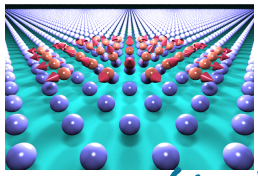

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Magnetism and magnetic interactions

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Outline

- **Introduction to magnetism:**

  single-particle magnetic hamiltonian; quantum origin; exchange interaction; atomic magnetism; band magnetism; DFT

- **Magnetic interactions I**

  local moments; magnetic force theorem, Liechstenstein formula and Heisenberg model; magnetic groundstates and spin spirals; disordered local moments; energies of spin spirals; competing interactions; magnetic multilayers

- **Magnetic interactions II**

  spin-orbit coupling; magnetic anisotropy, dipole-dipole interaction and magnetic stability; Dzyaloshinksii-Moriya interactions and chirality; chiral groundstates; symmetry; biquadratic and four-spin interactions

- **Beyond the groundstate**

  statistical physics; spin waves; dynamical magnetic susceptibility

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Introduction to magnetism

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Magnetic hamiltonian for a single particle

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- Schrödinger hamiltonian in Coulomb gauge: $\vec{A} = \vec{r} \times \vec{B}$

$$\mathcal{H} = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + V(\vec{r}) = \frac{p^2}{2m} - \frac{e}{2mc}(\vec{r} \times \vec{p}) \cdot \vec{B} + \frac{e^2}{8mc^2}(\vec{r} \times \vec{B})^2 + V(\vec{r})$$

- Magnetic part is paramagnetic plus diamagnetic

- Orbital magnetic moment:

$$\hbar\vec{L} = \vec{r} \times \vec{p} \implies -\frac{e}{2mc}(\vec{r} \times \vec{p}) \cdot \vec{B} = -\mu_{\mathrm{B}}\,\vec{L} \cdot \vec{B}\,, \quad \mu_{\mathrm{B}} = \frac{e\hbar}{2mc}$$

- Dirac hamiltonian gives also spin moment and spin-orbit coupling:

$$2\hbar\vec{S} = \hbar\vec{\sigma} \implies -\mu_{\mathrm{B}}\,\vec{\sigma} \cdot \vec{B} \qquad V_{\mathrm{soc}}(\vec{r}) \approx \frac{e\hbar^2}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\,\vec{L} \cdot \vec{\sigma} = \xi_{\mathrm{soc}}\,\vec{L} \cdot \vec{\sigma}$$

R.M. White, *Quantum Theory of Magnetism*, Springer (2007)

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Magnetism is a quantum effect

Bohr – van Leeuwen theorem: the equilibrium magnetization of a system described by classical physics is zero

- The dependence on the magnetic field can be removed from the classical expression for the magnetization by a simple change of integration variable

Magnetism comes from the interaction among the electrons: the classical magnetic dipole-dipole interaction is too weak to explain it

- The Pauli principle and the Coulomb repulsion among the electrons combine to give different energies to parallel and antiparallel spins

R.M. White, *Quantum Theory of Magnetism*, Springer (2007)

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Two electrons on one atom – I

- Schrödinger hamiltonian for two electrons:

$$\mathcal{H} = \frac{p_1^2}{2m} - \frac{Ze^2}{r_1} + \frac{p_2^2}{2m} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

- No spin dependence: why is energy spin dependent?

- Pauli exclusion:

$$\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \phi(\vec{r}_1, \vec{r}_2)\chi(s_1, s_2) = -\Psi(\vec{r}_2, s_2; \vec{r}_1, s_1)$$
$$\Longrightarrow \quad \phi(\vec{r}_1, \vec{r}_2) = \pm\phi(\vec{r}_2, \vec{r}_1) \;\; , \;\; \chi(s_1, s_2) = \mp\chi(s_2, s_1)$$

- Spinors:

$$\chi(s_1, s_2) = |\uparrow\uparrow\rangle \, , \; |\downarrow\downarrow\rangle \, , \; \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \, , \; \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

- Orbitals:

$$\phi(\vec{r}_1, \vec{r}_2) = |\, aa \,\rangle \, , \; |\, bb \,\rangle \, , \; \frac{|\, ab \,\rangle + |\, ba \,\rangle}{\sqrt{2}} \, , \; \frac{|\, ab \,\rangle - |\, ba \,\rangle}{\sqrt{2}} \;\; , \; |\, ab \,\rangle = \phi_a(\vec{r}_1)\phi_b(\vec{r}_2)$$

- Two electrons on the same orbital: spins antiparallel

R.M. White, *Quantum Theory of Magnetism*, Springer (2007)

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Two electrons on one atom – II

