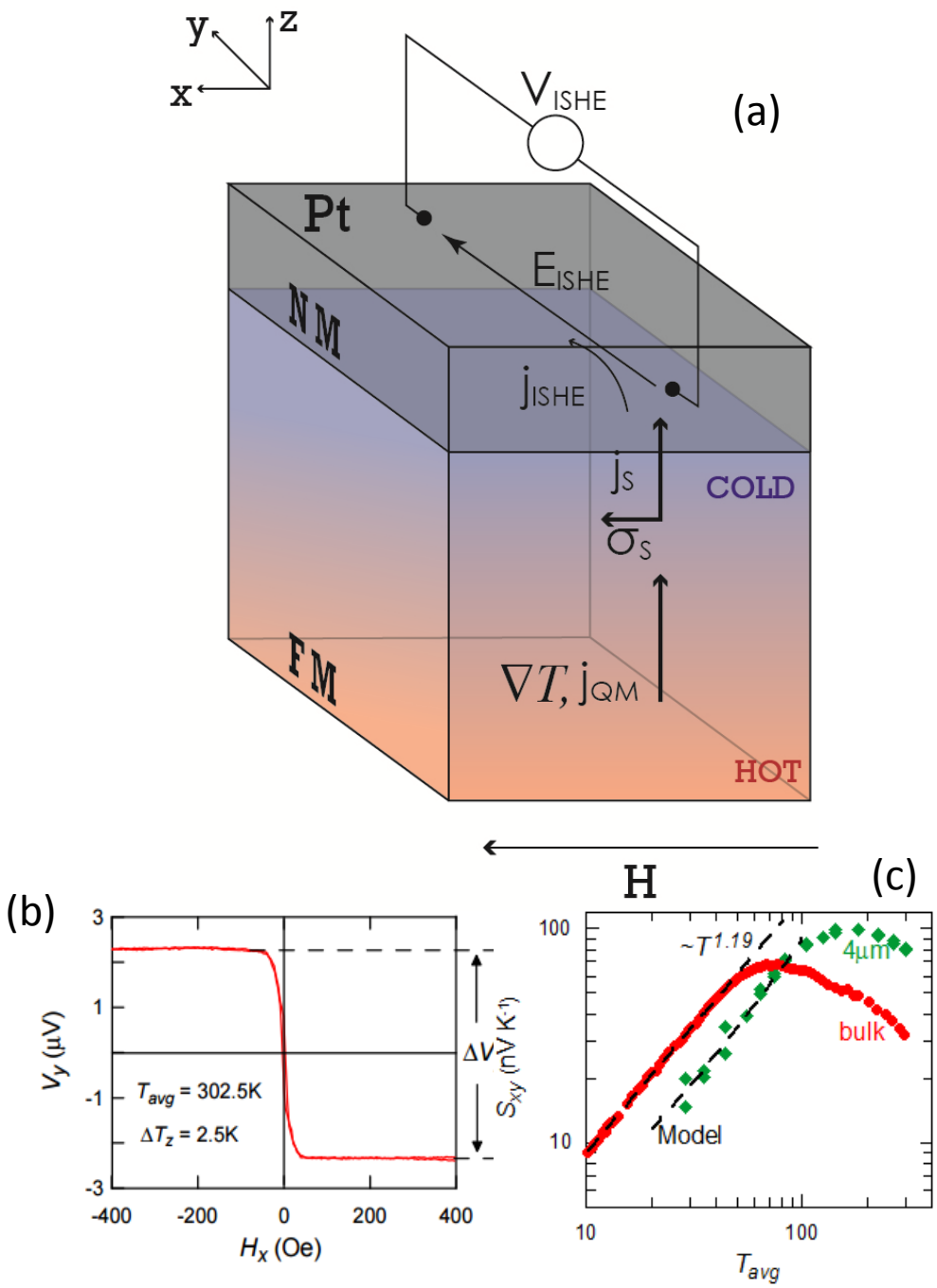

y
z
x
V ISHE
(a)
Pt
E ISHE
NM
j ISHE
j S
COLD
σ S
FM
∇T, j QM
HOT
H
(b)
3
1
-1
-3
V y (μV)
T avg = 302.5K
ΔT z = 2.5K
ΔV
S xy (nV K-1)
-400
-200
0
200
400
H x (Oe)
(c)
100
10
~T 1.19
4μm
bulk
Model
10
100
T avg

