Magnetisation dynamics

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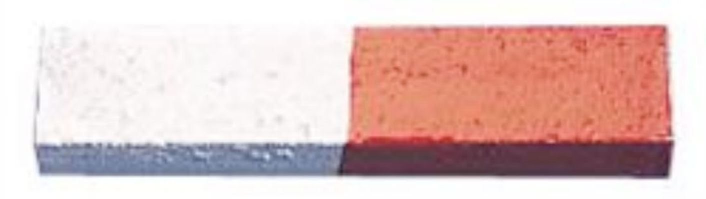
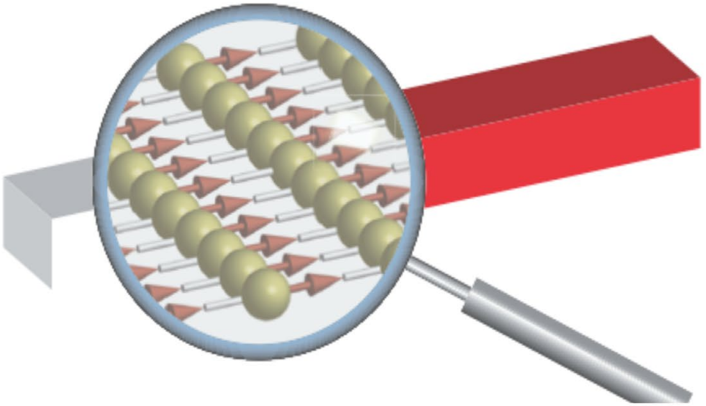
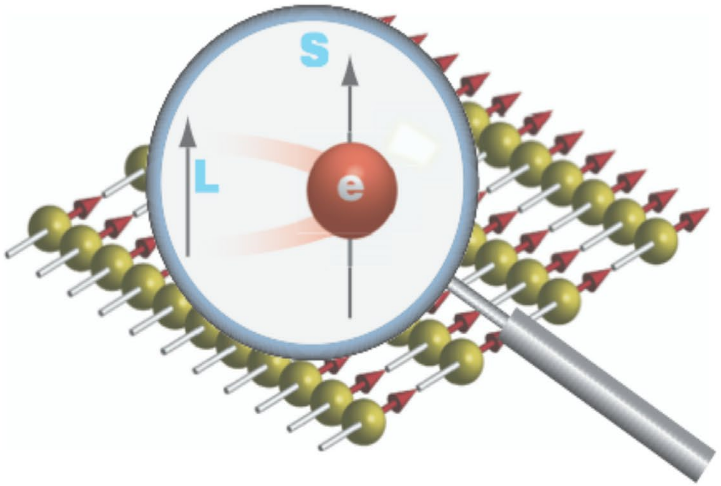
Spin dynamics



Micromagnetic simulations
Magnetization as $\mathbf{m}(\mathbf{r})$

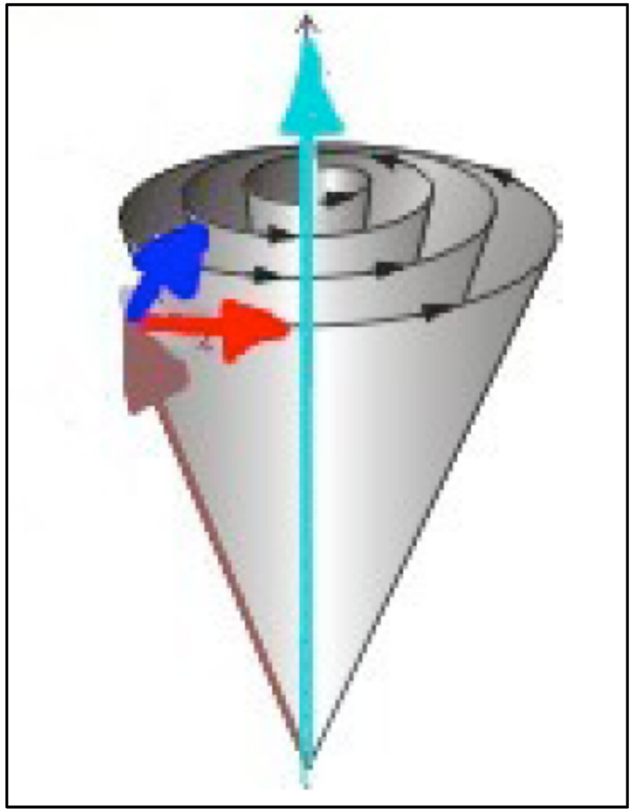


Atomistic spin dynamics
Discrete moments $\mathbf{m}_i$



Time dependent DFT
Magnetization as $\mathbf{m}(\mathbf{r})$

Separate fast variables (electrons) and slow (atomic spins) and the EOM together with Landau-Lifshitz damping term gives:



$$\boxed{\frac{\partial \mathbf{m}_i}{\partial t} = -\gamma \mathbf{m}_i \times \mathbf{B}_i - \gamma \frac{\alpha}{m} [\mathbf{m}_i \times [\mathbf{m}_i \times \mathbf{B}_i]]}$$

