Transport in strongly correlated systems

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Outline of lecture series

- Lecture 1: Linear response theory
- Lecture 2: Conductivities and their ratios
- Lecture 3: Transport with strong interactions
- Lecture 4: Transport at finite and infinite frequencies
- Lecture 5: Electro-magneto-thermal transport
  (the Nernst effect)

Lecture 1: Linear response theory

- Hydrodynamic requirements
- Kubo formulae
- Magnetization currents and the Onsager relations

Goal of studying transport

Apply perturbations to a system in equilibrium

Measure or calculate currents induced as a result

Typical perturbations: electric field and temperature gradient

Currents: Electrical, Energy and Heat currents

Linear response: Current linear in perturbation

Conductivity: ratio of a current to a perturbation

Linear response theory

Assumptions

- Small deviations from thermal equilibrium
- Large samples compared to microscopic scales
- Weak "slowly varying" perturbations
- Short range interactions

Hydrodynamic requirement

$$\boxed{\tau \gg \tau_m}$$

τ - timescale of variation of perturbation

τ_m - microscopic relaxation rate to equilibrium

System close to local equilibrium

All properties of interest can be described in terms of conserved densities and their derivatives

Conserved densities need not have attained their equilibrium values

The time scale for that can be macroscopic τ_M

Conserved densities like $n(\mathbf{r},t)$ and $h(\mathbf{r},t)$

$n(\mathbf{r},t)$: number density

$h(\mathbf{r},t)$: energy density

$$\dot{n} = -\nabla.\mathbf{J}$$

$$\dot{h} = -\nabla.\mathbf{J}^{E}$$

Physical quantity $P\left[n, h, \nabla n, \nabla h, \ldots\right]$

In operator form

$$\dot{\hat{n}} = -\nabla.\hat{\mathbf{J}}$$

$$\dot{\hat{h}} = -\nabla.\hat{\mathbf{J}}_{E}$$

τ_M is set by the diffusive dynamics of slow modes

$$\tau_M \sim L^2/D \sim 1/Dq^2 \text{ for } q \to 0$$

D: diffusion constant, L: size of system

In general $\tau_M \gg \tau_m$

Non-equilibrium steady state can result for

$$\tau_M \gg \tau \gg \tau_m$$

Equilibrium requires

$$\tau \gg \tau_M$$

The two most common perturbations in experimental situations

$\nabla\phi$: gradient of electrostatic potential

∇T: gradient of temperature

T and ϕ fundamentally different

ϕ couples as $\hat{H} \rightarrow \hat{H} + \int d\mathbf{r}\ \phi(\mathbf{r})\hat{n}(\mathbf{r})$

T is a "statistical" field, does not couple to $\hat{H}$

Linear response theory essentially perturbation theory in potentials that couple to $\hat{H}$

(as we will see)

How then do we handle ∇T?

Solution: Introduce a gradient in a "gravitational field" $\psi(\mathbf{r})$ which couples to $\hat{h}(\mathbf{r})$

[J. M. Luttinger *et. al.*, *Phys. Rev.* **135** 1505 (1964)]

Introducing $\nabla \psi$ gives the same answers as ∇T.

$$\hat{H} = \int d\mathbf{r}\ \hat{h}(\mathbf{r})$$

$$\hat{h}(\mathbf{r}) = \hat{h}^{(0)}(\mathbf{r}) + \phi(\mathbf{r})\hat{n}(\mathbf{r}) + \psi(\mathbf{r})\hat{h}^{(0)}(\mathbf{r})$$

Thermodynamic equilibrium

Density matrix: $\hat{w} = \frac{1}{Z} e^{-\beta(\hat{H} - \xi \hat{N})}$

Consider $\nabla\phi = \nabla\psi = 0$

$\hat{H}$ and $\hat{H}^{(0)}$ share the same eigenstates

$$\hat{w} = \frac{1}{Z} e^{-(\hat{H}^{(0)} - \mu \hat{N})/T}$$

$T^{-1} = \beta(1+\psi)$ and $\mu = (\xi - \phi)/(1+\psi)$

T and μ are "internal" temperature and chemical potential

Thermodynamic equilibrium

for $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$ varying "slowly enough"

$$T(\mathbf{r})^{-1} = \beta[1+\psi(\mathbf{r})] \text{ and } \mu(\mathbf{r}) = [\xi - \phi(\mathbf{r})]/[1+\psi(\mathbf{r})]$$