Fig. 1

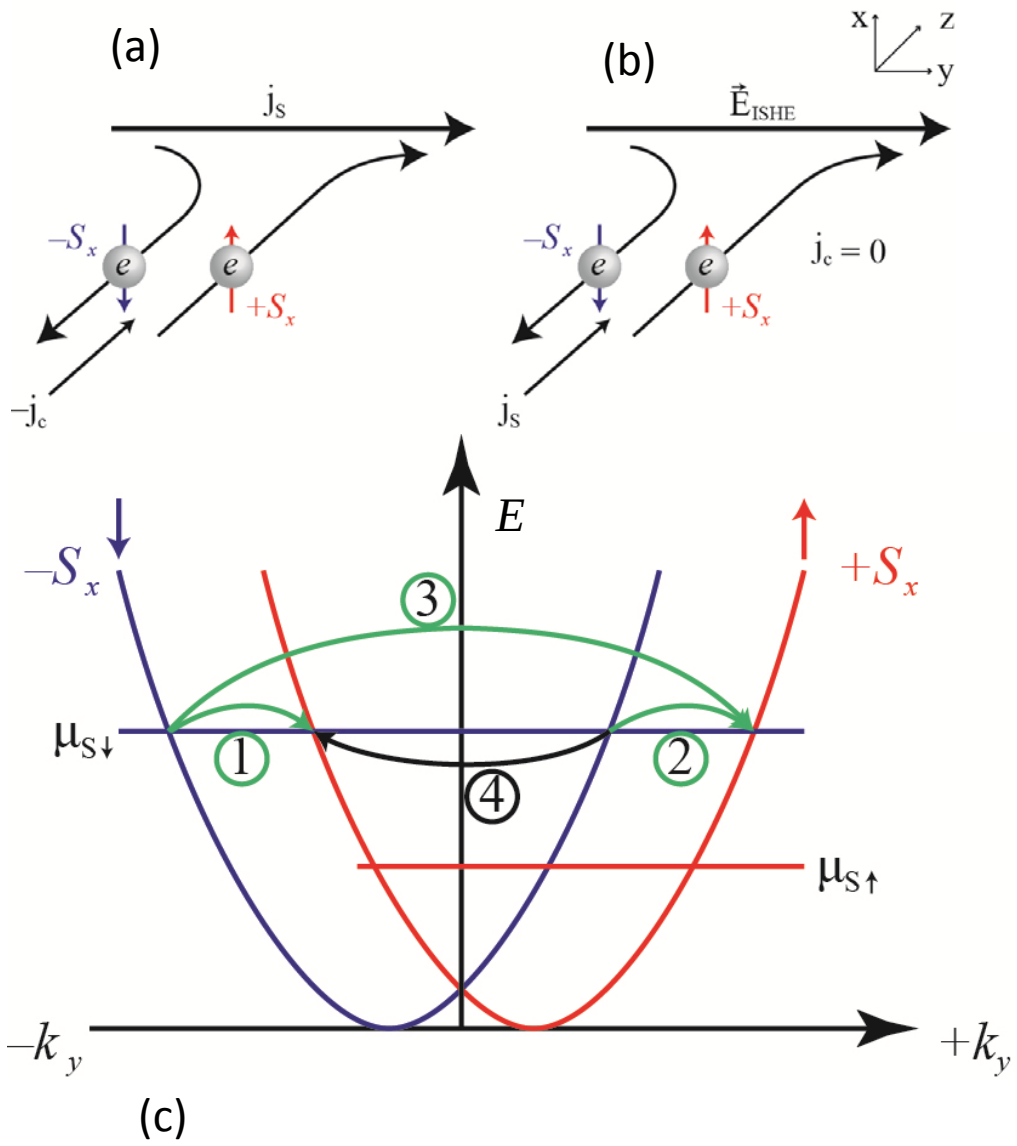

(a)
j_S
$-S_x$
$+S_x$
$-j_c$
(b)
x
z
y
$\vec{E}_{ISHE}$
$-S_x$
$+S_x$
$j_c = 0$
j_S
E
$-S_x$
$+S_x$
3
$\mu_{S\downarrow}$
1
2
4
$\mu_{S\uparrow}$
$-k_y$
$+k_y$
(c)

Fig. 2

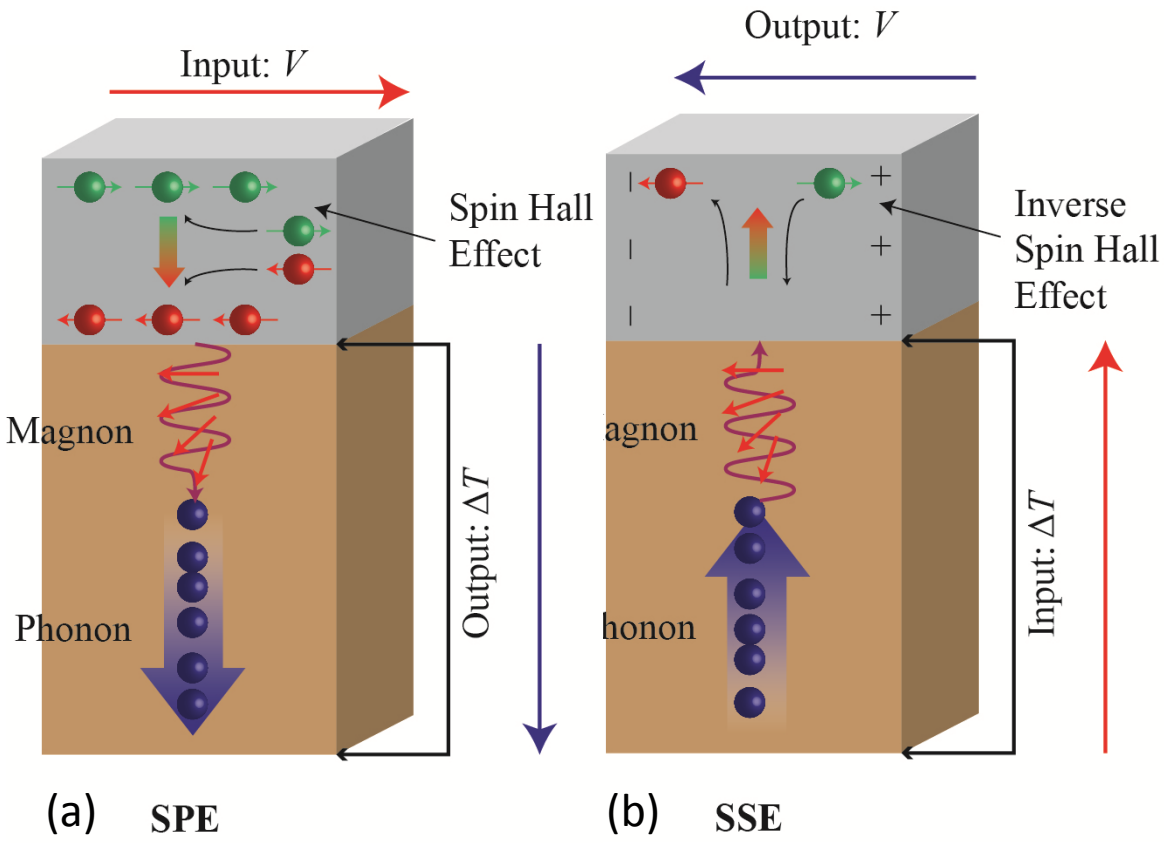

Input: V
Spin Hall Effect
Magnon
Phonon
Output: ΔT
(a) SPE
Output: V
Inverse Spin Hall Effect
agnon
honon
Input: ΔT
(b) SSE