Precession Damping

The effective field B is given by

$$\boxed{\mathbf{B}_i = -\frac{\partial \mathscr{H}}{\partial \mathbf{m}_i}}$$

Antropov et al. PRB **54**, 1019 (1996)

Spin dynamics

$$\boxed{\mathbf{B}_i = -\frac{\partial \mathscr{H}}{\partial \mathbf{m}_i}}$$

Heisenberg exchange

$$\mathscr{H}_{\text{iex}} = -\frac{1}{2}\sum_{i \neq j} J_{ij}\mathbf{m}_i \cdot \mathbf{m}_j$$

dipole-dipole

$$\mathscr{H}_{\text{dd}} = -\frac{1}{2}\sum_{i \neq j} Q_{ij}^{\mu\nu} m_i^{\mu} m_j^{\nu}$$

Magnetocrystalline anisotropy

$$\mathscr{H}_{\text{ma}} = K\sum_{i}(\mathbf{m}_i \cdot \mathbf{e}_K)^2$$

Dzyaloshinskii-Moriya

$$\mathcal{H}_{DM} = \sum_{i,j}\mathbf{D}_{ij}\left(\mathbf{m}_i \times \mathbf{m}_j\right)$$

Zeeman term

$$\mathscr{H}_{\text{ext}} = -\mathbf{B}_{\text{ext}} \cdot \sum_{i}\mathbf{m}_i$$

Spin dynamics

Langevin dynamics:

Stochastic contribution to the effective field

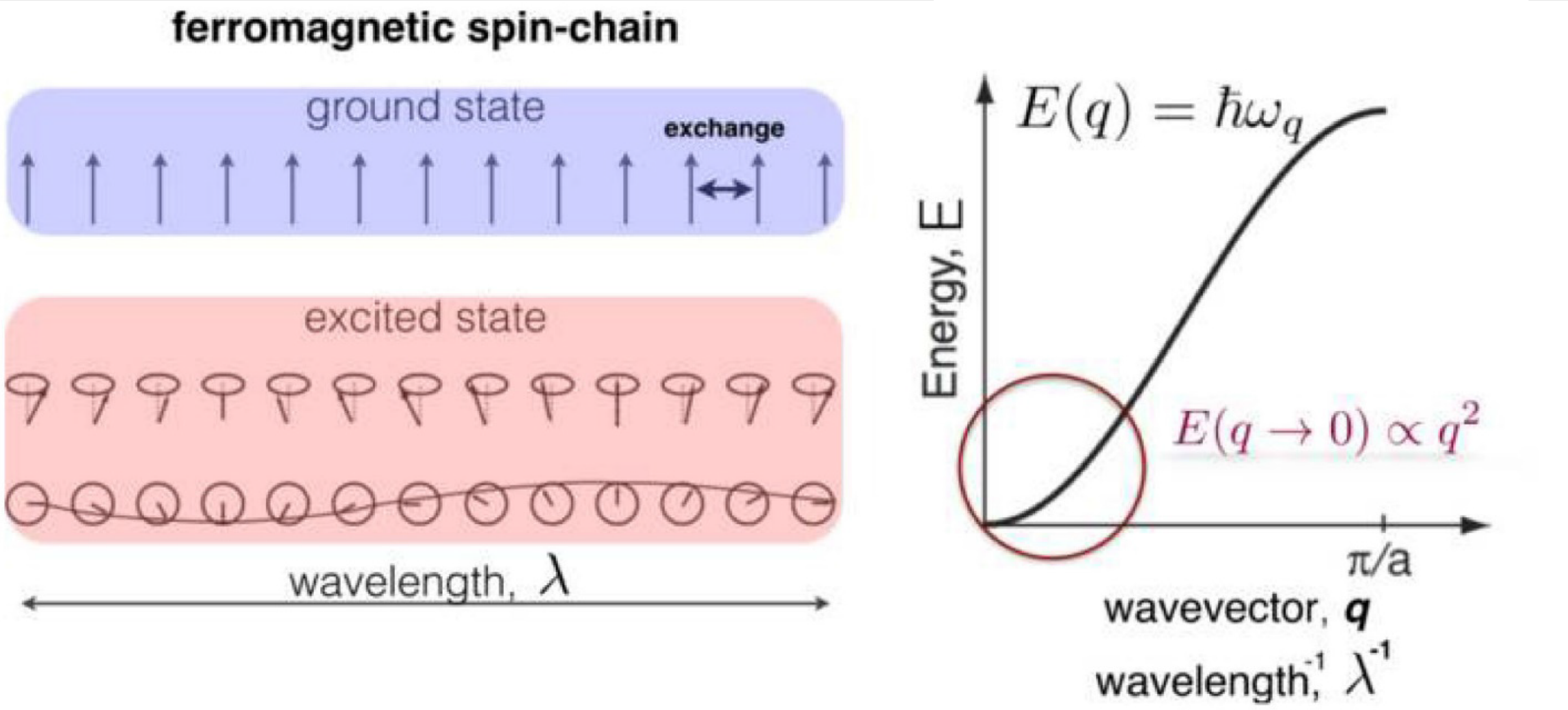
$$\langle b_{i,\mu}(t)\rangle = 0, \qquad D_{SLLG} = \frac{\alpha}{1+\alpha^2}\frac{k_B T}{\gamma m}$$