$n(\mathbf{r}) = \langle \hat{n}(\mathbf{r}) \rangle$ and $h(\mathbf{r}) = \langle \hat{h}(\mathbf{r}) \rangle$ can be defined in terms of $\mu(\mathbf{r})$ and $T(\mathbf{r})$

$$\delta(\mu/T) = -\phi(\mathbf{r})/T_0$$

$$\delta(1/T) = \psi(\mathbf{r})/T_0$$

$$T_0 = 1/\beta$$

With no magnetic fields in equilibrium

$$\mathbf{J} = \langle \hat{\mathbf{J}}(\mathbf{r}) \rangle = 0$$

$$\mathbf{J}^E = \langle \hat{\mathbf{J}}^E(\mathbf{r}) \rangle = 0$$

Thus $\mathbf{J}$ and $\mathbf{J}^E$ can only depend on $\nabla\phi + T\nabla\left(\mu/T\right)$ and $\nabla\psi - T\nabla\left(1/T\right)$ in the general non-equlibrium case.

(Einstein conditions)

Note that in the non-equilibrium case

$$\delta(\mu/T) \neq -\phi(\mathbf{r})/T_0$$

$$\delta(1/T) \neq \psi(\mathbf{r})/T_0$$

$$J_\alpha = L^{11}_{\alpha\beta}\left[-\nabla_\beta \phi - T\nabla_\beta\left(\mu/T\right)\right] + L^{12}_{\alpha\beta}\left[-\nabla_\beta \psi + T\nabla_\beta\left(1/T\right)\right]$$

$$J^E_\alpha = L^{21}_{\alpha\beta}\left[-\nabla_\beta \phi - T\nabla_\beta\left(\mu/T\right)\right] + L^{22}_{\alpha\beta}\left[-\nabla_\beta \psi + T\nabla_\beta\left(1/T\right)\right]$$

The same coefficient for $T = cons$ and $\nabla\psi \neq 0$
as for $\nabla T \neq 0$ and $\psi = 0$

Currents due to $\nabla\mu$ and ∇T: diffusion currents

Currents due to $\nabla\phi$ and $\nabla\psi$: drift currents

Determining $L_{\alpha\beta}$

Assume $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$ are switched on over a timescale τ such that $\tau_M \gg \tau \gg \tau_m$

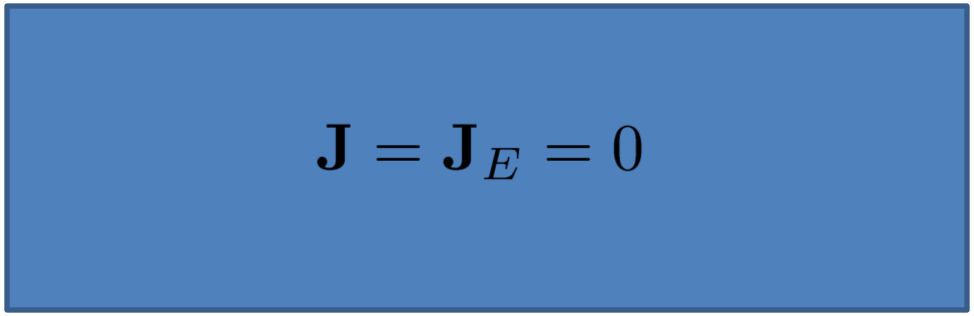
The system does not get time to attain a state of thermal equlibrium

It can be shown from the continuity equations that $\nabla\mu = \nabla T = 0$ and do not change from their initial values.

