Irreversible thermodynamics of transport and relaxation of magnetic dipoles with applications for spin caloritronics

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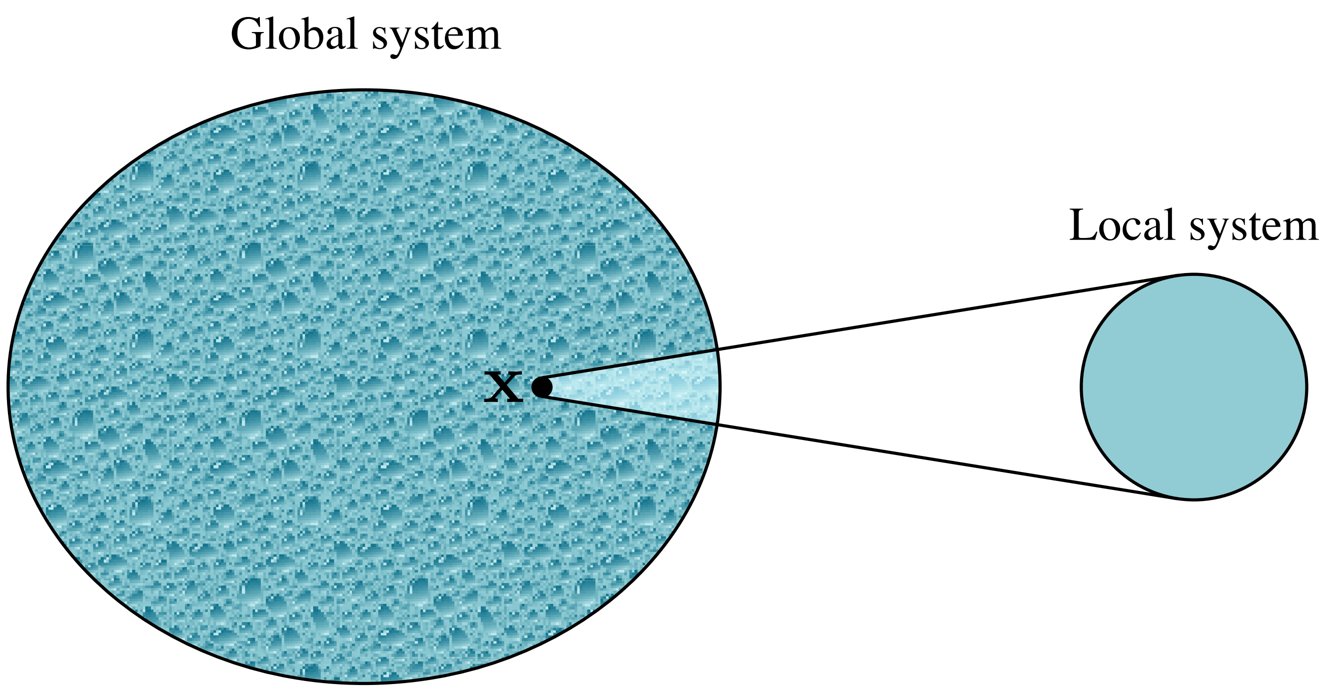
SWISS CONTRIBUTION

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

NANOSPIN

Outline

Global and local systems



Global system

- Not at equilibrium
- Inhomogeneous
- Non-uniform

Local System (i.e. x)

- At equilibrium
- Homogeneous
- Uniform

Continuous medium with magnetisation

State fields

- $s(\mathbf{x}, t)$: entropy density field
- $n_A(\mathbf{x}, t)$: density fields of chemical substances $A \quad \forall\ A$
- $q(\mathbf{x}, t)$: electric charge density field
- $\mathbf{v}(\mathbf{x}, t)$: velocity field
- $\mathbf{M}(\mathbf{x}, t)$: magnetisation field

State field functions

- $e(s, n_A, q, \mathbf{v}, \mathbf{M})$: energy density
- $\mathbf{p}(n_A, \mathbf{v})$: momentum density
- $m(n_A)$: mass density