$$\langle b_{i,\mu}(t) b_{j,\nu}(s)\rangle = 2D\delta_{\mu\nu}\delta_{ij}\delta(t-s)$$

Gaussian distribution
One thermal reservoir

$$\boxed{\frac{\partial \mathbf{m}_i}{\partial t} = -\gamma[\mathbf{m}_i \times [\mathbf{B}_i + \mathbf{b}_i(t)]] - \gamma\frac{\alpha}{m}[\mathbf{m}_i \times [\mathbf{m}_i \times [\mathbf{B}_i + \mathbf{b}_i(t)]]]}$$

Magnons



ferromagnetic spin-chain
ground state
exchange
excited state
wavelength, λ
$E(q) = \hbar\omega_q$
Energy, E
$E(q \to 0) \propto q^2$
π/a
wavevector, q
wavelength^{-1}, λ^{-1}

Workflow, similar to MD simulations

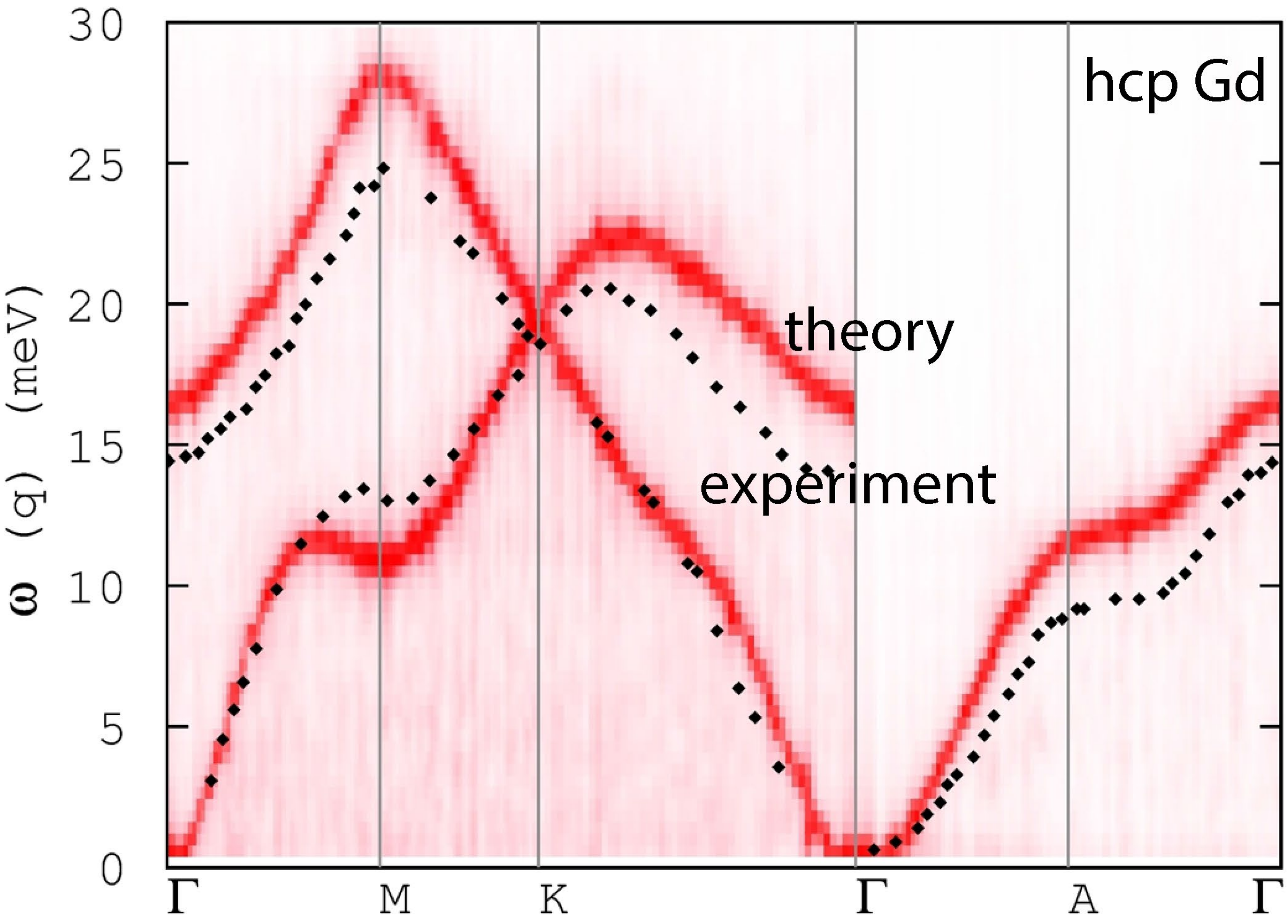
- For given temperature equilibrate
- Sample a property, e.g. spin-spin correlations