[J. M. Luttinger, *Phys. Rev.* **135** 1505 (1964)]

$$J_\alpha = L^{11}_{\alpha\beta}\left(-\nabla_\beta\phi\right) + L^{12}_{\alpha\beta}\left(-\nabla_\beta\psi\right)$$

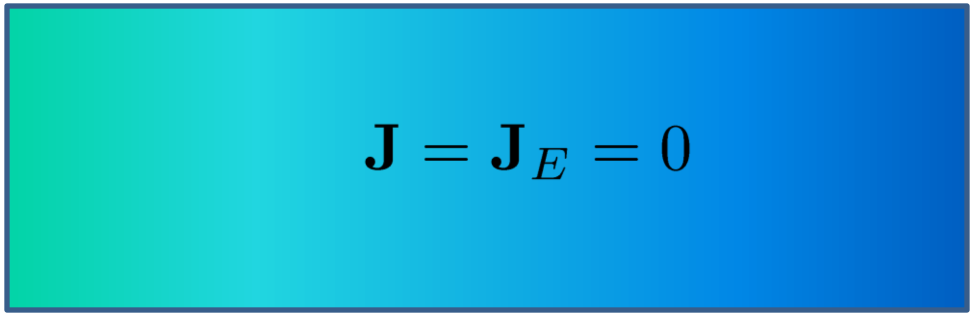
$$J^E_\alpha = L^{21}_{\alpha\beta}\left(-\nabla_\beta\phi\right) + L^{22}_{\alpha\beta}\left(-\nabla_\beta\psi\right)$$



Equilibrium

$$\nabla\phi = \nabla\psi = 0$$

$$\nabla\mu = \nabla T = 0$$

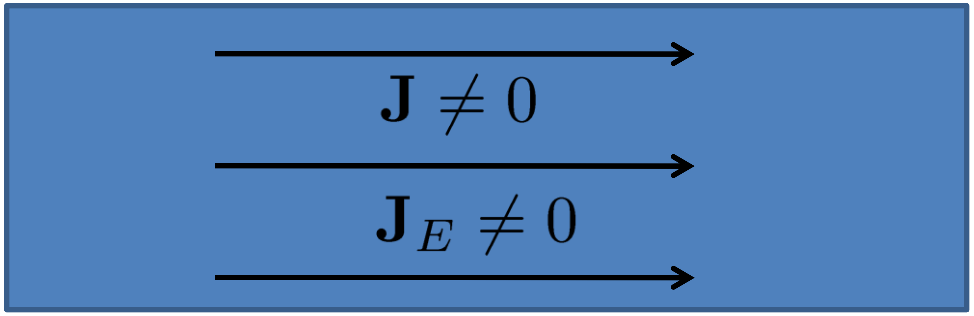


Equilibrium

$$\nabla\phi \neq 0,\ \nabla\psi \neq 0$$

$$\tau \gg \tau_M \gg \tau_m$$

$$\nabla\mu \neq 0,\ \nabla T \neq 0$$



Non-equilibrium

$$\nabla\phi \neq 0,\ \nabla\psi \neq 0$$

$$\tau_M \gg \tau \gg \tau_m$$

$$\nabla\mu = \nabla T = 0$$

Kubo formula

Calculate $L^{11}_{\alpha\beta}$ as an example

Set $\psi = 0$ and $-\nabla\phi = \mathbf{E}$, constant in space

Assume $\mathbf{E}$ has been switched on at $t = -\infty$ over timescale $\tau = 1/s$

Present time $t = 0$

$$\hat{H}(t) = \hat{H}^{(0)} + e^{st} \int d\mathbf{r}\ \hat{n}(\mathbf{r}, t)\phi(\mathbf{r}) = \hat{H}^{(0)} + e^{st}\hat{F}(t)$$

$$\hat{A}(t) = e^{i\hat{H}^{(0)}t}\hat{A}e^{-i\hat{H}^{(0)}t}$$

Using a spatially constant $\mathbf{E}$ at the outset sets $\tau_M = \infty$

$$(q = 0,\ \tau_M \sim 1/Dq^2)$$

To effect $\tau \gg \tau_m$, we will finally take the limit $s \to 0$

Obtain a solution of the Liouville equation that is a density matrix of the form $\hat{w}(t) = \hat{w}^{(0)} + e^{st}\hat{f}(t)$

Equilibrium density matrix: $\hat{w}^{(0)} = \frac{1}{Z}e^{-\beta(\hat{H}^{(0)} - \mu\hat{N})}$