Extensive state fields

- $\dot{s} + (\nabla \cdot \mathbf{v})\, s + \nabla \cdot \mathbf{j}_s = \rho_s \geqslant 0$ **2nd law Thermo**
- $\dot{n}_A + (\nabla \cdot \mathbf{v})\, n_A + \nabla \cdot \mathbf{j}_A = \sum_a \nu_{aA}\, \omega_a$ **Chemical balance**
- $\dot{q} + (\nabla \cdot \mathbf{v})\, q + \nabla \cdot \mathbf{j}_q = 0$ **Electric charge balance**
- $\dot{\mathbf{M}} + (\nabla \cdot \mathbf{v})\, \mathbf{M} + \nabla \cdot \mathrm{j}_{\mathrm{M}} = \sum_A \left(\gamma_A\, n_A\, (\mathbf{m}_A \times \mathbf{B}) + \boldsymbol{\Omega}_A \times \mathbf{m}_A \right)$ **Mag. balance**

Extensive state field functions

- $\dot{e} + (\nabla \cdot \mathbf{v})\, e + \nabla \cdot \mathbf{j}_e = \mathbf{f}^{\,\text{ext}} \cdot \mathbf{v}$ **1st law Thermo**
- $\dot{\mathbf{p}} + (\nabla \cdot \mathbf{v})\, \mathbf{p} - \nabla \cdot \boldsymbol{\sigma} = \mathbf{f}^{\,\text{ext}}$ **Momentum balance**
- $\dot{m} + (\nabla \cdot \mathbf{v})\, m = 0$ **Mass balance**

2nd law Newton:

- $\mathbf{p}\,(n_A, \mathbf{v}) = m\,(n_A)\;\mathbf{v} \qquad \Rightarrow \qquad m\,\dot{\mathbf{v}} = \mathbf{f}^{\,\text{ext}} + \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}$

Energy density (Kinetic + Internal)

- $e\,(s, n_A, q, \mathbf{v}, \mathbf{M}) = \dfrac{1}{2}\,m\,(n_A)\;\mathbf{v}^2 + u\,(s, n_A, q, \mathbf{M})$

Internal energy balance

- $\dot{u} + (\boldsymbol{\nabla}\cdot\mathbf{v})\,u + \boldsymbol{\nabla}\cdot\mathbf{j}_u = \boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\odot\mathbf{v})$

Stress energy tensor (Elastic + Viscous)

- $\boldsymbol{\sigma} = -\,P\,\mathbb{1} + \tilde{\boldsymbol{\sigma}}$

Mass and electric current density vectors

- $m = \sum_A n_A \, m_A \quad \Rightarrow \quad \mathbf{j}_m = \sum_A m_A \, \mathbf{j}_A = \mathbf{0}$
- $q = \sum_A n_A \, q_A \quad \Rightarrow \quad \mathbf{j}_q = \sum_A q_A \, \mathbf{j}_A$

Magnetisation current and stress tensors

- $\mathbf{M} = \sum_A n_A \, \mathbf{m}_A \quad \Rightarrow \quad \mathsf{j}_M = \sum_A \mathbf{m}_A \odot \mathbf{j}_A$
- $\mathbf{p} = \sum_A n_A \, m_A \, \mathbf{v}_A \quad \Rightarrow \quad \tilde{\boldsymbol{\sigma}} = -\sum_A m_A \, \mathbf{v}_A \odot \mathbf{j}_A$

Mass and electric charge conservation laws

- $$\sum_A \nu_{aA}\, m_A = 0$$
- $$\sum_A \nu_{aA}\, q_A = 0$$

Time evolution of magnetic dipoles and dynamics

- $$n_A\,\dot{\mathbf{m}}_A = \gamma_A\, n_A\left(\mathbf{m}_A \times \mathbf{B}\right) - \mathbf{m}_A \times \boldsymbol{\Omega}_A - \left(\mathbf{j}_A \cdot \boldsymbol{\nabla}\right)\mathbf{m}_A$$
$$+ \sum_B \gamma_{AB}\, n_A\left(\mathbf{m}_A \times n_B\,\mathbf{m}_B\right) - \sum_a \nu_{aA}\,\omega_a\,\mathbf{m}_A$$
- $$n_A\, m_A\,\dot{\mathbf{v}}_A = \mathbf{f}_A^{\,\text{ext}} + \sum_B \mathbf{f}_{B\rightarrow A}^{\,\text{int}} - \boldsymbol{\nabla} P_A - m_A\left(\mathbf{j}_A \cdot \boldsymbol{\nabla}\right)\mathbf{v}_A$$

