Lecture 6
Thermo-electronic Applications

- Currents and forces:
  - Electrical and thermal currents
  - Mechanical and statistical forces
- Anomalous transport effects:
  - Hall, Nernst, and thermal Hall
- Transport relations:
  - Einstein, Onsager, Mott, Wiedemann-Franz, Luttinger
- Generalizations:
  - Spin density response, gravitational forces

Dipole correction to density distribution

- Density of a physical quantity

$$\mathcal{O}(\boldsymbol{r}) = \int \frac{d\boldsymbol{r}_c d\boldsymbol{q}_c}{(2\pi)^3} g(\boldsymbol{r}_c, \boldsymbol{q}_c) \langle W | \hat{\mathcal{O}} \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}) | W \rangle$$

- Expanding to first order in $\hat{\boldsymbol{r}} - \boldsymbol{r}_c$:

$$\mathcal{O}(\boldsymbol{r}) = \int \frac{d\boldsymbol{q}}{(2\pi)^3} g(\boldsymbol{r}, \boldsymbol{q}) \langle W | \hat{\mathcal{O}} | W \rangle |_{\boldsymbol{r}_c = \boldsymbol{r}}$$

$$- \nabla \cdot \int \frac{d\boldsymbol{q}}{(2\pi)^3} g(\boldsymbol{r}, \boldsymbol{q}) \langle W | \hat{\mathcal{O}} (\hat{\boldsymbol{r}} - \boldsymbol{r}_c) | W \rangle |_{\boldsymbol{r}_c = \boldsymbol{r}}$$

- Wave packet dipole:

$$\boldsymbol{P}_{\hat{\mathcal{O}}} = \langle W | \hat{\mathcal{O}} (\hat{\boldsymbol{r}} - \boldsymbol{r}_c) | W \rangle \qquad \boldsymbol{P}_s = \langle u | s \left(i \frac{\partial}{\partial \boldsymbol{q}} - \mathcal{A}_{\boldsymbol{q}} \right) | u \rangle$$

Electric current density

Local current density

$$\boldsymbol{j}^L = \int \frac{d\boldsymbol{q}}{(2\pi)^3} g(\boldsymbol{r},\boldsymbol{q})\dot{\boldsymbol{r}} + \boldsymbol{\nabla} \times \int \frac{d\boldsymbol{q}}{(2\pi)^3} g(\boldsymbol{r},\boldsymbol{q})\boldsymbol{m}(\boldsymbol{q})$$

Transport current density $\boldsymbol{j} = \boldsymbol{j}^L - \boldsymbol{\nabla} \times M(\boldsymbol{r})$

$$\boldsymbol{j}^{\mathrm{tr}} = -e \int \mathrm{d}\boldsymbol{k}\, g(\boldsymbol{r},\boldsymbol{k})\dot{\boldsymbol{r}} - \boldsymbol{\nabla} \times \ M_f$$

Magnetization at local equilibrium:

$$\begin{aligned} \boldsymbol{M} &= \int \mathrm{d}\boldsymbol{k}\, f(\boldsymbol{k})\boldsymbol{m}(\boldsymbol{k}) + k_B T \int \mathrm{d}\boldsymbol{k}\, \frac{e}{\hbar}\boldsymbol{\Omega} \log(1 + e^{-\beta(\varepsilon-\mu)}) \\ &= \boldsymbol{M}_{\mathrm{moment}} + \ M_f \end{aligned}$$

Free energy from a single state $g(\varepsilon) = -(1/\beta)\log(1 + e^{-\beta(\varepsilon-\mu)})$

Anomalous Hall and Nernst effects

Intrinsic charge current due to statistical forces:

$$\boldsymbol{j}_{\text{in}} = -\nabla \times \boldsymbol{M}_{\text{f}}$$

Response to chemical potential gradient: anomalous Hall

$$-\nabla\mu \times (e/\hbar) \int [d\boldsymbol{k}] f(\boldsymbol{k}) \boldsymbol{\Omega}(\boldsymbol{k}).$$