μ is the equilibrium chemical potential with $\mathbf{E} = 0$

$$i\hbar\dot{\hat{w}} = \left[\hat{H}, \hat{w}\right] \approx e^{st}\left(\left[\hat{F}, \hat{w}^{(0)}\right] + \left[\hat{H}^{(0)}, \hat{f}\right]\right)$$

$$(\left[\hat{H}^{(0)}, \hat{w}^{(0)}\right] = 0 \text{ and } \left[\hat{F}, \hat{f}\right] \text{ is small})$$

$$\hat{f}(t=0) = -i\int_0^\infty dt\; e^{-st}\left[\hat{F}(-t), \hat{w}^{(0)}\right]$$

$$\left[\hat{F}(-t), \hat{w}^{(0)}\right] = -i\hat{w}^{(0)}\int_0^\beta d\beta'\,\frac{\partial}{\partial t'}\hat{F}\left(-t - i\beta'\right)$$

$$J_\alpha = \frac{1}{V}\int_0^\infty dt\; e^{-st}\int_0^\beta d\beta' \langle \hat{J}_\beta(-t-i\beta')\hat{J}_\alpha(0)\rangle E_\beta$$

$$L^{11}_{\alpha\beta} = \lim_{s\to 0}\;\frac{1}{V}\int_0^\infty dt\; e^{-st}\int_0^\beta d\beta' \langle \hat{J}_\beta(-t-i\beta')\hat{J}_\alpha(0)\rangle$$

$$\hat{\mathbf{J}}(t) = \frac{1}{V}\int d\mathbf{r}\;\hat{\mathbf{J}}(\mathbf{r},t)$$

$$L^{ab}_{\alpha\beta} = \lim_{s\to 0}\;\frac{1}{V}\int_0^\infty dt\; e^{-st}\int_0^\beta d\beta' \langle \hat{J}^{(b)}_\beta(-t-i\beta')\hat{J}^{(a)}_\alpha(0)\rangle$$

Kubo formula

$$\hat{\mathbf{J}}^{(1)} = \hat{\mathbf{J}},\; \hat{\mathbf{J}}^{(2)} = \hat{\mathbf{J}}^E$$

Kubo's original derivation was for all ω

$$L^{ab}_{\alpha\beta}(\omega) = \frac{1}{V}\int_0^\infty dt\; e^{i\omega t}\int_0^\beta d\beta' \langle \hat{J}^{(b)}_\beta(-t-i\beta')\hat{J}^{(a)}_\alpha(0)\rangle$$

$$L^{ab}_{\alpha\beta}(\omega) = \frac{\pi\left(1-e^{-\beta\hbar\omega}\right)}{\hbar\omega V}\int_0^\infty dt\; e^{i\omega t}\langle \hat{J}^{(b)}_\beta(t)\hat{J}^{(a)}_\alpha(0)\rangle$$

$$= \frac{\pi\left(1-e^{-\beta\hbar\omega}\right)}{\hbar\omega V Z}\sum_{n,m} e^{-\beta E_n}\langle n|\hat{J}^{(b)}_\beta|m\rangle\langle m|\hat{J}^{(a)}_\alpha|n\rangle\delta\left(E_m-E_n-\hbar\omega\right)$$

in the limit $\omega \to 0$ matches previous expression

[R. Kubo, *J. Phys. Soc. Jpn.* **12** 570 (1957)]

$$L^{ab}_{\alpha\beta} = \frac{\pi\beta}{VZ}\sum_{n,m} e^{-\beta E_n}\langle n|\hat{J}^{(b)}_\beta|m\rangle\langle m|\hat{J}^{(a)}_\alpha|n\rangle\delta\left(E_m-E_n\right)$$

$$\boxed{L^{ab}_{\alpha\beta} = L^{ba}_{\beta\alpha}}$$

(Onsager relations)

Let us set $\psi = 0$

$$J_\alpha = L^{11}_{\alpha\beta}\left(-\nabla_\beta \bar{\mu}\right) + \left(L^{12} - \mu L^{11}\right)_{\alpha\beta} T \nabla_\beta \left(1/T\right)$$

$$J^E_\alpha = L^{21}_{\alpha\beta}\left(-\nabla_\beta \bar{\mu}\right) + \left(L^{22} - \mu L^{21}\right)_{\alpha\beta} T \nabla_\beta \left(1/T\right)$$

$$\bar{\mu} = \mu + \phi$$

The coefficients of $\nabla\bar{\mu}$ and $T\nabla(1/T)$ do not satisfy the Onsager relations