- Thermodynamics of a continuous medium $\subset$ continuity equation for $u\,(s, n_A, q, \mathbf{M})$:

$$\dot{u} + (\boldsymbol{\nabla}\cdot\mathbf{v})\,(u+P) + \boldsymbol{\nabla}\cdot\mathbf{j}_u = \sum_A \mathbf{j}_A \cdot \Big(-\; m_A\,\mathbf{v}_A\,\boldsymbol{\nabla}\,\mathbf{v}\Big)$$

where $\mathbf{v} \equiv$ velocity local center of mass

$$\mathbf{v} = \frac{\sum_A n_A\, m_A\, \mathbf{v}_A}{\sum_A n_A\, m_A}$$

- Intensive fields $\equiv$ conjugate of extensive state fields :

$$T \equiv \frac{\partial u}{\partial s}\;;\quad \mu_A \equiv \frac{\partial u}{\partial n_A}\;;\quad V \equiv \frac{\partial u}{\partial q}\;;\quad \mathbf{B} \equiv -\frac{\partial u}{\partial \mathbf{M}}$$

- Time evolution of $u\,(s, n_A, q, \mathbf{M})$:

$$\dot{u} = T\,\dot{s} + \sum_A \mu_A\,\dot{n}_A + V\,\dot{q} - \mathbf{B}\cdot\dot{\mathbf{M}}$$

- **Thermostatics**
- **Reversible thermodynamics**
- **Irreversible thermodynamics**

$$
\begin{aligned}
&\Big(u - T\,s + P - \sum_A \big(\mu_A + q_A\,V - \mathbf{m}_A\cdot\mathbf{B}\big)\,n_A\Big)\,(\boldsymbol{\nabla}\cdot\mathbf{v})\\
&+\boldsymbol{\nabla}\cdot\Big(\mathbf{j}_u - T\,\mathbf{j}_s - \sum_A \big(\mu_A + q_A\,V - \mathbf{m}_A\cdot\mathbf{B}\big)\,\mathbf{j}_A\Big)\\
&+T\,\rho_s - \sum_a \omega_a\,\mathcal{A}_a - \sum_A \boldsymbol{\Omega}_A\cdot\big(\mathbf{m}_A\times\mathbf{B}\big)\\
&-\sum_A \mathbf{j}_A\cdot\Big(-\boldsymbol{\nabla}\mu_A - q_A\,\boldsymbol{\nabla}\,V - m_A\,\mathbf{v}_A\,\boldsymbol{\nabla}\,\mathbf{v} + \mathbf{m}_A\,\boldsymbol{\nabla}\,\mathbf{B}\Big) = 0
\end{aligned}
$$

- **Thermostatics**

$$u = T\,s - P + \sum_A \Big(\mu_A + q_A\,V - \mathbf{m}_A \cdot \mathbf{B}\Big)\,n_A$$

- **Reversible thermodynamics**

$$\mathbf{j}_u = T\,\mathbf{j}_s + \sum_A \Big(\mu_A + q_A\,V - \mathbf{m}_A \cdot \mathbf{B}\Big)\,\mathbf{j}_A$$

- **Irreversible thermodynamics**

$$\rho_s = \frac{1}{T}\Bigg\{\sum_a \omega_a\,\mathcal{A}_a + \sum_A \boldsymbol{\Omega}_A \cdot \Big(\mathbf{m}_A \times \mathbf{B}\Big) + \mathbf{j}_s \cdot \left(-\,\boldsymbol{\nabla}\,T\right)$$
$$+ \sum_A \mathbf{j}_A \cdot \Big(-\,\boldsymbol{\nabla}\mu_A - q_A\,\boldsymbol{\nabla}\,V - m_A\,\mathbf{v}_A\,\boldsymbol{\nabla}\,\mathbf{v} + \mathbf{m}_A\,\boldsymbol{\nabla}\,\mathbf{B}\Big)\Bigg\}$$