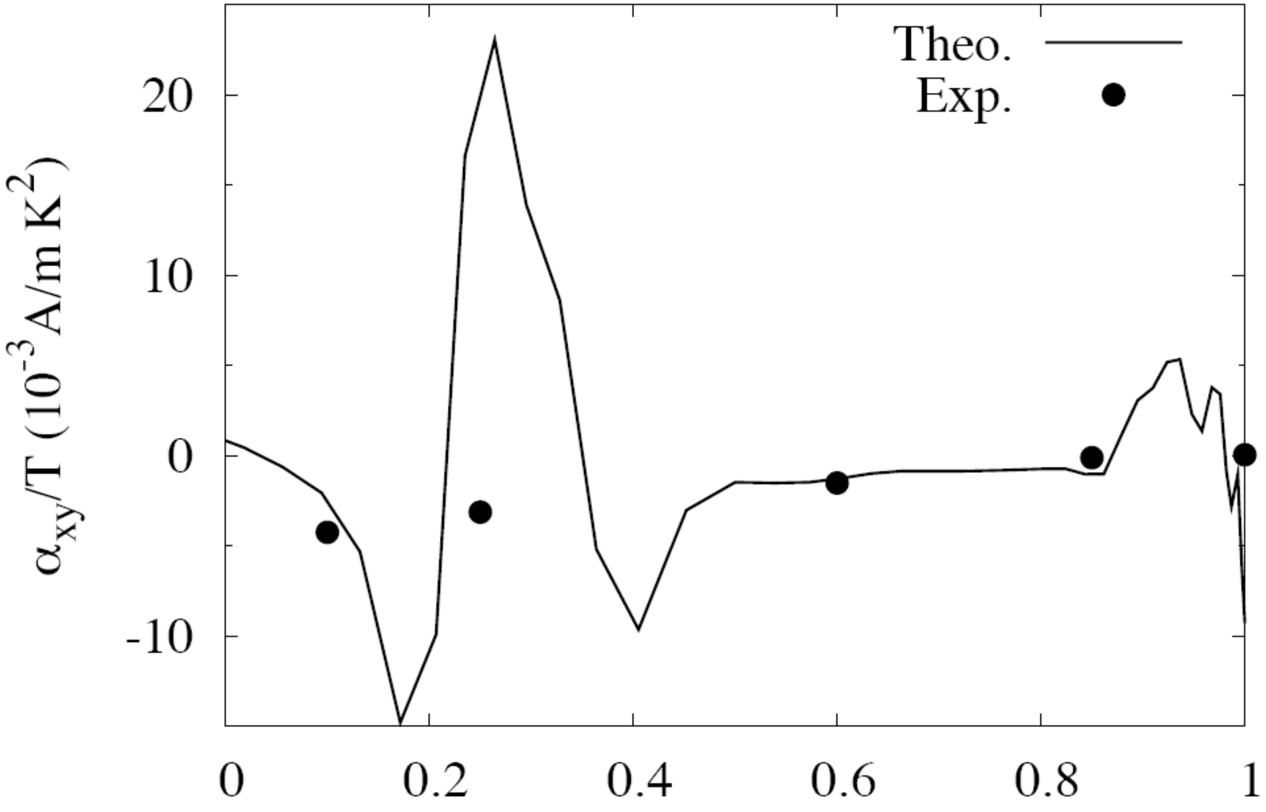
Einstein relation

Response to temperature gradient: anomalous Nernst

$$\boldsymbol{j}_{\text{in}} = -\frac{\nabla T}{T} \times \frac{e}{\hbar} \int [d\boldsymbol{k}] \boldsymbol{\Omega} \Big[(\varepsilon - \mu) f + k_B T \log(1 + e^{-\beta(\varepsilon - \mu)}) \Big].$$