Heat current $\mathbf{J}^Q = \mathbf{J}^E - \mu \mathbf{J}$

$$J_\alpha = -N^{11}_{\alpha\beta} \nabla_\beta \bar{\mu} - N^{12}_{\alpha\beta} \nabla_\beta T$$

$$J^Q_\alpha = -T N^{21}_{\alpha\beta} \nabla_\beta \bar{\mu} - \frac{N^{22}_{\alpha\beta}}{T} \nabla_\beta T$$

$$N^{11}_{\alpha\beta} = L^{11}_{\alpha\beta}$$

$$N^{12}_{\alpha\beta} = \frac{L^{12}_{\alpha\beta} - \mu L^{11}_{\alpha\beta}}{T}$$

$$N^{22}_{\alpha\beta} = L^{22}_{\alpha\beta} - \mu \left(L^{12}_{\alpha\beta} + L^{21}_{\alpha\beta} \right) + \mu^2 L^{11}_{\alpha\beta}$$

$$L^{ab}_{\alpha\beta} = \lim_{s \to 0} \frac{1}{V} \int_0^\infty dt\, e^{-st} \int_0^\beta d\beta' \langle \hat{J}^{(b)}_\beta(-t - i\beta') \hat{J}^{(a)}_\alpha(0) \rangle$$

$$L^{ab}_{\alpha\beta} = L^{ba}_{\beta\alpha}$$

$$N^{ab}_{\alpha\beta} = N^{ba}_{\beta\alpha}$$

Non-zero applied magnetic field ($\mathbf{B} \neq \mathbf{0}$)

Currents now flow even in thermal equilibrium

Bulk magnetization currents

$$\mathbf{J}_{\mathrm{mag}} = \nabla \times \mathbf{M}$$

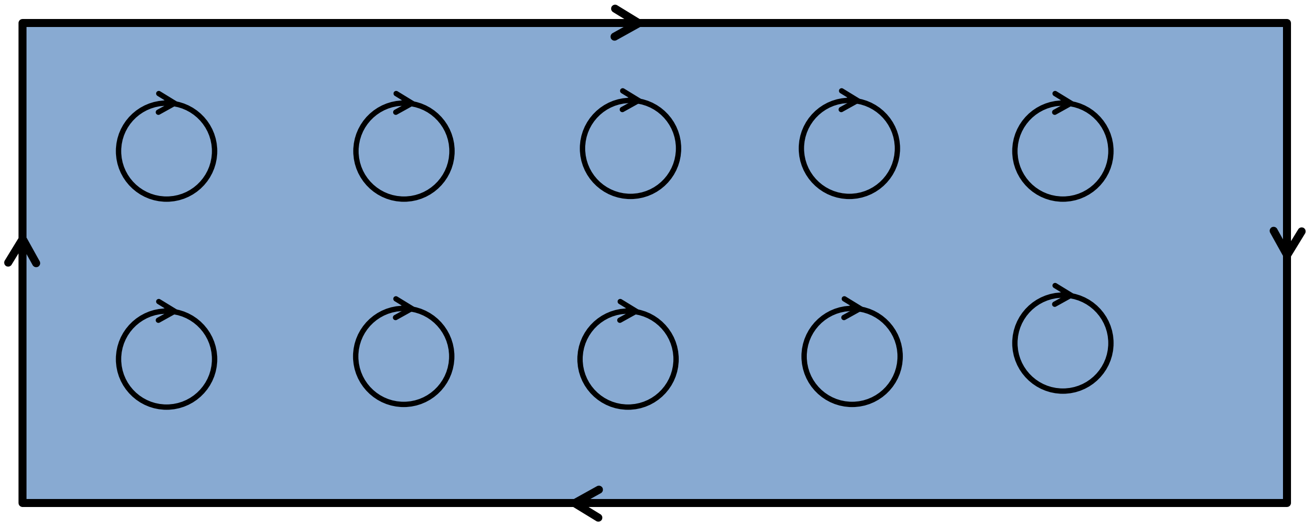
$$\mathbf{J}^{E}_{\mathrm{mag}} = \nabla \times \mathbf{M}^{E}$$