Fig. 3

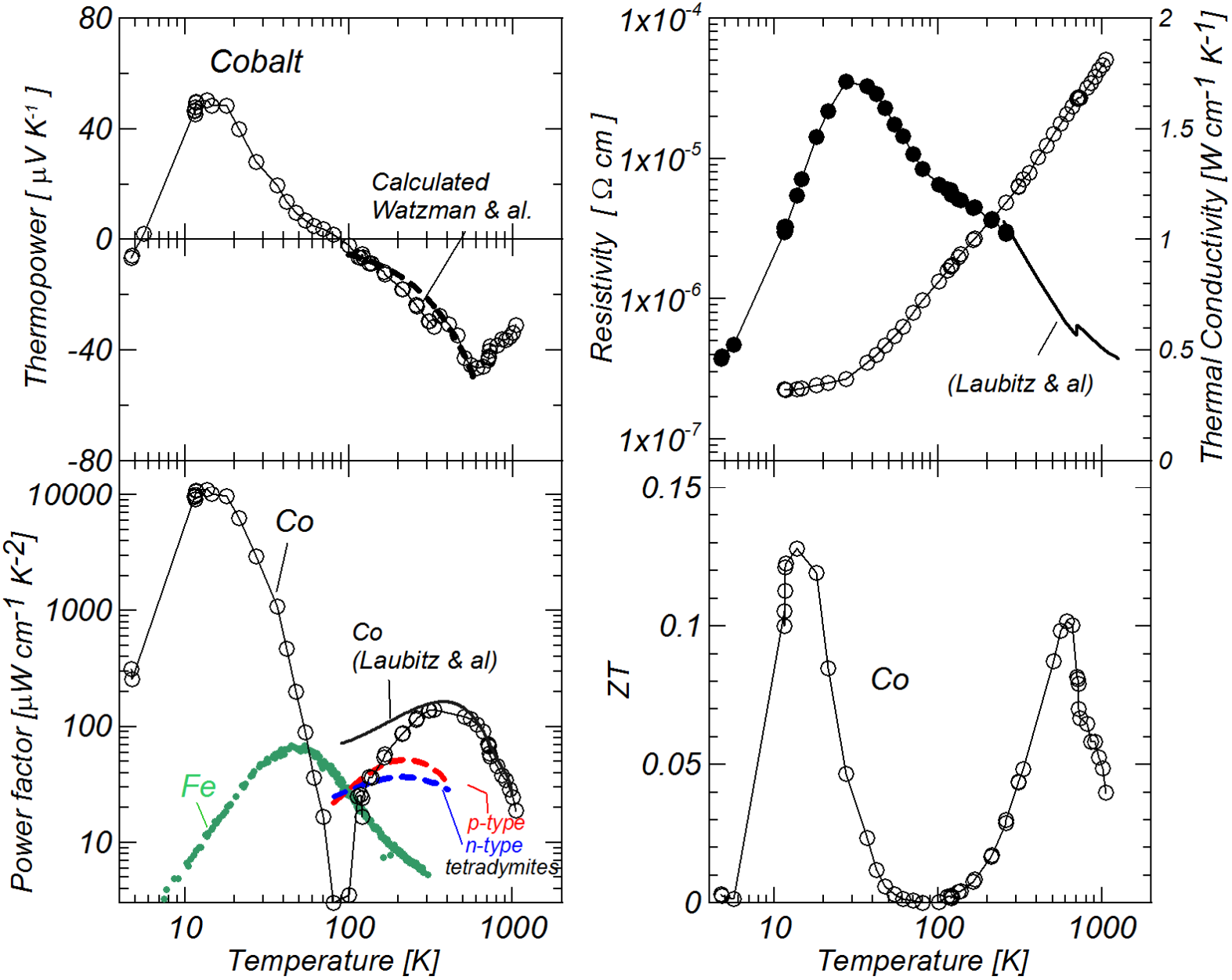
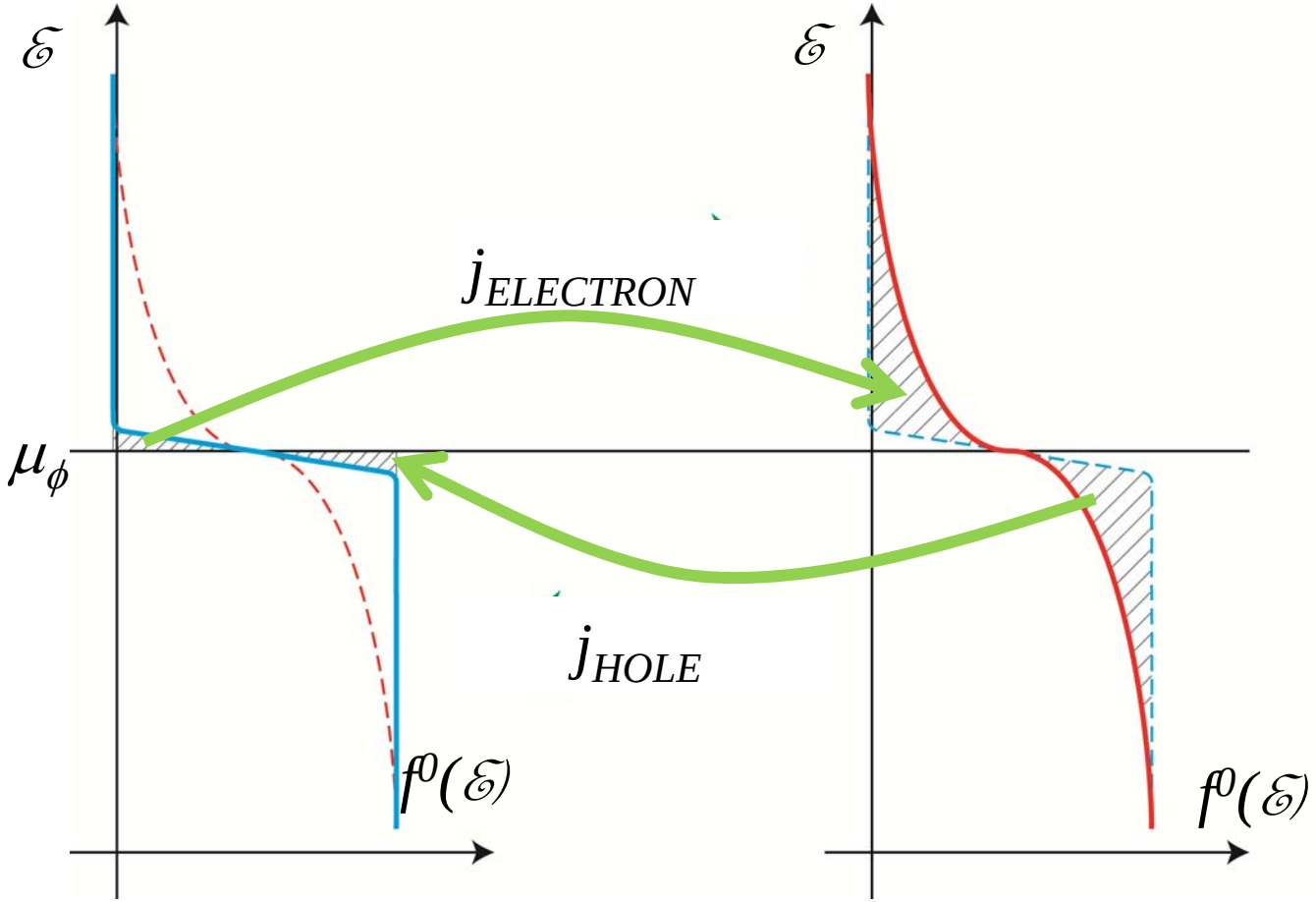