- Kinetic plus nuclear part: $\langle ab | \frac{p_1^2}{2m} - \frac{Ze^2}{r_1} + \frac{p_2^2}{2m} - \frac{Ze^2}{r_2} | ab \rangle = E_a + E_b$
- Coulomb repulsion part: $\langle ab | \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} | ab \rangle = U_{abab}$
- Triplet (degenerate): $E_a + E_b + \frac{U_{abab} - U_{abba}}{2}$
- Singlet block:

$$\begin{pmatrix} 2E_a + U_{aaaa} & U_{aabb} & \frac{U_{aaab}+U_{aaba}}{\sqrt{2}} \\ U_{bbaa} & 2E_b + U_{bbbb} & \frac{U_{bbab}+U_{bbba}}{\sqrt{2}} \\ \frac{U_{abaa}+U_{baaa}}{\sqrt{2}} & \frac{U_{abbb}+U_{babb}}{\sqrt{2}} & E_a + E_b + \frac{U_{abab}+U_{abba}}{2} \end{pmatrix}$$

- Coulomb repulsion lowers the energy of the triplet against the singlet
- Hamiltonian independent of spin + Pauli exclusion = spin-dependent energy

R.M. White, *Quantum Theory of Magnetism*, Springer (2007)

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Hund's rules – groundstate of an atom

- Russel-Saunders coupling scheme: $\vec{L} = \sum_{i=1}^{N_e} \vec{L}_i \,, \quad \vec{S} = \sum_{i=1}^{N_e} \vec{S}_i$
- First rule: maximize the total spin (think triplet vs singlet)
- Second rule: maximize the total orbital angular momentum (matrix elements of the Coulomb repulsion are smaller)
- Third rule: decide on the total angular momentum as to minimize the spin-orbit coupling energy, $E_{\mathrm{soc}} \approx \xi \vec{L} \cdot \vec{S}$
- In molecules and solids the orbitals can spread across several atoms, and the rules hold approximately for those electrons localized on a single atom
- How to describe the magnetism of delocalized electrons?

R.M. White, *Quantum Theory of Magnetism*, Springer (2007)

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Itinerant electrons – Stoner model

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- All the tricks in the book (spin up and spin down with same energy):

$$E_{\text{band}} = 2\sum_{\vec{k}}^{k\le k_{\text{F}}} \frac{\hbar^2 k^2}{2m} = 2\int^{\varepsilon_{\text{F}}} \mathrm{d}\varepsilon\, \varepsilon\, \frac{V}{(2\pi)^3} \int \mathrm{d}\vec{k}\, \delta(\varepsilon - \varepsilon_{\vec{k}}) = \int^{\varepsilon_{\text{F}}} \mathrm{d}\varepsilon\, \varepsilon \left(n_\uparrow(\varepsilon) + n_\downarrow(\varepsilon)\right)$$

- Stoner exchange energy: $E_{\text{total}} = E_{\text{band}} - \frac{I}{2}(N_\uparrow - N_\downarrow)^2 = E_{\text{band}} - \frac{I}{2}M^2$

- Splitting the non-magnetic state: $\delta M = \int^{\varepsilon_{\text{F}}} \mathrm{d}\varepsilon \left(n_\uparrow(\varepsilon - \Delta) - n_\downarrow(\varepsilon + \Delta)\right) \approx 2\, n(\varepsilon_{\text{F}})\, \Delta$

- Magnetic instability: $\delta E_{\text{total}} \approx \left(\frac{1}{n(\varepsilon_{\text{F}})} - I\right) \frac{(\delta M)^2}{2} < 0 \;\text{ if }\; n(\varepsilon_{\text{F}})\, I > 1$

- Contrast: localized electrons favour magnetism, itinerant ones not really

- How to describe the magnetism of real materials?

J. Kübler, *Theory of Itinerant Electron Magnetism*, OUP (2000)

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Density functional theory

- Kohn-Sham hamiltonian and Green function (cell-centered coordinates):

$$\mathcal{H}_i^{\mathrm{KS}}(\vec{r}) = -\nabla_{\vec{r}}^2 + 2\sum_j \int \mathrm{d}\vec{r}\,' \frac{n_j(\vec{r}\,') - Z_j\,\delta(\vec{r}\,')}{|\vec{r} - \vec{r}\,' + \vec{R}_{ij}|} + V_i^{\mathrm{xc}}(\vec{r}) + \left[\vec{B}_i^{\mathrm{xc}}(\vec{r}) + \vec{B}_i^{\mathrm{soc}}(\vec{r})\right] \cdot \vec{\sigma}$$

$$= -\nabla_{\vec{r}}^2 + V_i^{\mathrm{KS}}(\vec{r}) + \vec{B}_i^{\mathrm{KS}}(\vec{r}) \cdot \vec{\sigma} \quad , \quad \left[\varepsilon - \mathcal{H}_i^{\mathrm{KS}}(\vec{r})\right] G_{ij}(\vec{r}, \vec{r}\,'; \varepsilon) = \delta_{ij}\,\delta(\vec{r} - \vec{r}\,')$$

- Total energy: $E_{\mathrm{tot}} = \underbrace{E_{\mathrm{band}} - E_{\mathrm{dc}}}_{T_s} + E_{\mathrm{Coulomb}} + E_{\mathrm{xc}} + E_{\mathrm{ext}}$

- Each electron moves in mean-field created by all other electrons

- Complicated electron-electron interactions approximated by xc functional

- Structure similar to Stoner model – when should DFT perform well?