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}\left[\mu(\mathbf{r}), T(\mathbf{r})\right] \text{ and } \mathbf{M}^{E}(\mathbf{r}) = \mathbf{M}^{E}\left[\mu(\mathbf{r}), T(\mathbf{r})\right]$$

$$\mathbf{J} = \mathbf{J}_{\mathrm{mag}} + \mathbf{J}_{\mathrm{tr}}$$

$$\mathbf{J}^{E} = \mathbf{J}^{E}_{\mathrm{mag}} + \mathbf{J}^{E}_{\mathrm{tr}}$$

Magnetization currents



Do not contribute to net flows

Only transport currents contribute to flow measured in experiments

How do we deal with magnetization currents in linear response?

$$\hat{\mathbf{J}}_{\mathrm{mag}}(\mathbf{r}) = \hat{\mathbf{J}}^{(0)}_{\mathrm{mag}}(\mathbf{r})\left[1+\psi\right]$$

$$\hat{\mathbf{J}}^{E}_{\mathrm{mag}}(\mathbf{r}) = \left(\hat{\mathbf{J}}^{E}_{\mathrm{mag}}\right)^{(0)}(\mathbf{r})\left[1+2\psi\right] + \phi\hat{\mathbf{J}}^{(0)}_{\mathrm{mag}}(\mathbf{r})$$

for constant ϕ and ψ

$$\mathbf{M} = (1+\psi)\mathbf{M}^{(0)}(\mu, T)$$

$$\mathbf{M}^{E} = (1+2\psi)\left(\mathbf{M}^{E}\right)^{(0)}(\mu, T) + \phi\mathbf{M}^{(0)}(\mu, T)$$

These expressions continue to hold with gradients

$$\mathbf{J}_{\rm mag}(\mathbf{r}) = -\frac{\partial \mathbf{M}}{\partial \mu}\times\nabla\mu - \frac{\partial \mathbf{M}}{\partial T}\times\nabla T - \mathbf{M}\times\nabla\psi$$

$$\mathbf{J}^E_{\rm mag}(\mathbf{r}) = -\frac{\partial \mathbf{M}^E}{\partial \mu}\times\nabla\mu - \frac{\partial \mathbf{M}^E}{\partial T}\times\nabla T - \mathbf{M}\times\nabla\phi - 2\mathbf{M}^E\times\nabla\psi$$

Leading order in ϕ and ψ

$\mathbf{M}$ and $\mathbf{M}^E$ are equilibrium magnetizations here

Again for $\tau_M \gg \tau$

$$\mathbf{J}_{\rm mag}(\mathbf{r}) = -\mathbf{M}\times\nabla\psi$$

$$\mathbf{J}^E_{\rm mag}(\mathbf{r}) = -\mathbf{M}\times\nabla\phi - 2\mathbf{M}^E\times\nabla\psi$$

$$L^{ab}_{\alpha\beta}(\mathbf{B}) = L^{ba}_{\beta\alpha}(-\mathbf{B})$$ (Onsager relations)

[N. R. Cooper, B. I. Halperin, I. M. Ruzin, *Phys. Rev. B* **55** 2344 (1997)]

$$(J_\alpha)_{\rm tr} = L^{11}_{\alpha\beta}\left(-\nabla_\beta\phi\right) + \left(L^{12}_{\alpha\beta} - \epsilon_{\alpha\beta\gamma}M_\gamma\right)\left(-\nabla_\beta\psi\right)$$

$$\left(J^E_\alpha\right)_{\rm tr} = \left(L^{21}_{\alpha\beta} - \epsilon_{\alpha\beta\gamma}M_\gamma\right)\left(-\nabla_\beta\phi\right) + \left(L^{22}_{\alpha\beta} - 2\epsilon_{\alpha\beta\gamma}M^E_\gamma\right)\left(-\nabla_\beta\psi\right)$$