Anomalous Nernst Effect in $CuCr_2Se_{4-x}Br_x$

Lee, *et al*, Science 2004; PRL 2004,   Xiao et al, PRL 2006



Magnetization from boundary current

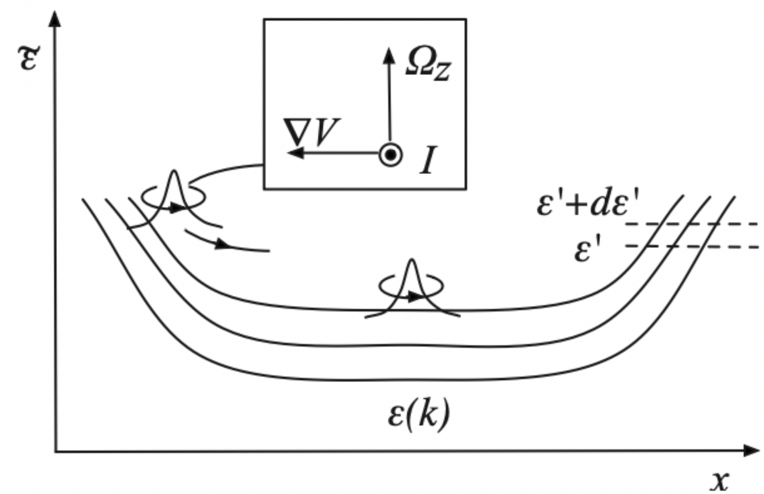
Boundary potential modification: $\tilde{\varepsilon}(\boldsymbol{r},\boldsymbol{q}) = \varepsilon(\boldsymbol{q}) + V(\boldsymbol{r})$

Hall velocity due to boundary force:

$$\frac{1}{\hbar}\boldsymbol{\nabla} V(\boldsymbol{r}) \times \boldsymbol{\Omega}(\boldsymbol{q})$$

Boundary current:

$$I = \frac{e}{\hbar}\int dx \int \frac{d\boldsymbol{q}}{(2\pi)^2}\frac{dV}{dx} f[\varepsilon(\boldsymbol{q}) + V]\Omega_z(\boldsymbol{q})$$



Contribution to magnetization:

$$M_f = \frac{1}{e}\int d\varepsilon f(\varepsilon)\sigma_{xy}(\varepsilon)$$

where

$$\sigma_{xy}(\varepsilon) = \frac{e^2}{\hbar}\int \frac{d\boldsymbol{q}}{(2\pi)^d}\Theta(\varepsilon - \varepsilon(\boldsymbol{q}))\Omega_z(\boldsymbol{q})$$

Reproduces earlier result, if we note that $f(\varepsilon)$ is the derivative of

$$g(\varepsilon) = -(1/\beta)\log\left(1 + e^{-\beta(\varepsilon-\mu)}\right)$$

Relation to Hall conductivity at T=0

Intrinsic charge current due to statistical forces:

$$\boldsymbol{j}_{\text{in}} = -\nabla \times M_{\text{f}}$$

Magnetization from boundary current:

$$M_f = \frac{1}{e}\int d\varepsilon f(\varepsilon)\sigma_{xy}(\varepsilon) \qquad \text{where} \qquad \sigma_{xy}(\varepsilon) = \frac{e^2}{\hbar}\int \frac{d\boldsymbol{q}}{(2\pi)^d}\Theta(\varepsilon - \varepsilon(\boldsymbol{q}))\Omega_z(\boldsymbol{q})$$

Hall current driven by chemical potential gradient:

$$j_x = \sigma_{xy} \nabla_y \mu / e$$

Hall conductivity at finite temperature

$$\sigma_{xy} = \int d\varepsilon \frac{\partial f}{\partial \mu}\sigma_{xy}(\varepsilon)$$

Mott relation

- Nernst conductivity $$j_x = \alpha_{xy}(-\nabla_y T)$$

- Relation to Hall conductivity at T=0

$$\alpha_{xy} = \frac{1}{e}\int d\varepsilon \frac{\partial f}{\partial \mu}\sigma_{xy}(\varepsilon)\frac{\varepsilon - \mu}{T}$$