Spin-correlation function and dynamic structure factor

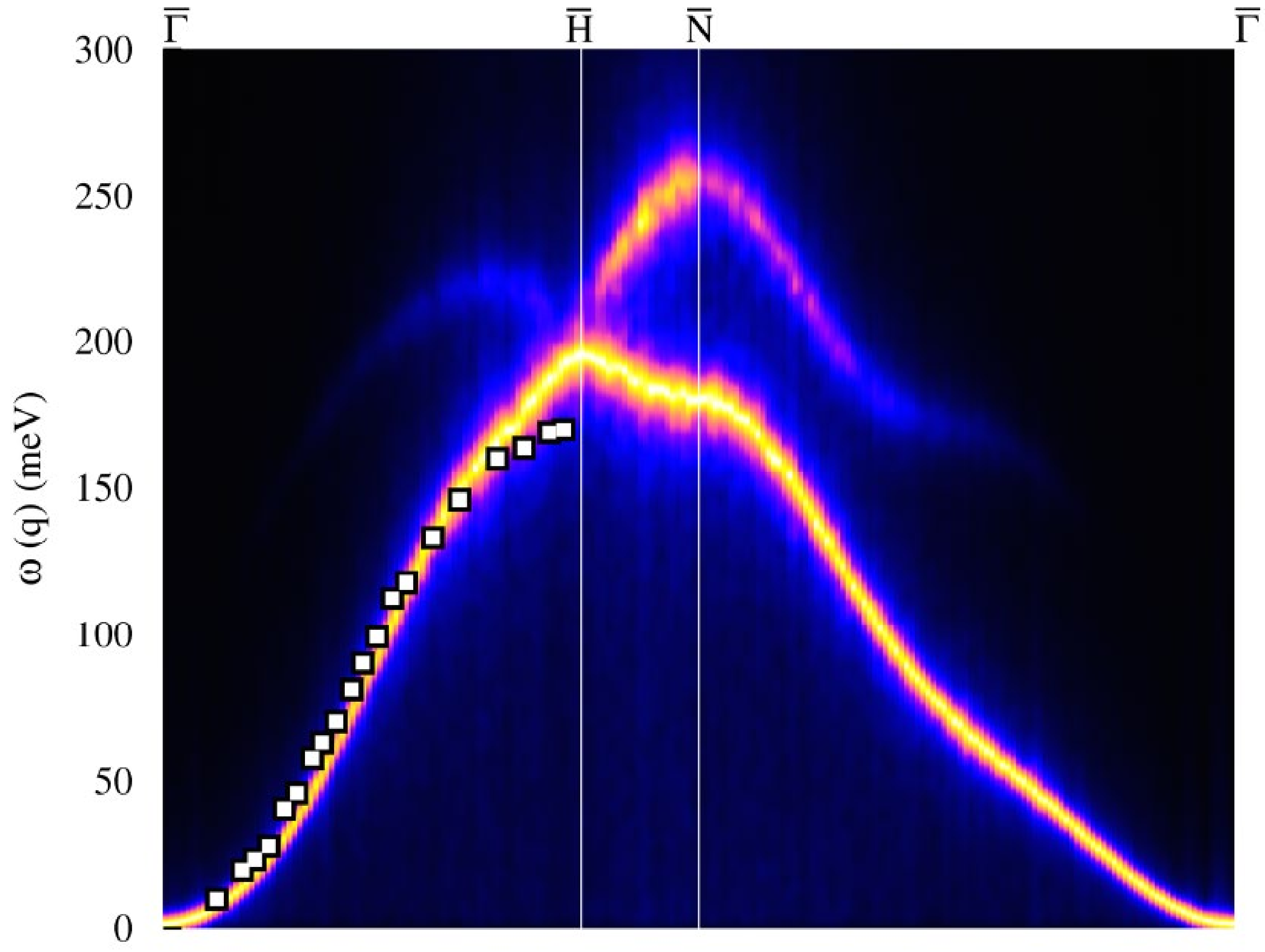
$$C^k(\mathbf{r}-\mathbf{r}',t) = \langle m^k_{\mathbf{r}}(t) m^k_{\mathbf{r}'}(0)\rangle - \langle m^k_{\mathbf{r}}(t)\rangle\langle m^k_{\mathbf{r}'}(0)\rangle,$$