Cobalt
Calculated
Watzman & al.
Thermopower [μV K-1]
80
40
0
-40
-80
Resistivity [Ω cm]
1x10-4
1x10-5
1x10-6
1x10-7
(Laubitz & al)
Thermal Conductivity [W cm-1 K-1]
2
1.5
1
0.5
0
Power factor [μW cm-1 K-2]
10000
1000
100
10
Co
Co
(Laubitz & al)
Fe
p-type
n-type
tetradymites
ZT
0.15
0.1
0.05
0
Co
10
100
1000
Temperature [K]
10
100
1000
Temperature [K]

Fig. 4

Thermopower: Fermions, DOS uniform

Cold side, distribution function

Hot side side, distribution function

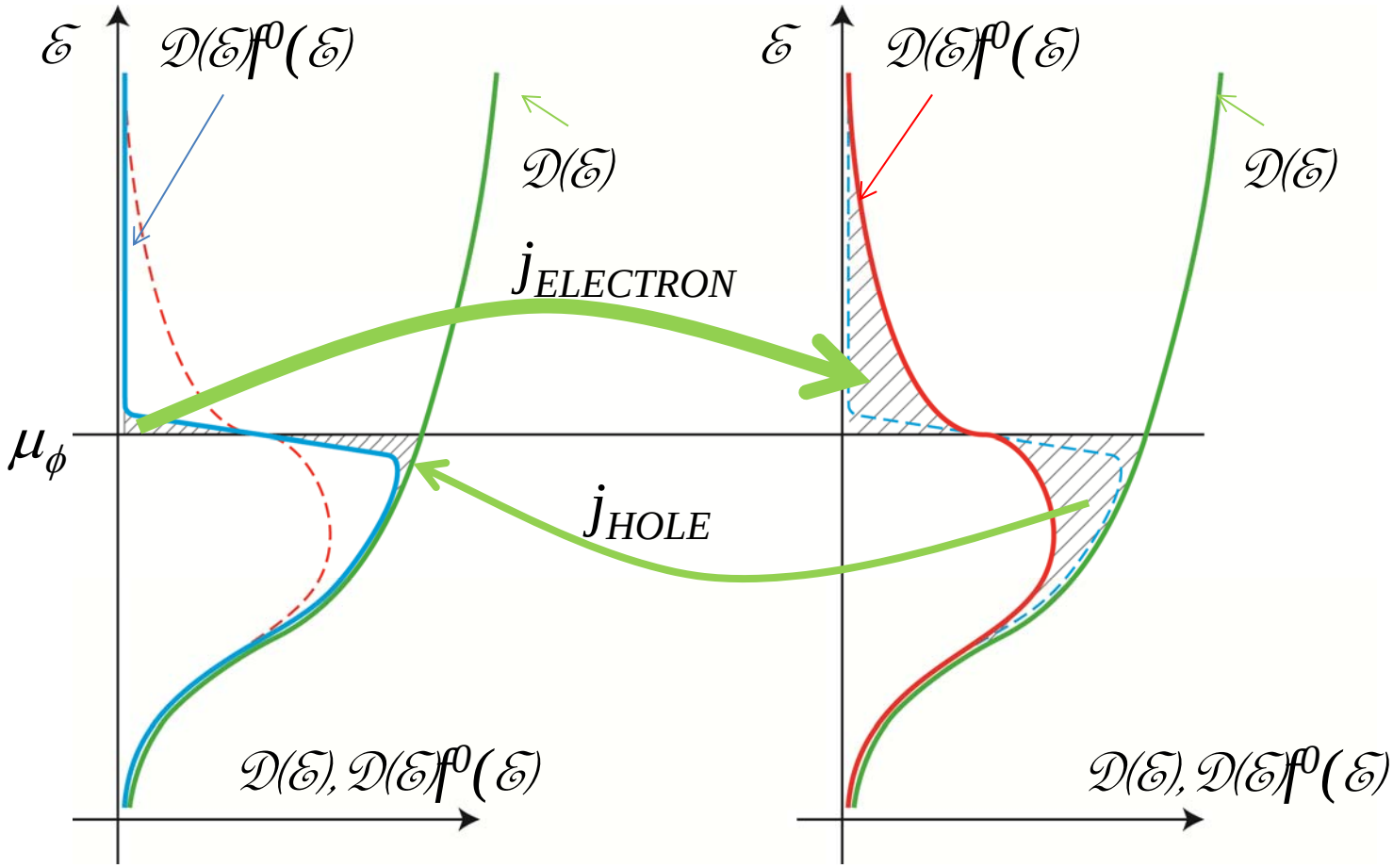


$$j_{ELECTRON} = j_{HOLE} \qquad \alpha = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)(k_B T)\left.\frac{d\ln(\sigma_{\mathcal{E}}(\mathcal{E}))}{d\mathcal{E}}\right|_{\mu_\phi} = 0$$

Conduction band

Cold side, electron concentration

Hot side side, electron concentration