- **Scalar part: Chemistry**
- **Pseudo-vectorial part: Relaxation**
- **Vectorial part: Transport**

$$\rho_s = \frac{1}{T}\Bigg\{\sum_a \omega_a\,\mathcal{A}_a + \sum_A \mathbf{\Omega}_A \cdot \Big(\mathbf{m}_A \times \mathbf{B}\Big) + \mathbf{j}_s \cdot (-\,\boldsymbol{\nabla}\,T)$$

$$+ \sum_A \mathbf{j}_A \cdot \Big(-\,\boldsymbol{\nabla}\mu_A - q_A\,\boldsymbol{\nabla}\,V - m_A\,\mathbf{v}_A\,\boldsymbol{\nabla}\,\mathbf{v} + \mathbf{m}_A\,\boldsymbol{\nabla}\,\mathbf{B}\Big)\Bigg\}$$

- **Scalar part: Chemistry**
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$$\rho_s = \frac{1}{T}\left\{\sum_a \omega_a \mathcal{A}_a + \sum_A \boldsymbol{\Omega}_A \cdot \Big(\mathbf{m}_A \times \mathbf{B}\Big) + \mathbf{j}_s \cdot (-\boldsymbol{\nabla} T)\right.$$
$$\left. + \sum_A \mathbf{j}_A \cdot \Big(-\boldsymbol{\nabla}\mu_A - q_A \boldsymbol{\nabla} V - m_A \mathbf{v}_A \boldsymbol{\nabla} \mathbf{v} + \mathbf{m}_A \boldsymbol{\nabla} \mathbf{B}\Big)\right\}$$

$$\rho_s = \frac{1}{T}\left\{\sum_a \omega_a\,\mathcal{A}_a + \sum_A \boldsymbol{\Omega}_A\cdot\mathbf{T}_A + \sum_\alpha \mathbf{j}_\alpha\cdot\mathbf{F}_\alpha\right\} \geqslant 0$$

- **Scalar part: Chemistry**
  1. $$\sum_a \omega_a\,\mathcal{A}_a$$
- **Pseudo-vectorial part: Relaxation**
  1. $$\sum_A \boldsymbol{\Omega}_A\cdot(\mathbf{m}_A\times\mathbf{B})$$
- **Vectorial part: Transport**
  1. $$\mathbf{j}_s\cdot(-\boldsymbol{\nabla}\,T)$$
  2. $$\sum_A \mathbf{j}_A\cdot(-\boldsymbol{\nabla}\mu_A - q_A\boldsymbol{\nabla}\,V - m_A\mathbf{v}_A\boldsymbol{\nabla}\,\mathbf{v} + \mathbf{m}_A\boldsymbol{\nabla}\,\mathbf{B})$$

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- $\rho_s \geqslant 0 \Rightarrow$ **quadratic forms (near equilibrium):**

$$\rho_s = \frac{1}{T}\Big(\sum_{a,\,b} L_{ab}\,\mathcal{A}_a\,\mathcal{A}_b + \sum_{\alpha,\,\beta} \mathsf{L}_{\alpha\beta}\cdot\left(\mathbf{F}_\alpha \odot \mathbf{F}_\beta\right) + \sum_{A,\,B} \mathsf{L}_{AB}\cdot\left(\mathbf{T}_A \odot \mathbf{T}_B\right)\Big) \geqslant 0$$

- **Symmetries (Onsager reciprocity relations):**

$$L_{ab}\left(s, n_A, q, \mathbf{M}\right) = L_{ba}\left(s, n_A, q, -\mathbf{M}\right)$$

$$\mathsf{L}_{\alpha\beta}\left(s, n_A, q, \mathbf{M}\right) = \mathsf{L}_{\beta\alpha}\left(s, n_A, q, -\mathbf{M}\right)$$

$$\mathsf{L}_{AB}\left(s, n_A, q, \mathbf{M}\right) = \mathsf{L}_{BA}\left(s, n_A, q, -\mathbf{M}\right)$$

Linear phenomenological relations (Onsager)

- **Scalar linear relations (Chemistry):**

$$\omega_a = \sum_b L_{ab}\,\mathcal{A}_b$$

- **Pseudo-vectorial linear relations (Relaxation):**

$$\boldsymbol{\Omega}_A = \sum_B \mathsf{L}_{AB} \cdot (\mathbf{m}_B \times \mathbf{B})$$