$$S^k(\mathbf{q},\omega) = \frac{1}{N\sqrt{2\pi}} \sum_{\mathbf{r},\mathbf{r}'} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \int_{-\infty}^{+\infty} e^{i\omega t} C^k(\mathbf{r}-\mathbf{r}',t)dt,$$

Magnons of Gd



Magnons of 2 ML Fe on W (110)



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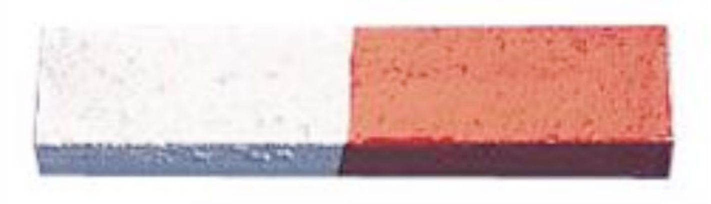
Spin dynamics



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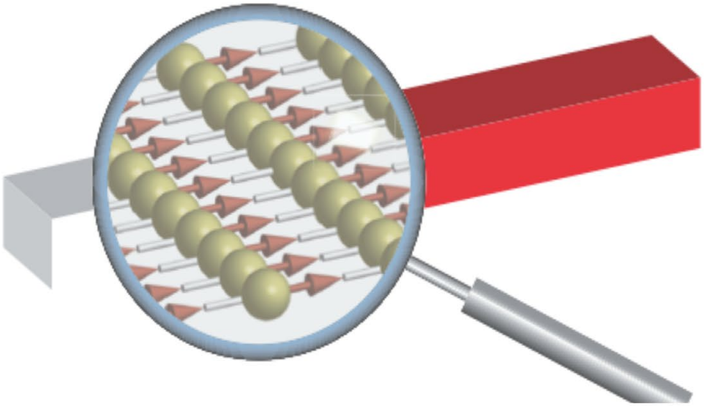