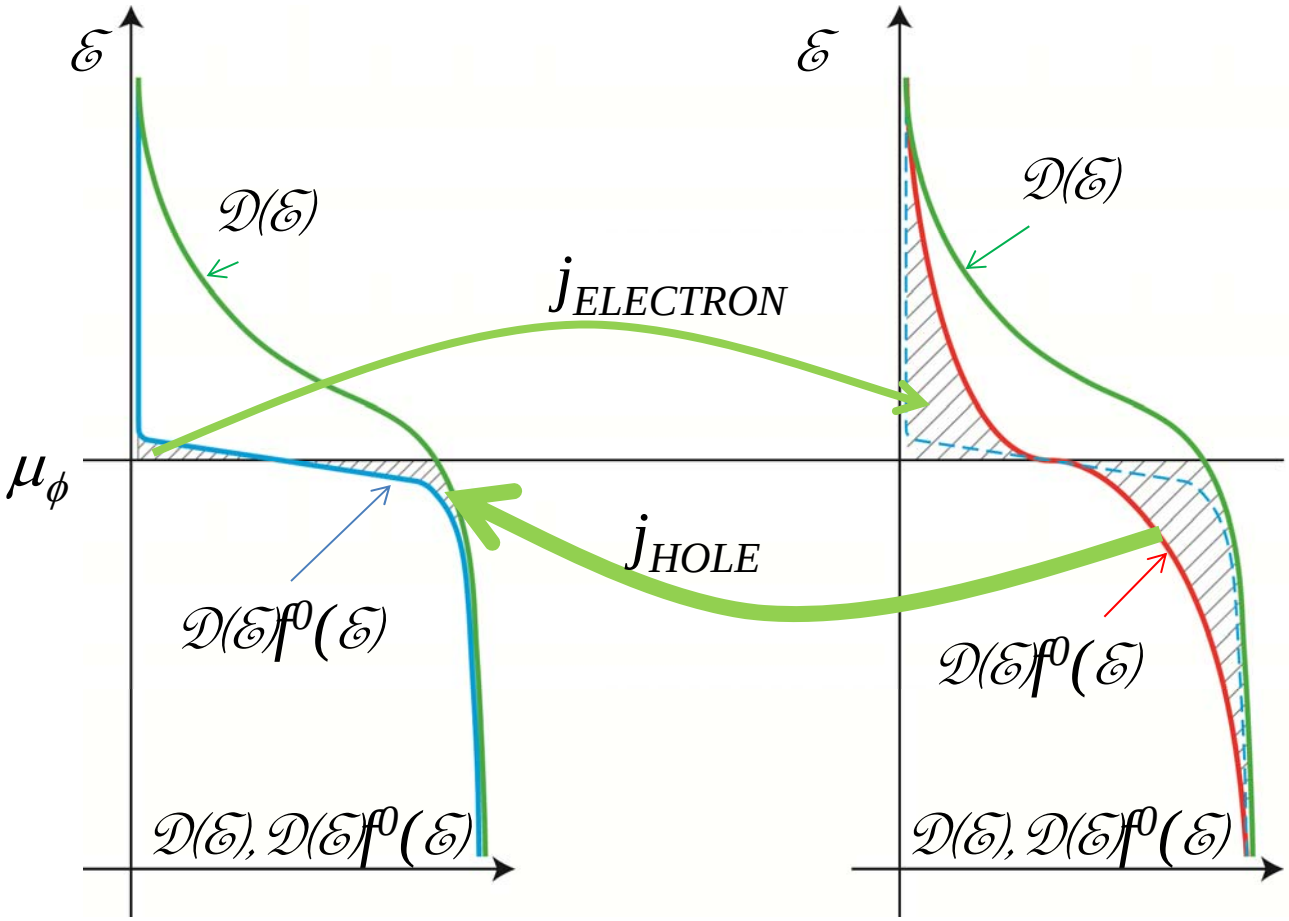


$$j_{ELECTRON} > j_{HOLE} \qquad \alpha = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)(k_B T)\left.\frac{d\ln(\sigma_{\mathcal{E}}(\mathcal{E}))}{d\mathcal{E}}\right|_{\mu_\phi} < 0$$

Valence band

Cold side, electron concentration

Hot side side, electron concentration



$$j_{ELECTRON} < j_{HOLE} \qquad \alpha = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)(k_B T)\left.\frac{d\ln(\sigma_{\mathcal{E}}(\mathcal{E}))}{d\mathcal{E}}\right|_{\mu_\phi} > 0$$

Limitations of band transport

1. Atomic potentials can be not weak at all, but very strong:
    1. Bands become flat (little energy change per momentum change)
    2. Impurities can have much deeper potentials that the atoms of the host solid and electrons can get trapped over them.

