Inter-atomic exchange interaction

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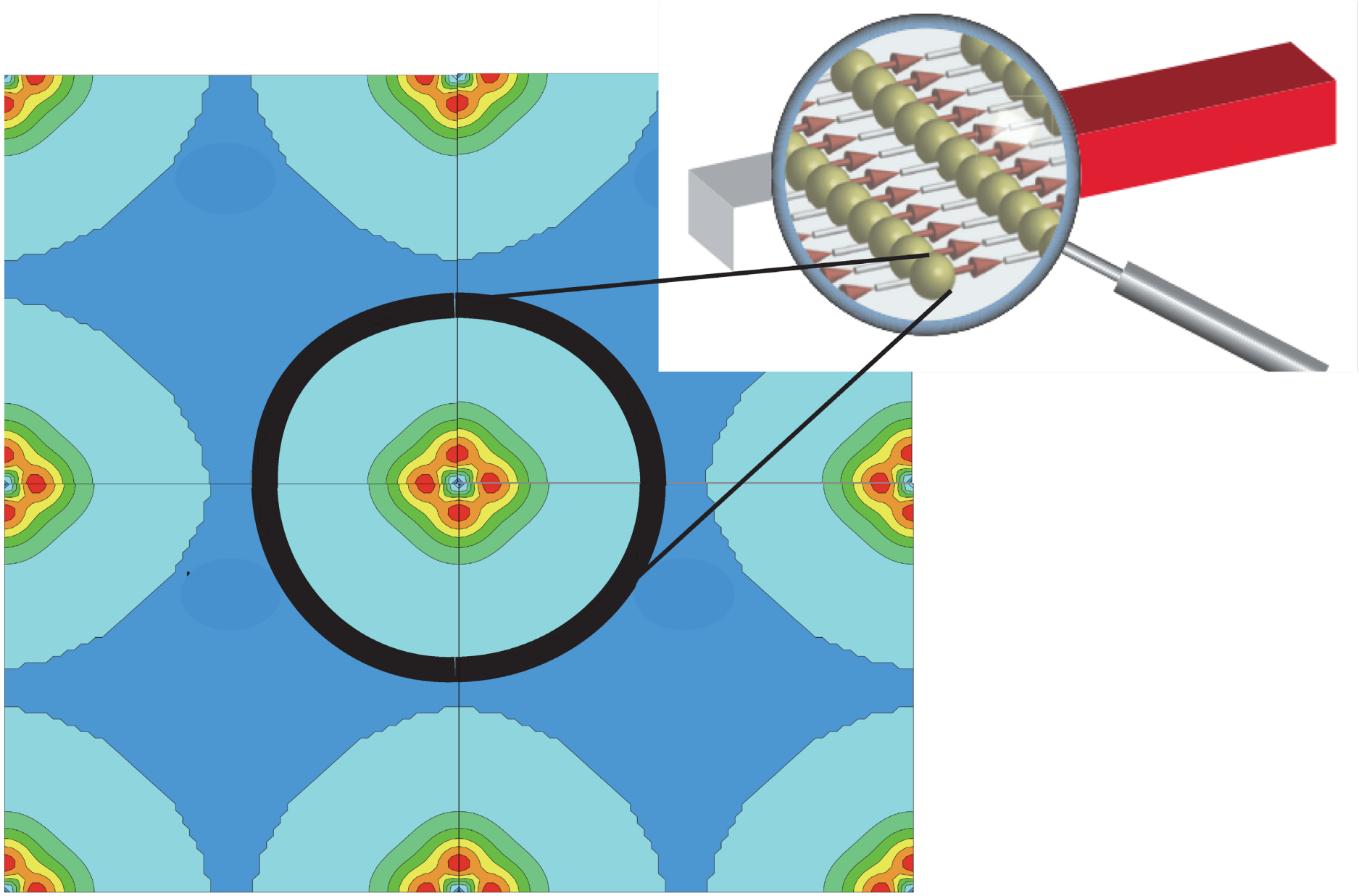
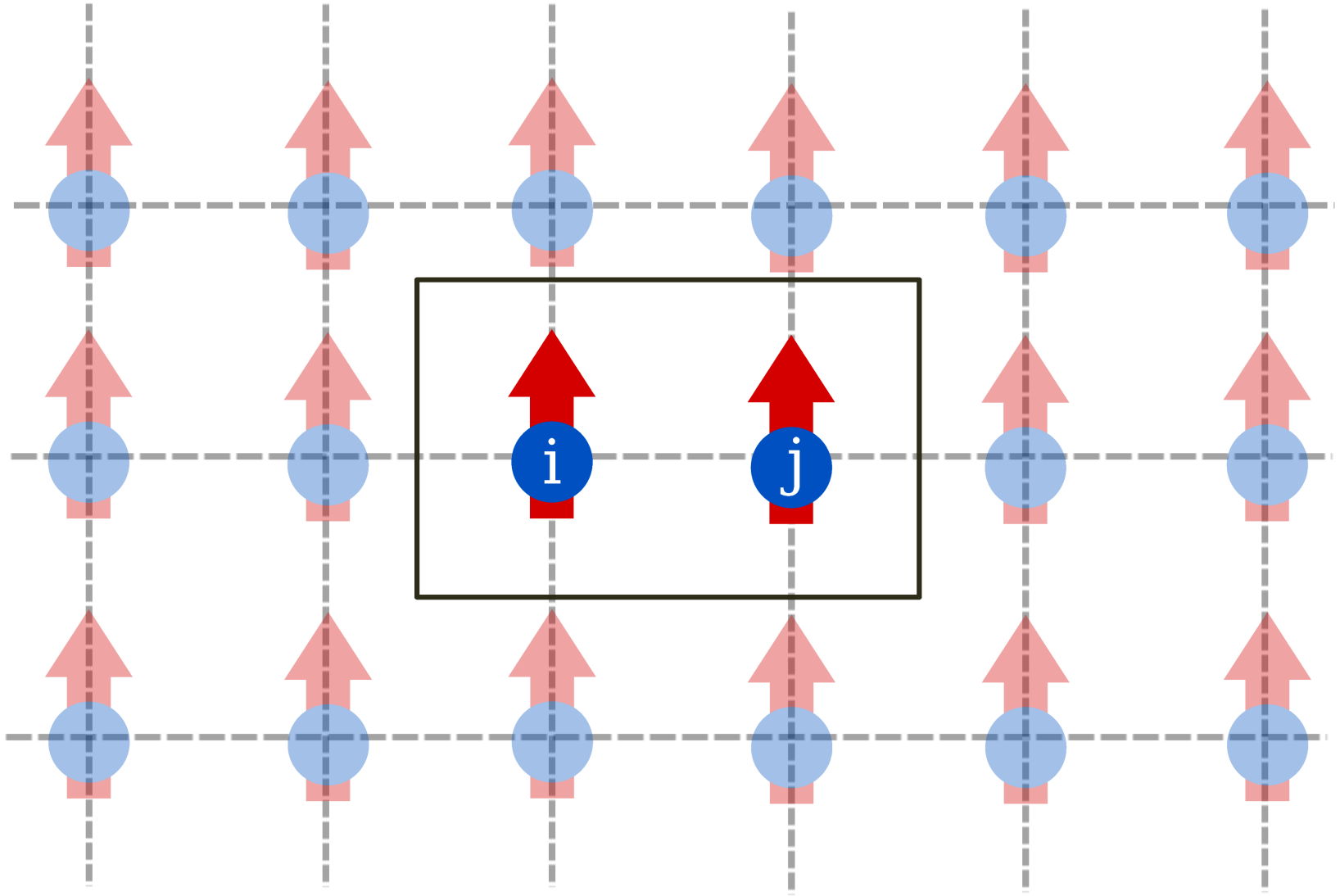