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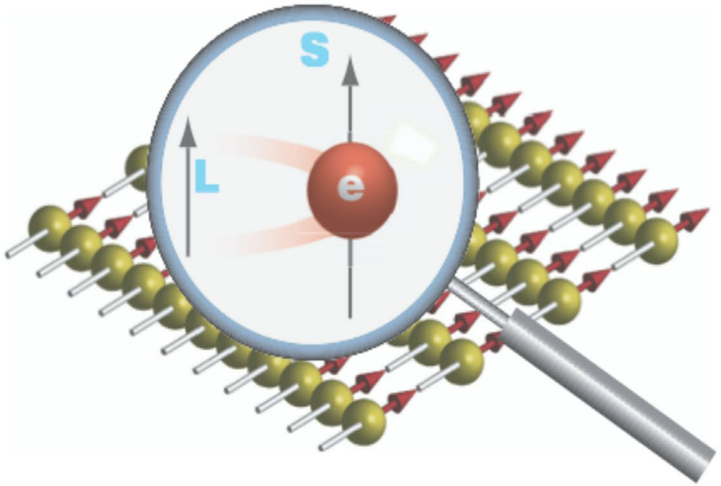
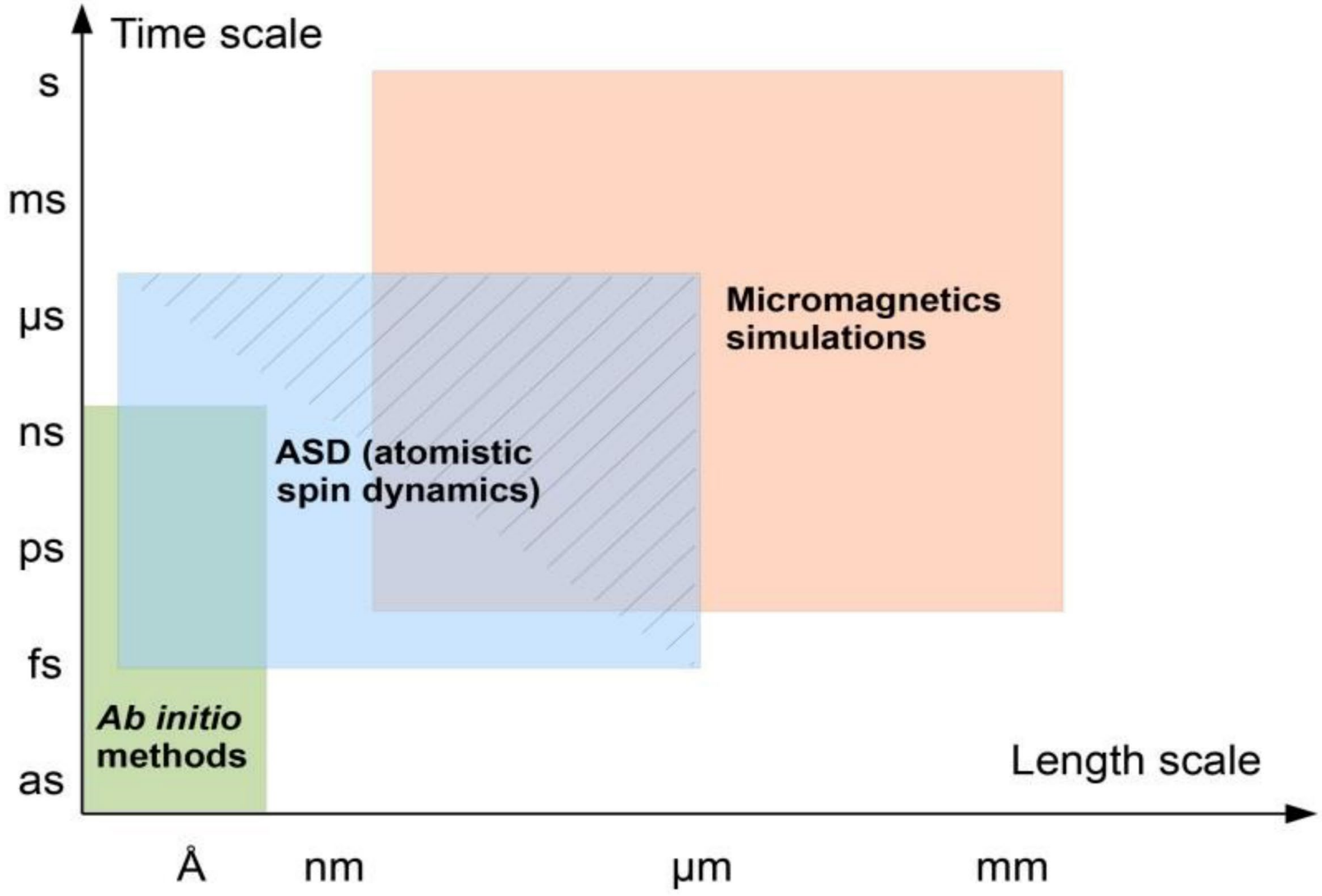


Time dependent DFT
Magnetization as $\mathbf{m}(\mathbf{r})$

Multiscale simulations



LLG equation for spin dynamics

Atomistic

$$\frac{d\vec{s}_i}{dt} = -\gamma \vec{s}_i \times \vec{H}_i - \alpha \vec{s}_i \times \left(\vec{s}_i \times \vec{H}_i\right)$$

$$\vec{H}_i^{\text{exc}} = \sum_{j \neq i} J_{ij} \vec{s}_j$$

$$\vec{H}_i^{\text{D}} = \sum_{j \neq i} \vec{D}_{ij} \times \vec{s}_j$$

$$\vec{H}_i^{\text{ani}} = Ka \cdot \vec{s}_i$$

$$\vec{H}^e = \mu \vec{H}^{\text{app}}$$

$$\vec{H}^i = \vec{H}_i^{\text{exc}} + \vec{H}_i^D + \vec{H}_i^{\text{ani}} + \vec{H}^e$$