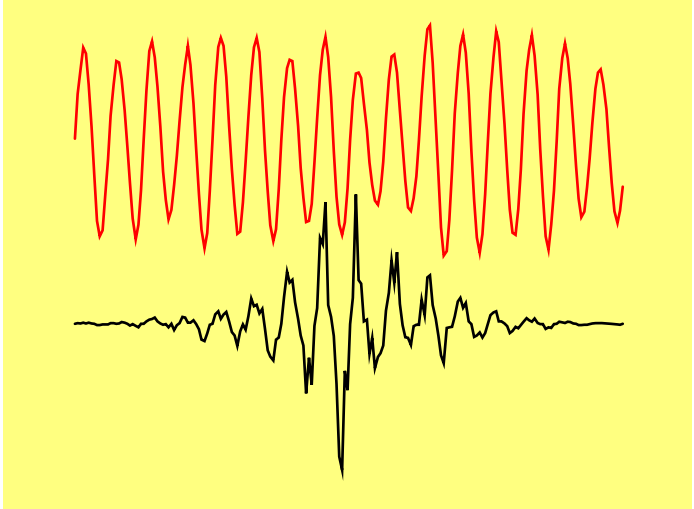
2. Potentials can be non-periodic in disordered solids and in liquids => no Bragg condition, no band structure at all, only the notion of density of available energy states can be used

3. Electron wavefunctions can be affected by things other than the periodic electrostatic potentials of the atoms:
    1. External magnetic fields => Landau levels
    2. Spin-orbit interactions => Dirac bands
    3. Finite size effects => Quantum confinement
    4. Interference effects => Weak Localization
    5. Strong electron interactions
        1. electron – electron => Correlation effects
        2. electron – impurity => Resonant levels
        3. electron – magnetic impurity => Kondo effect
        4. electron – phonon => Polarons

The Anderson (Ioffe-Regel) limit

Difference between insulator and metal in any arbitrary solid ?

Wave origin of the electrons can be propagating wave or standing wave



Delocalized states conduct

Localized states don't conduct

The states' wavefunction at the Fermi energy must extend beyond one mean free path

$$\ell < \frac{1}{k_F}$$

If $k_F \ell > 1$ => **band conduction**

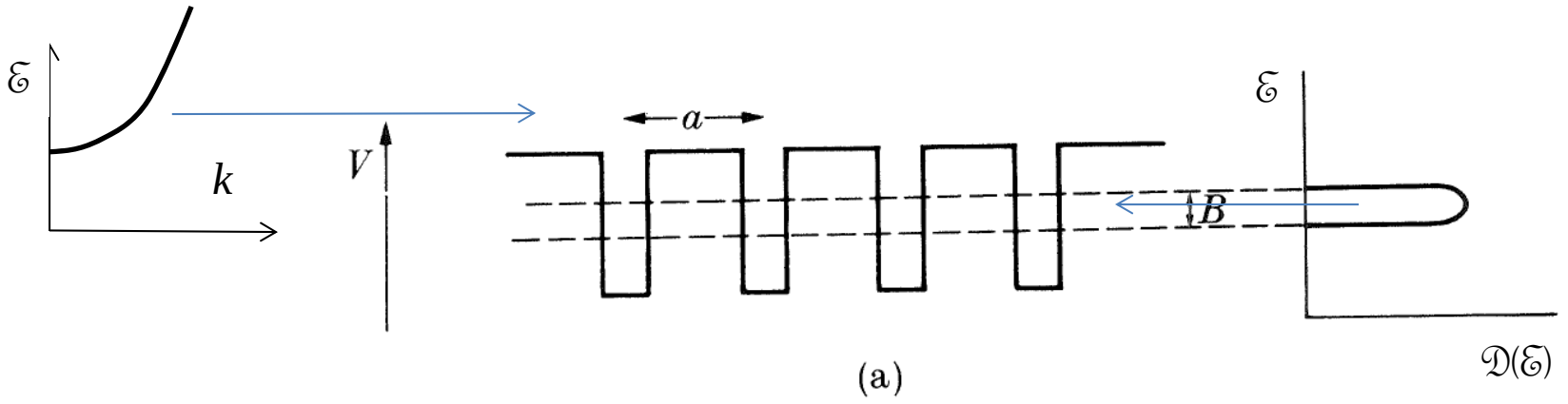
If $k_F \ell < 1$ => **localization**

Rigorous demonstration in N. F. Mott & E. A. Davis "electronic Processes in Non-crystalline Materials"