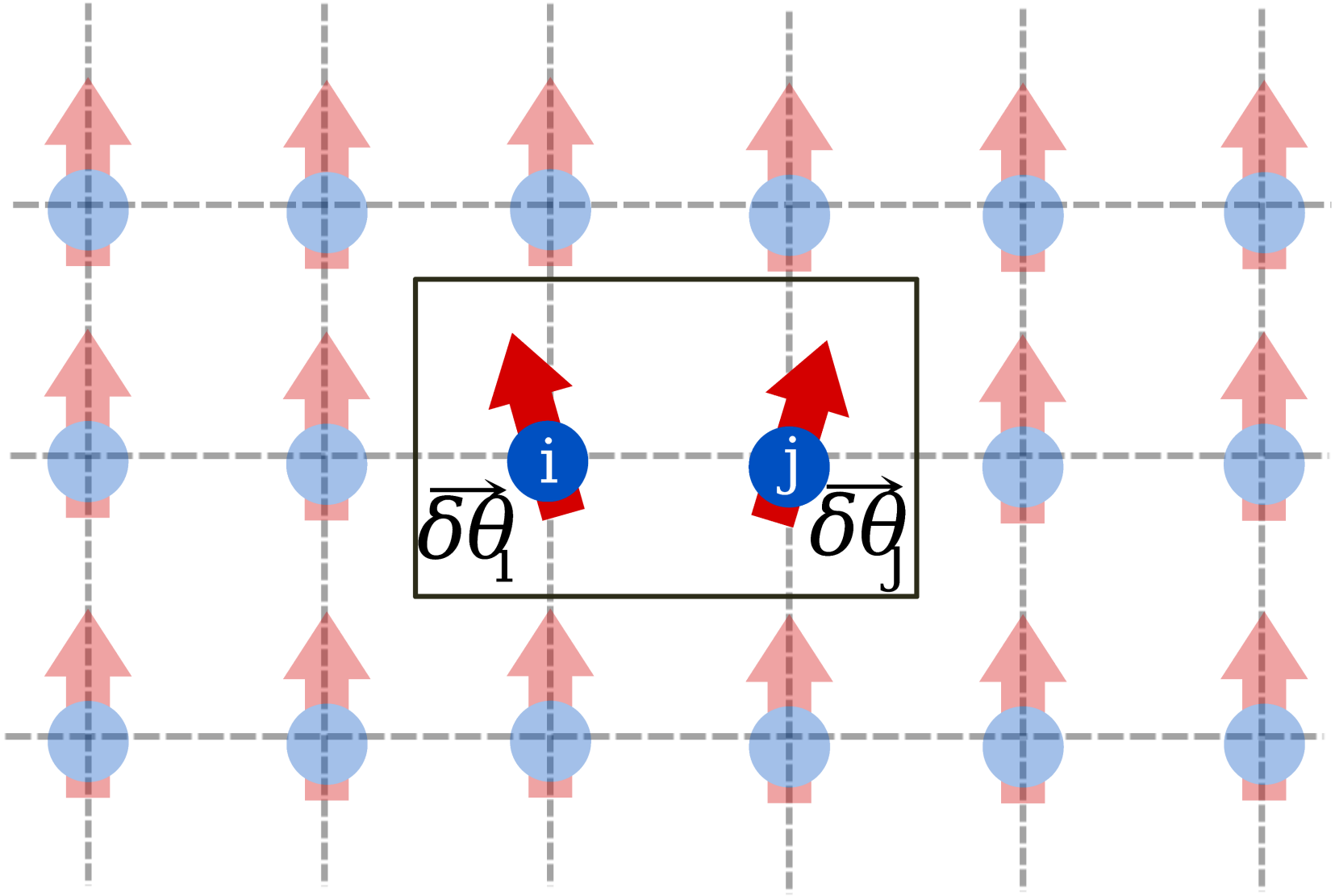
Atomistic spin dynamics