Micromagnetics

$$\frac{\partial \vec{m}}{\partial t} = -\gamma \vec{m} \times \vec{H} - \alpha \vec{m} \times \left(\vec{m} \times \vec{H}\right)$$

$$\vec{H}^{\text{exc}} = Ae \cdot \nabla\nabla \vec{m}$$

$$\vec{H}^D = \nabla \cdot (De \times \vec{m})$$

$$\vec{H}^{\text{ani}} = Ka \cdot \vec{m}$$

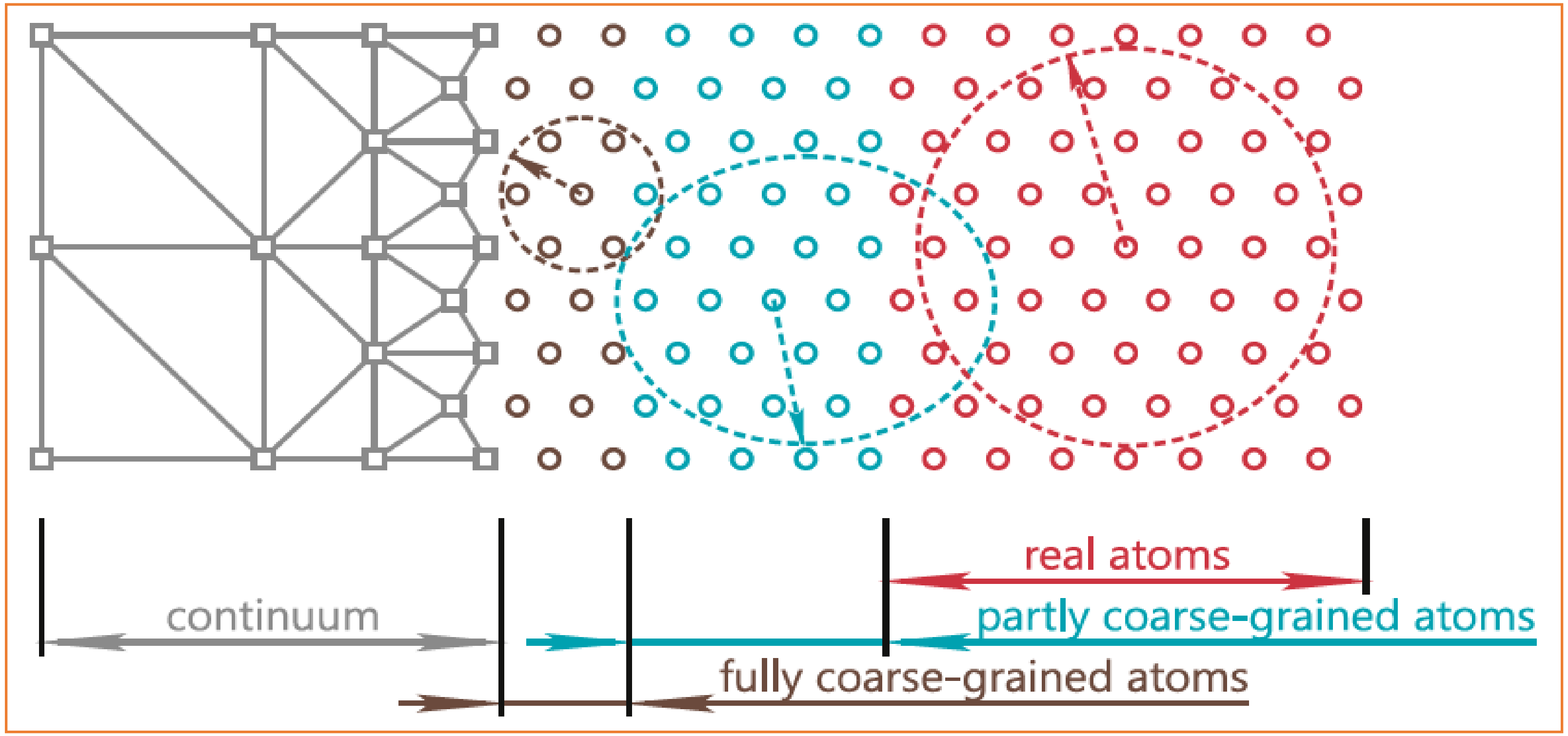
$$\vec{H}^e = \mu \vec{H}^{\text{app}}$$

$$\vec{H} = \vec{H}^{\text{exc}} + \vec{H}^D + \vec{H}^{\text{ani}} + \vec{H}^e.$$