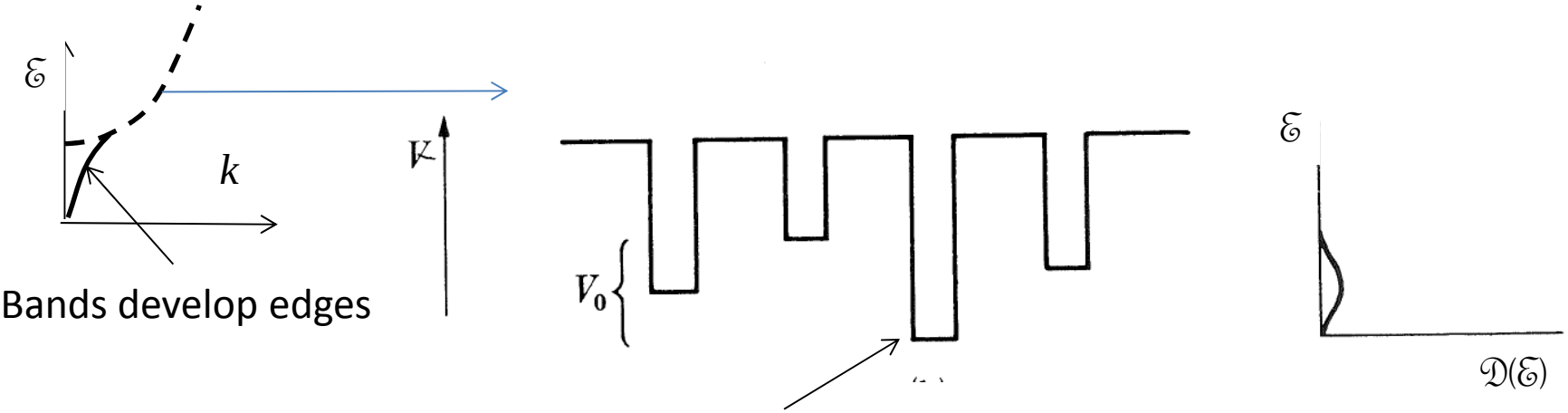
P. W. Anderson, Phys. Rev. ***109*** *1492 (1958); A.F. Ioffe and A.R. Regel, Prog. Semicond.* ***4****, 237 (1960).*

Minimum metallic conductivity (consequence of Anderson criterion)

A. This solid is fully periodic: Bands are fully developed



B. with disorder: one can still define *k*-vectors, but wavefunctions are not fully periodic



Bands develop edges

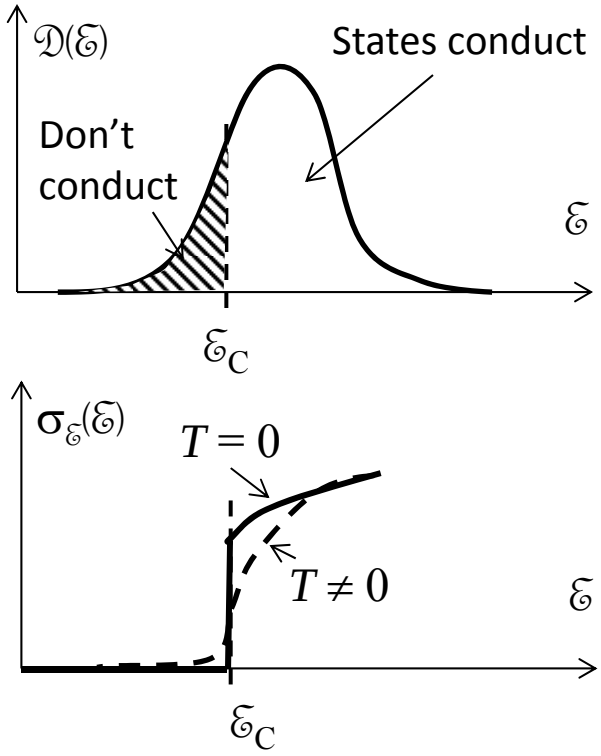
One deep potential can be so deep (V_0) that the Anderson criterion is locally not satisfied:
the level will pin the electron => there exists a critical pinning energy $\mathcal{E}_C$

Minimum metallic conductivity

There is a critical value of $\mathcal{E}_C$ so that, at $T = 0$

$$\sigma = 0 \quad \text{if } \mathcal{E} < \mathcal{E}_C$$

$$\sigma \neq 0 \quad \text{if } \mathcal{E} > \mathcal{E}_C$$



Also called the mobility edge

At finite temperature $T \neq 0$

if $\mu_\phi < \mathcal{E}_C$ => **hopping conduction**

if $\mu_\phi > \mathcal{E}_C$ => **band conduction**

Calculate the critical value of $\mathcal{E}_C$ and the corresponding critical conductivity

$$\sigma_{\min} = \frac{\pi^2}{z}\frac{e^2}{h}\frac{1}{a}$$

At finite temperature $T \neq 0$

if $\sigma < \sigma_{\min}$ => **hopping conduction**

if $\sigma > \sigma_{\min}$ => **band conduction**

N. F. Mott and E. A. Davis, Electronic Processes in Non-crystalline Materials, Oxford (1979), sec 2.6

Natural units for electrical conductance

The Fermi liquid, spherical Fermi surface

Energy dispersion: $E_F = \frac{\hbar^2 k_F^2}{2m^*}; v_F = \frac{1}{\hbar}\frac{\partial E_F}{\partial k_F} = \frac{\hbar k_F}{m} = \frac{2\pi h k_F}{m}$

=> Drude conductivity: $\sigma = \frac{n e^2 \ell}{m v_F} = 2\pi \left(\frac{e^2}{h}\right)\frac{n\ell}{k_F}$

	3-dimensions	2-dimensions	1-dimension
Number of *k*-points per volume	$V/8\pi^3$	$V/4\pi^2$	$V/2\pi$
Volume of Fermi surface	$4\pi k_F^3/3$	πk_F^2	$2k_F$
Concentration of electrons (x2)	$n_{3D} = k_F^3/3\pi^2$	$n_{2D} = k_F^2/2\pi$	$n_{1D} = 2k_F/\pi$
Drude conductivity:	$\sigma_{3D} = \left(\frac{e^2}{h}\right)\frac{2}{3\pi}k_F^2\ell$	$\sigma_{2D} = \left(\frac{e^2}{h}\right)k_F\ell$	$\sigma_{1D} = \left(\frac{e^2}{h}\right)4\ell$
units	$\Omega^{-1}\mathrm{m}^{-1}$	Ω^{-1}	$\Omega^{-1}\mathrm{m}$