- Mott relation at low temperatures

$$\alpha_{xy} = \frac{\pi^2}{3}\frac{k_B^2 T}{e}\sigma'_{xy}(\varepsilon_F).$$

Thermal current

Local energy current to first order in electric field

$$\boldsymbol{J}^{E} = \int [d\boldsymbol{k}] g(\boldsymbol{k}) \varepsilon \dot{\boldsymbol{r}} - \boldsymbol{E} \times \int [d\boldsymbol{k}] f(\boldsymbol{k}) \boldsymbol{m}(\boldsymbol{k})$$

Transport energy current and heat current

$$\boldsymbol{j}^{E} = \boldsymbol{J}^{E} + \boldsymbol{E} \times \boldsymbol{M} \qquad \boldsymbol{j}^{Q} \equiv \boldsymbol{j}^{E} - \mu \boldsymbol{j}$$

Intrinsic response to electric field:

$$\boldsymbol{j}_{\text{in}}^{Q} = \boldsymbol{E} \times \frac{e}{\hbar} \int [d\boldsymbol{k}] \boldsymbol{\Omega} [(\varepsilon - \mu) f + k_B T \log(1 + e^{-\beta(\varepsilon - \mu)})]$$

Compare with anomalous Nernst: Onsager relation

$$\boldsymbol{j}_{\text{in}} = -\frac{\boldsymbol{\nabla} T}{T} \times \frac{e}{\hbar} \int [d\boldsymbol{k}] \boldsymbol{\Omega} [(\varepsilon - \mu) f + k_B T \log(1 + e^{-\beta(\varepsilon - \mu)})]$$

Revisit anomalous Nernst

- Earlier result on anomalous Nernst:

$$\boldsymbol{j}_{\text{in}}^{Q} = \boldsymbol{E} \times \frac{e}{\hbar} \int [d\boldsymbol{k}] \boldsymbol{\Omega} [(\varepsilon - \mu) f + k_B T \log(1 + e^{-\beta(\varepsilon - \mu)})],$$

- Response to chemical potential gradient:

$$\boldsymbol{j}_{\text{in}}^{Q} = -\nabla \times M_{\text{f}}^{E} + \mu \nabla \times M_{\text{f}}$$

$$= \nabla \mu \times \frac{1}{e} \int d\varepsilon \frac{\partial f}{\partial \mu} \sigma_{xy}(\varepsilon)(\varepsilon - \mu)$$

- Einstein relation is satisfied.

Anomalous Thermal Hall effect

Energy magnetization due to boundary current

$$M_f^E = \frac{1}{e^2}\int d\varepsilon f(\varepsilon)\sigma_{xy}(\varepsilon)\, \varepsilon \qquad \text{where} \qquad \sigma_{xy}(\varepsilon) = \frac{e^2}{\hbar}\int \frac{d\boldsymbol{q}}{(2\pi)^d}\Theta(\varepsilon - \varepsilon(\boldsymbol{q}))\Omega_z(\boldsymbol{q})$$

Intrinsic heat current due to statistical force

$$\boldsymbol{j}_{\mathrm{in}}^Q = -\nabla \times M_{\mathrm{f}}^E + \boldsymbol{\mu}\, \nabla \times M_{\mathrm{f}}$$

Thermal Hall conductivity:

$$j_x^Q = \kappa_{xy}(-\nabla_y T)$$

Relation to Hall conductivity:

$$\kappa_{xy} = -\frac{1}{e^2 T}\int \mathrm{d}\epsilon(\epsilon-\mu)^2\sigma_{xy}(\epsilon) f'(\epsilon)$$

Wiedemann-Franz Law at low temperature:

$$\kappa_{xy} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T\sigma_{xy}$$

Magnon anomalous thermal Hall

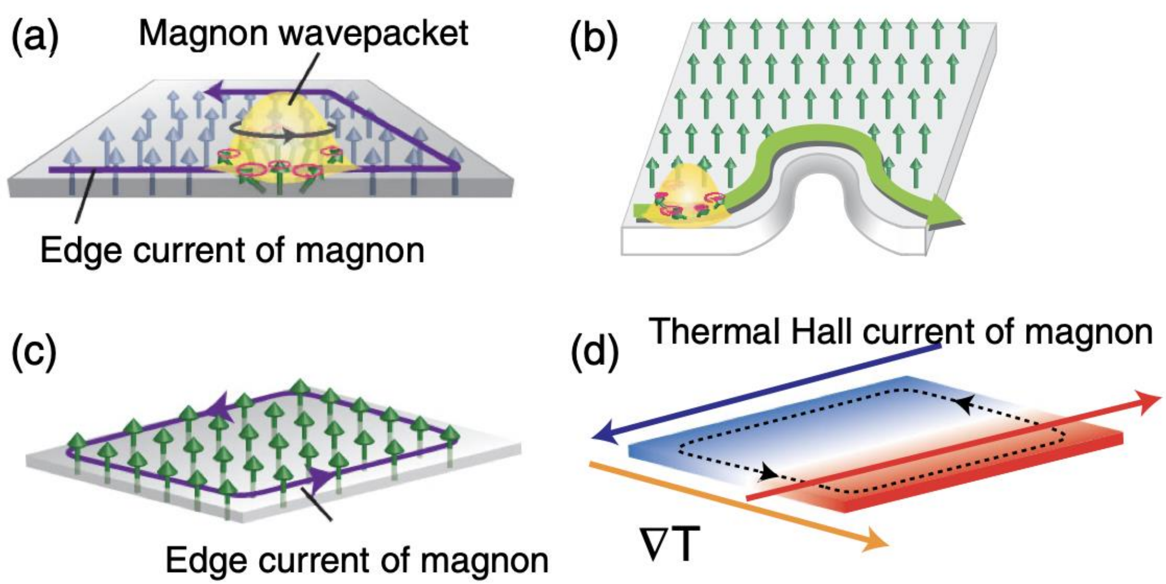


FIG. 1 (color online). (a) Self-rotation of a magnon wave packet and a magnon edge current. (b) The magnon near the boundary proceeds along the boundary, irrespective of the edge shape. (c) Magnon edge current in equilibrium. (d) Under the temperature gradient, the amount of the transverse heat current are not balanced between the two edges, and a finite thermal Hall current will appear.

Matsumoto & Murakami (2011)

Spin waves in ferromagnet

Use Bose-Einstein distribution with μ=0

Spin density response

Dong, et al PRL (2020)

System Hamiltonian:

$$\hat{\mathcal{H}} = \hat{H}_0 + \hat{\boldsymbol{\theta}} \cdot \boldsymbol{h}(\boldsymbol{r}_c, t) - e\phi(\boldsymbol{r}_c)$$

Density response:

$$\rho^{\boldsymbol{\theta}}_{\text{loc}} = \int Df(\partial_{\boldsymbol{h}}\varepsilon_{\text{tot}} - \Omega_{\boldsymbol{h}\mathcal{T}}) - \partial_{r^i}\int f m^{i\boldsymbol{\theta}}$$

Energy correction:

$$\Delta\varepsilon = \boldsymbol{m}^{i\boldsymbol{\theta}} \cdot \partial_{r^i}\boldsymbol{h}$$

Dipole moment:

$$\boldsymbol{m}^{i\boldsymbol{\theta}} = \text{Im}\langle\partial_{q_i}u|\varepsilon - \hat{\mathcal{H}}|\partial_{\boldsymbol{h}}u\rangle$$

Berry curvature:

$$\Omega_{\boldsymbol{h}\mathcal{T}} = \Omega_{\boldsymbol{h}\boldsymbol{r}}\dot{\boldsymbol{r}} + \Omega_{\boldsymbol{h}\boldsymbol{q}}\dot{\boldsymbol{q}} + \Omega_{\boldsymbol{h}t}$$

Equilibrium and transport responses

Equilibrium response:

$$\rho^{\theta}_{\text{eq}} = \partial_{h} G_{\text{tot}} - \partial_i M^{i\theta}$$

Free energy correction:

$$-(1/\beta)\log(1+e^{-\beta(\varepsilon-\mu)})$$

$$\Delta G = \int [f \Delta \varepsilon + \Omega_{q_i r_i} g]$$

Dipole Density:

$$M^{i\theta} = \int (f m^{i\theta} + g \Omega_{q_i h})$$

Transport response:

$$\rho^{\theta}_{\text{neq}} = \sigma^{i\theta}(E_i + \partial_i \mu / e) - \alpha^{i\theta} \partial_i T$$