$$Ae = \frac{1}{2} \sum_{j \neq i} J_{ij} \vec{r}_{ij} \vec{r}_{ij}$$

$$De = \sum_{j \neq i} \vec{r}_{ij} \vec{D}_{ij}$$

Multiscale Mechanism



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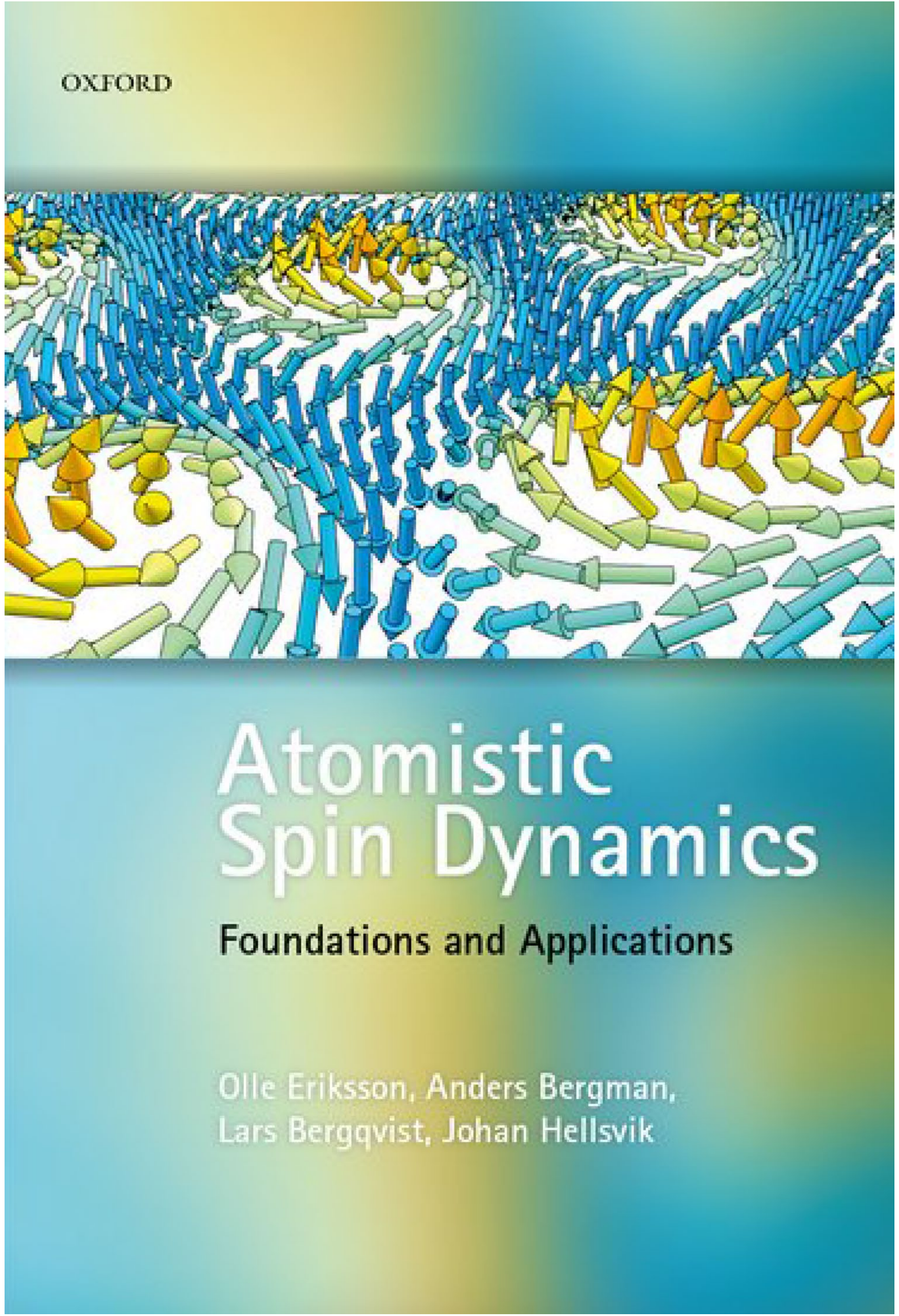
E.Mendez, M.Pouletkov, G.Kreiss, O.Eriksson and M.Pereiro, Physical Review Research **2**, 013092 (2020)
N.Salehi, O.Eriksson and M.Pereiro, https://arxiv.org/pdf/2504.14019


OXFORD
Atomistic
Spin Dynamics
Foundations and Applications
Olle Eriksson, Anders Bergman,
Lars Bergqvist, Johan Hellsvik