- **Vectorial linear relations (Transport):**

$$\begin{cases} \mathbf{j}_s = \mathsf{L}_{ss} \cdot (-\boldsymbol{\nabla}\, T) + \sum_B \mathsf{L}_{sB} \cdot (-\boldsymbol{\nabla}\mu_B - \; q_B\,\boldsymbol{\nabla}\, V - \; m_B\,\mathbf{v}_B\,\boldsymbol{\nabla}\,\mathbf{v} + \mathbf{m}_B\,\boldsymbol{\nabla}\,\mathbf{B}) \\ \mathbf{j}_A = \mathsf{L}_{As} \cdot (-\boldsymbol{\nabla}\, T) + \sum_B \mathsf{L}_{AB} \cdot (-\boldsymbol{\nabla}\mu_B - \; q_B\,\boldsymbol{\nabla}\, V - \; m_B\,\mathbf{v}_B\,\boldsymbol{\nabla}\,\mathbf{v} + \mathbf{m}_B\,\boldsymbol{\nabla}\,\mathbf{B}) \end{cases}$$

- **Time evolution equation:**

$$n_A \, \dot{\mathbf{m}}_A = \gamma_A \, n_A \, (\mathbf{m}_A \times \mathbf{B}) - \mathbf{m}_A \times \boldsymbol{\Omega}_A - (\mathbf{j}_A \cdot \boldsymbol{\nabla}) \, \mathbf{m}_A$$

$$+ \sum_B \gamma_{AB} \, n_A \, (\mathbf{m}_A \times n_B \, \mathbf{m}_B) - \sum_a \nu_{aA} \, \omega_a \, \mathbf{m}_A$$

- **Relaxation:**

$$\boldsymbol{\Omega}_A = \sum_B \mathsf{L}_{AB} \cdot (\mathbf{m}_B \times \mathbf{B})$$

- **Transport:**

$$\mathbf{j}_A = \mathsf{L}_{As} \cdot (-\boldsymbol{\nabla} \, T) + \sum_B \mathsf{L}_{AB} \cdot (-\boldsymbol{\nabla} \mu_B - q_B \, \boldsymbol{\nabla} \, V - m_B \, \mathbf{v}_B \, \boldsymbol{\nabla} \, \mathbf{v} + \mathbf{m}_B \, \boldsymbol{\nabla} \, \mathbf{B})$$

- **Magnetisation current tensor:**

$$\mathsf{j}_M = \sum_A \mathbf{m}_A \odot \mathbf{j}_A \, .$$

- **Time evolution of magnetic dipoles of core electrons** d

$$n_d\,\dot{\mathbf{m}}_d = \gamma_d\,n_d\,\mathbf{m}_d \times \mathbf{B} - \,\mathbf{m}_d \times \boldsymbol{\Omega}_d$$

- **Relaxation**

$$\boldsymbol{\Omega}_d = L_{dd}\,\left(\mathbf{m}_d \times \mathbf{B}\right)$$

Relaxation of magnetic dipoles

- $\dot{\mathbf{m}}_d = \gamma_d\,\mathbf{m}_d \times \mathbf{B} - \,\beta_d\,\mathbf{m}_d \times \left(\mathbf{m}_d \times \mathbf{B}\right)$

- **Magnetisation waves**

$$\mathbf{B} = \mathbf{B}^{\,\text{ext}} + A\,\boldsymbol{\nabla}^2\left(n_d\,\mathbf{m}_d\right)$$

Electrically driven transport of magnetic dipoles

- **Electrically driven transport of conduction electrons** s

$$\mathbf{j}_s = -\frac{\sigma_{s\|}}{q_s}\,\boldsymbol{\nabla} V - \frac{\sigma_{s\perp}}{q_s}\left(\frac{\mathbf{B}}{B}\times\boldsymbol{\nabla} V\right)$$

Time evolution of magnetic dipoles $\left(t_{\textbf{transport}} \gg t_{\textbf{relaxation}}\right)$

- $\dot{\mathbf{m}}_s = \frac{\sigma_{s\|}}{q_s\,n_s}\,\boldsymbol{\nabla} V\cdot\boldsymbol{\nabla}\,\mathbf{m}_s + \frac{\sigma_{s\perp}}{q_s\,n_s}\left(\frac{\mathbf{B}}{B}\times\boldsymbol{\nabla} V\right)\cdot\boldsymbol{\nabla}\,\mathbf{m}_s$
  $+\,\gamma_{sd}\left(\mathbf{m}_s\times n_d\,\mathbf{m}_d\right)$