Transport coefficients:

$$\sigma^{i\theta} = -e \int f \Omega_{q_i h},$$

$$\alpha^{i\theta} = \frac{1}{T} \int \Omega_{q_i h} [(\varepsilon - \mu) f(\varepsilon) - g(\varepsilon)]$$

Response to gravitational field

Luttinger (1964): thermal transport as a linear response to a gravitational field

$$\hat{h}_{\phi,\psi}(\boldsymbol{r}) = [1+\psi(\boldsymbol{r})]\left[\hat{h}(\boldsymbol{r}) + \phi(\boldsymbol{r})\hat{n}(\boldsymbol{r})\right]$$

Local equilibrium:

$$\hat{\rho}_{\,\mathrm{leq}} = \frac{1}{Z}\exp\left[-\int d\boldsymbol{r}\,\frac{\hat{h}(\boldsymbol{r}) - \mu(\boldsymbol{r})\hat{n}(\boldsymbol{r})}{k_B T(\boldsymbol{r})}\right].$$

Global equilibrium: the following fields are constant

$$\alpha(\boldsymbol{r}) \equiv [1+\psi(\boldsymbol{r})][\phi(\boldsymbol{r}) + \mu(\boldsymbol{r})] \qquad \beta(\boldsymbol{r}) \equiv 1/k_B[1+\psi(\boldsymbol{r})]T(\boldsymbol{r})$$

Equilibrium Currents:

$$\boldsymbol{J}_1^{\mathrm{eq}}(\boldsymbol{r}) = [1+\psi(\boldsymbol{r})]\,\boldsymbol{\nabla}\times\boldsymbol{M}_N(\boldsymbol{r}),$$

$$\boldsymbol{J}_2^{\mathrm{eq}}(\boldsymbol{r}) = [1+\psi(\boldsymbol{r})]^2\,[\boldsymbol{\nabla}\times\boldsymbol{M}_E(\boldsymbol{r}) - \mu(\boldsymbol{r})\boldsymbol{\nabla}\times\boldsymbol{M}_N(\boldsymbol{r})]$$

Transport currents

$$\begin{bmatrix} \boldsymbol{J}_1 \\ \boldsymbol{J}_2 \end{bmatrix}_{\rm tr} = \begin{bmatrix} \overleftrightarrow{L}^{(11)} & \overleftrightarrow{L}^{(12)} - \frac{1}{\beta V}\boldsymbol{M}_N \times \\ \overleftrightarrow{L}^{(21)} - \frac{1}{\beta V}\boldsymbol{M}_N \times & \overleftrightarrow{L}^{(22)} - \frac{2}{\beta V}\boldsymbol{M}_Q \times \end{bmatrix} \begin{bmatrix} \boldsymbol{X}_1 \\ \boldsymbol{X}_2 \end{bmatrix}$$

Cooper-Halperin-Ruzin, PRB **55**, 2344(1997)

Flux

$$\boldsymbol{J}_1^{\phi,\psi} \equiv \boldsymbol{J}_N^{\phi,\psi}$$

$$\boldsymbol{J}_2^{\phi,\psi} \equiv \boldsymbol{J}_E^{\phi,\psi} - \alpha(\boldsymbol{r})\boldsymbol{J}_N^{\phi,\psi}$$

Force

$$\boldsymbol{X}_1 = -\beta(\boldsymbol{r})\boldsymbol{\nabla}\alpha(\boldsymbol{r})$$

$$\boldsymbol{X}_2 = \boldsymbol{\nabla}\beta(\boldsymbol{r})$$

The L’s are given by standard Kubo formula

Heat Magnetization
Qin, Niu and Shi PRL (2011)

$$\boldsymbol{M}_Q(\boldsymbol{r}) \equiv \boldsymbol{M}_E(\boldsymbol{r}) - \mu_0 \boldsymbol{M}_N(\boldsymbol{r})$$

Summary

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