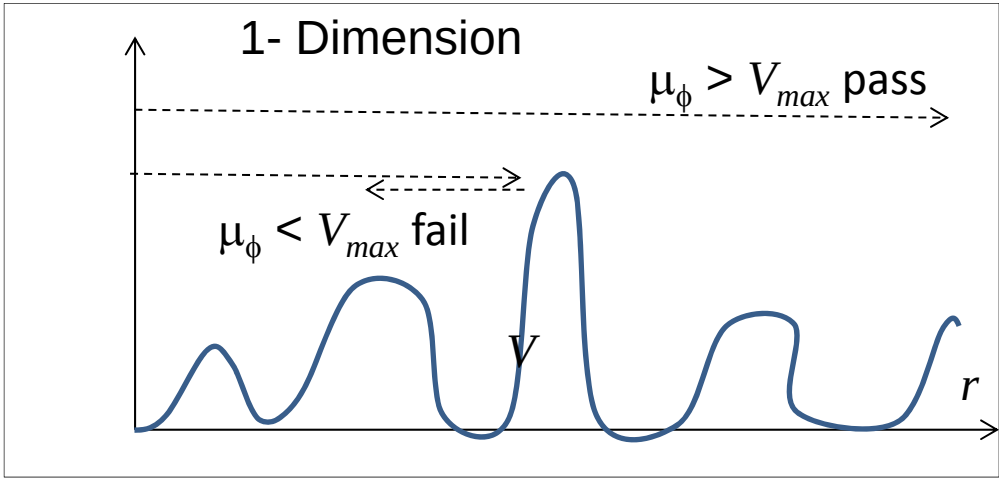
All are expressed in terms of $G_0 = \frac{e^2}{h} = 3.874\times10^{-5}\,\Omega^{-1}\mathrm{m}^{-1}$

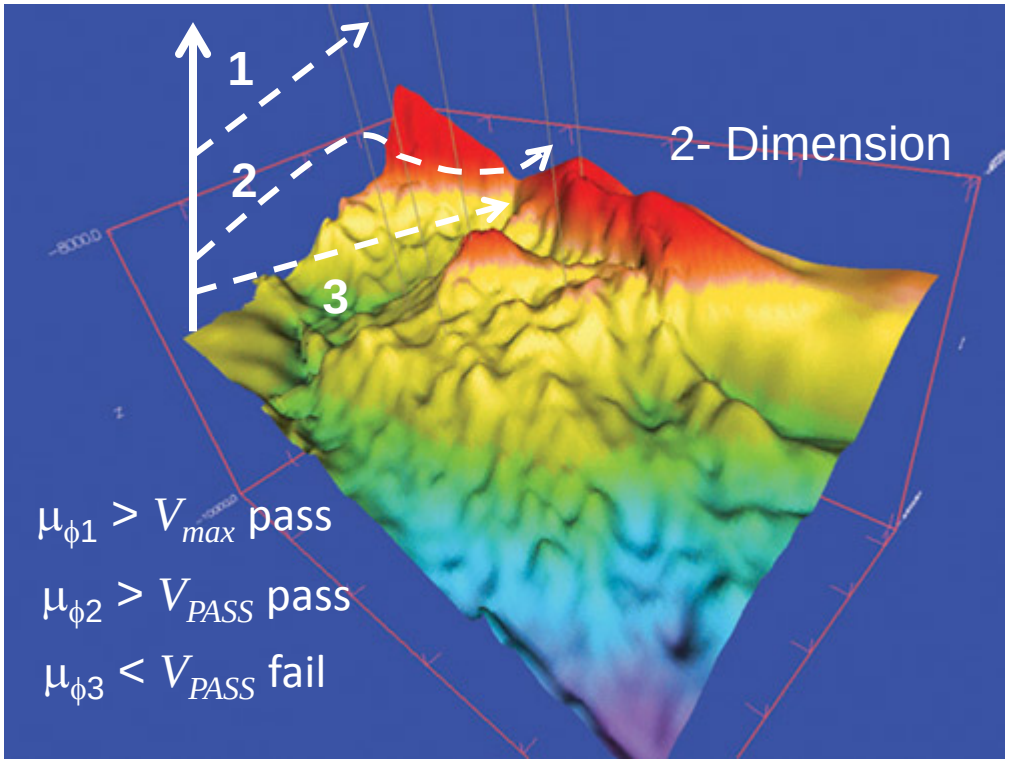
Fundamental unit for electrical conductance

Dimensionality dependence

The criteria are always less stringent in 3-D, most stringent in 1-D

In 1-dimension: particle at any energy below the highest peak fails => conduction is interrupted





In 2-dimension: particle at any energy below the highest peak can find a way around. Only those below the potential of a saddle point fail

In 3-dimension: better yet

Specific heat by magnons (heavy RE elements)

O. V. Lounasmaa & L. J. Sundström, Phys. Rev. ***150*** *399 (1966)*

TABLE VII. Percentage contributions of C_L, C_E, C_M, and C_N in the total C_p.

Sample	T(°K)	C_L(%)	C_E(%)	C_M(%)	C_N(%)	C_p(mJ/mole °K)[b]
Gd[a]	5	20	31	39	···	180
	10	59	18	23	···	625
	20	77	5	18	···	4470
Tb[a]	5	33	51	7	9	110
	10	64	21	15	<1	590
	20	73	5	22	···	4690
Dy[a]	5	23	35	41	<1	160
	10	60	18	22	···	630
	20	61	4	35	···	5640
Ho	5	7	11	49	33	530
	10	14	4	80	2	2725
	20	36	2	62	···	9550
Tm	5	9	14	77	···	400
	10	19	6	75	···	1990
	20	32	2	66	···	10600