- **Magnetisation current**

$$\mathrm{j}_M = -\frac{\sigma_{s\|}}{q_s}\,\mathbf{m}_s\odot\boldsymbol{\nabla} V - \frac{\sigma_{s\perp}}{q_s}\,\mathbf{m}_s\odot\left(\frac{\mathbf{B}}{B}\times\boldsymbol{\nabla} V\right)$$

- **Thermally driven transport of conduction electrons** s

$$\mathbf{j}_s = -\frac{\sigma_{s\parallel}\,\varepsilon_{s\parallel}}{q_s}\,\nabla T - \frac{\sigma_{s\parallel}\,\varepsilon_{s\perp} + \sigma_{s\perp}\,\varepsilon_{s\parallel}}{q_s}\left(\frac{\mathbf{B}}{B}\times\nabla T\right)$$

Time evolution of magnetic dipoles ($t_{\text{transport}} \gg t_{\text{relaxation}}$)

- $\dot{\mathbf{m}}_s = \frac{\sigma_{s\parallel}\,\varepsilon_{s\parallel}}{q_s\,n_s}\,\nabla T\cdot\nabla\,\mathbf{m}_s + \frac{\sigma_{s\parallel}\,\varepsilon_{s\perp}+\sigma_{s\perp}\,\varepsilon_{s\parallel}}{q_s\,n_s}\left(\frac{\mathbf{B}}{B}\times\nabla T\right)\cdot\nabla\,\mathbf{m}_s$
  $+\,\gamma_{sd}\left(\mathbf{m}_s\times n_d\,\mathbf{m}_d\right)$

- **Magnetisation current**

$$\mathrm{j}_{\mathrm{M}} = -\frac{\sigma_{s\parallel}\,\varepsilon_{s\parallel}}{q_s}\,\mathbf{m}_s\odot\nabla T - \frac{\sigma_{s\parallel}\,\varepsilon_{s\perp} + \sigma_{s\perp}\,\varepsilon_{B\parallel}}{q_s}\,\mathbf{m}_s\odot\left(\frac{\mathbf{B}}{B}\times\nabla T\right)$$

- **Magnetic induction field**

$$\mathbf{B} = \mathbf{B}^{\,\text{ext}} + A\,\boldsymbol{\nabla}^2\left(n_d\,\mathbf{m}_d\right) + \mathbf{B}^{\,\text{th}} \ ,$$

- **Thermomagnetic effect (i.e. $\mathbf{j}_d = \mathbf{0}$)**

$$\mathbf{B}^{\,\text{th}} = -\,\varepsilon_{\mathbf{M}}\ \left(\mathbf{j}_{\mathbf{M}}^{-1} \times \boldsymbol{\nabla}\,T\right) \ ,$$

where $\qquad \mathbf{j}_{\mathbf{M}} = \boldsymbol{\nabla} \times \left(n_d\,\mathbf{m}_d\right)$

Thermally driven magnetisation waves

- $$\dot{\mathbf{m}}_d = \gamma_d\,\mathbf{m}_d \times \Big(\mathbf{B}^{\,\text{ext}} + A\,\boldsymbol{\nabla}^2\left(n_d\,\mathbf{m}_d\right) - \varepsilon_{\mathbf{M}}\ \left(\mathbf{j}_{\mathbf{M}}^{-1} \times \boldsymbol{\nabla}\,T\right)\Big) - \beta_d\,\mathbf{m}_d \times \Big(\mathbf{m}_d \times \Big(\mathbf{B}^{\,\text{ext}} + A\,\boldsymbol{\nabla}^2\left(n_d\,\mathbf{m}_d\right) - \varepsilon_{\mathbf{M}}\ \left(\mathbf{j}_{\mathbf{M}}^{-1} \times \boldsymbol{\nabla}\,T\right)\Big)\Big)$$

Summary

- Thermodynamics of continuous medium with magnetisation:
  1. **Thermostatics**
  2. **Reversible thermodynamics**
  3. **Irreversible thermodynamics**
- Irreversible linear phenomenological relations:
  1. **Scalar: Chemistry**
  2. **Pseudo-vectorial: Relaxation**
  3. **Vectorial: Transport**
- Applications for spintronics and spin-caloritronics
  1. **Relaxation of magnetic dipoles**
  2. **Electrically and thermally driven transport of mag. dip.**
  3. **Thermally driven magnetisation waves**

THANK YOU

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