when $\nabla\mu = \nabla T = 0$

In the general case

$$(J_\alpha)_{\rm tr} = \mathcal{L}^{11}_{\alpha\beta}\left[-\nabla_\beta\phi - T\nabla_\beta\left(\mu/T\right)\right] + \mathcal{L}^{12}_{\alpha\beta}\left[-\nabla_\beta\psi + T\nabla_\beta\left(1/T\right)\right]$$

$$\left(J^E_\alpha\right)_{\rm tr} = \mathcal{L}^{21}_{\alpha\beta}\left[-\nabla_\beta\phi - T\nabla_\beta\left(\mu/T\right)\right] + \mathcal{L}^{22}_{\alpha\beta}\left[-\nabla_\beta\psi + T\nabla_\beta\left(1/T\right)\right]$$

$$\mathcal{L}^{11}_{\alpha\beta} = L^{11}_{\alpha\beta} \qquad \mathcal{L}^{12}_{\alpha\beta} = L^{12}_{\alpha\beta} - \epsilon_{\alpha\beta\gamma}M_\gamma$$

$$\mathcal{L}^{21}_{\alpha\beta} = L^{21}_{\alpha\beta} - \epsilon_{\alpha\beta\gamma}M_\gamma \qquad \mathcal{L}^{22}_{\alpha\beta} = L^{22}_{\alpha\beta} - \epsilon_{\alpha\beta\gamma}M^E_\gamma$$

$$L^{ab}_{\alpha\beta}(\mathbf{B}) = L^{ba}_{\beta\alpha}(-\mathbf{B})$$ (Onsager relations)

Transport currents obey the Onsager relations

But the magnetization currents do not!

Hence neither do the total currents!

$$\mathbf{J}_{\mathrm{tr}}^{Q} = \mathbf{J}_{\mathrm{tr}}^{E} - \mu \mathbf{J}_{\mathrm{tr}}$$

$$(J_\alpha)_{\mathrm{tr}} = -\mathcal{N}_{\alpha\beta}^{11} \nabla_\beta \bar{\mu} - \mathcal{N}_{\alpha\beta}^{12} \nabla_\beta T$$

$$\left(J_\alpha^Q\right)_{\mathrm{tr}} = -T \mathcal{N}_{\alpha\beta}^{21} \nabla_\beta \bar{\mu} - \frac{\mathcal{N}_{\alpha\beta}^{22}}{T} \nabla_\beta T$$

$$\mathcal{N}_{\alpha\beta}^{11} = L_{\alpha\beta}^{11}$$

$$\mathcal{N}_{\alpha\beta}^{12} = L_{\alpha\beta}^{12} - \mu L_{\alpha\beta}^{11} - \epsilon_{\alpha\beta\gamma} M_\gamma \qquad \mathcal{N}_{\alpha\beta}^{21} = L_{\alpha\beta}^{21} - \mu L_{\alpha\beta}^{11} - \epsilon_{\alpha\beta\gamma} M_\gamma$$

$$\mathcal{N}_{\alpha\beta}^{22} = L_{\alpha\beta}^{22} - \mu \left(L_{\alpha\beta}^{12} + L_{\alpha\beta}^{21} \right) + \mu^2 L_{\alpha\beta}^{11} - 2\epsilon_{\alpha\beta\gamma} \left(M_\gamma^E - M_\gamma \right)$$

Various conductivities

Charge conductivities: $\nabla T = 0$, apply $\nabla\phi$, measure $\mathbf{J}$

$$\boxed{\sigma_{\alpha\beta} = \mathcal{N}^{11}_{\alpha\beta}}$$

Peltier conductivities: $\nabla T = 0$, apply $\nabla\phi$, measure $\mathbf{J}^Q$

or $\nabla\phi = 0$, apply ∇T, measure $\mathbf{J}$

$$\boxed{\alpha_{\alpha\beta} = \mathcal{N}^{12}_{\alpha\beta}}$$

Heat conductivities: $\nabla\phi = 0$, apply ∇T, measure $\mathbf{J}^Q$

$$\boxed{Q_{\alpha\beta} = \frac{1}{T}\mathcal{N}^{22}_{\alpha\beta}}$$

References

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Tomorrow

Lecture 2: Conductivities and their ratios

- Transport coefficients measured experimentally
- Boltzmann transport theory
- Thermopower and Lorenz number
- The Nernst effect