Inter-atomic exchange



Inter-atomic exchange



Heisenberg Hamiltonian

$$\Delta E = -J_{ij}\, \mathbf{m}_i\, \mathbf{m}_j$$

$$H = -J_{ij}\, \mathbf{m}_i\, \mathbf{m}_j$$

Some useful expressions

O.K.Andersen et al., PURE AND APPLIED CHEMISTRY 52(1), pp.93-118 (1980)
Green's Functions in Quantum Physics, EN Economou

Energy expression:

$$E = \int_{-\infty}^{\infty} d\varepsilon\, \varepsilon f(\varepsilon) n(\varepsilon)$$

Grand canonical potential:

$$\Omega = E - TS - \mu N$$

Green function:

$$G(z) = (z - H)^{-1} \qquad G(z) = \sum_{\mu} \frac{|\varphi_\mu\rangle\langle\varphi_\mu|}{z - \varepsilon_\mu}$$

$$G(z) = \sum_{ij\mu} \frac{|\phi_i\rangle\langle\phi_i|\varphi_\mu\rangle\langle\varphi_\mu|\phi_j\rangle\langle\phi_j|}{z - \varepsilon_\mu} = \sum_{ij} |\phi_i\rangle G_{ij}(z) \langle\phi_j|$$

DFT-expressions of J_{ij}

A. Szilva et al. REVIEWS OF MODERN PHYSICS, VOLUME 95, 035004-1 (2023)

Energy cost of rotating one spin

$$\Omega' = \Omega + \delta\Omega_i^{\mathrm{one}}$$

Energy cost of rotating two spins

$$\Omega'' = \Omega + \delta\Omega_i^{\mathrm{one}} + \delta\Omega_j^{\mathrm{one}} + \delta\Omega_{ij}^{\mathrm{two}}$$

Part corresponding to Heisenberg exchange

DFT-expressions of J_{ij}

A. Szilva et al. REVIEWS OF MODERN PHYSICS, VOLUME 95, 035004-1 (2023)

DOS $$n(\varepsilon) = -\frac{1}{\pi}\Im \mathrm{Tr}_{L\sigma} G^{+}(\varepsilon) \qquad N = -\frac{1}{\pi}\Im \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \mathrm{Tr}_{L\sigma} G^{+}(\varepsilon)$$

$$\Omega = \int_{-\infty}^{\varepsilon_F} d\varepsilon\, \varepsilon n(\varepsilon) - \varepsilon_F N = -\int_{-\infty}^{\varepsilon_F} d\varepsilon N(\varepsilon)$$

$$G = -\frac{\partial \ln G}{\partial \varepsilon} \longrightarrow N = -\frac{1}{\pi}\Im \mathrm{Tr}_{iL\sigma}(-\ln G)$$

DFT-expressions of J_{ij}

A. Szilva et al. REVIEWS OF MODERN PHYSICS, VOLUME 95, 035004-1 (2023)

Dyson eqn. $$G' = G + G\,\delta V\,G'$$

Rotating one spin $$\delta V = -\sum_i \delta\vec{B}_i \cdot \vec{\sigma} = -\sum_i B_i \delta\vec{e}_i \cdot \vec{\sigma}$$

$$\delta N = -\frac{1}{\pi}\Im \mathrm{Tr}_{iL\sigma} \ln\left(1 - G\delta V\right) = \frac{1}{\pi}\Im \mathrm{Tr}_{iL\sigma} \sum_{k=1}^{\infty} \frac{(\delta V G)^k}{k}$$

Part of Grand canonical potential when rotating two spins

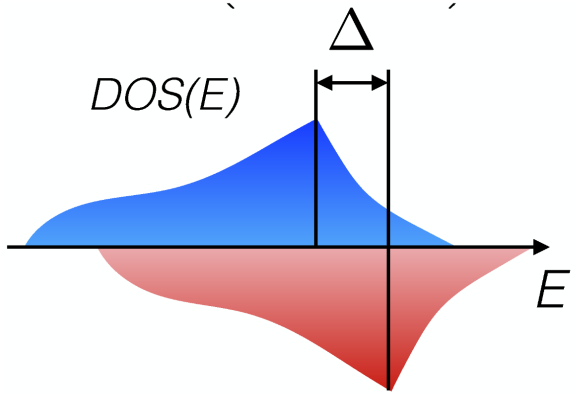
$$-\frac{1}{2\pi}\sum_{(i,j)} \int \Im \mathrm{Tr}_{L\sigma} \delta\vec{e}_i \cdot \vec{\sigma} B_i G_{ij} \delta\vec{e}_j \cdot \vec{\sigma} B_j G_{ji} d\varepsilon$$

Expansion of the Hamiltonian in $\delta\vec{\theta}_i$ and $\delta\vec{\theta}_j$ gives

$$J_{ij} = \frac{-1}{4\pi}\int_{-\infty}^{E_F} \delta\epsilon \mathrm{Tr}_m \left[\Delta_i \cdot G_{ij}^{\uparrow}(\epsilon) \cdot \Delta_j \cdot G_{ij}^{\downarrow}(\epsilon)\right]$$

Local exchange field

$$\Delta_i = (\hat{H}_i^{\uparrow} - \hat{H}_i^{\downarrow})$$



Inter-site Greens function

$$G_{ij}^{\sigma} = \left\langle i \left| \hat{G}(z) \right| j \right\rangle = \left\langle i \left| \frac{1}{z - \hat{H}^{\sigma}} \right| j \right\rangle$$

Lichtenstein *et al* JMMM **67** 65 (1987),
Katsnelson *et al* PRB **61** 8906 (2000),
Kvashnin *et al* PRB **91** 125133 (2015)
A.Szilva et al. RMP 95, 035004 (2023)

hcp Gd

Ferromagnetic metal (T_C=292 K)