R.M. Martin, *Electronic Structure – Basic Theory and Practical Methods*, CUP (2004)

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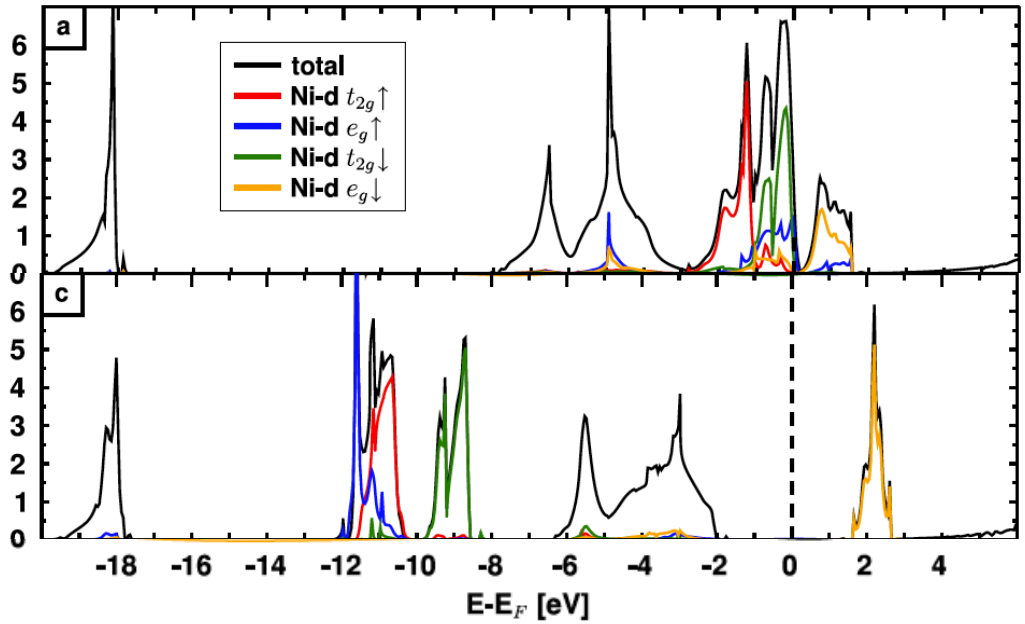
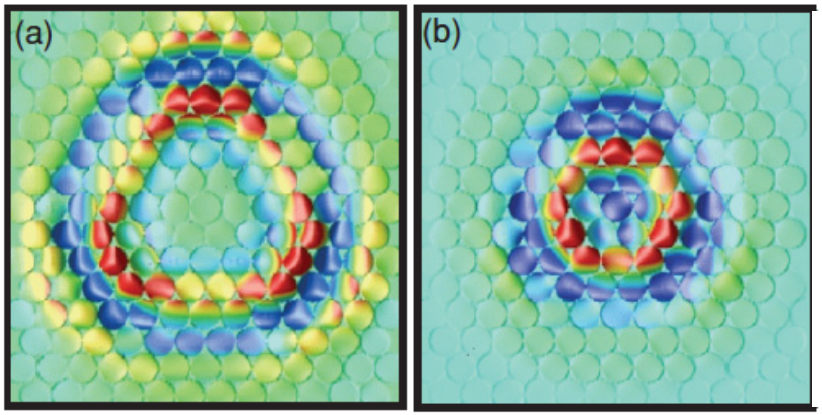
Examples of DFT+KKR calculations

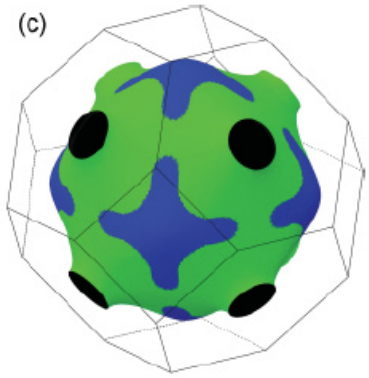
- Transition metal oxides:

Compound	SIC configuration
MnO	$3t_{2g}^{\uparrow} + 2e_g^{\uparrow}$
FeO	$3t_{2g}^{\uparrow} + 2e_g^{\uparrow} + 1t_{2g}^{\downarrow}$
CoO	$3t_{2g}^{\uparrow} + 2e_g^{\uparrow} + 2t_{2g}^{\downarrow}$
NiO	$3t_{2g}^{\uparrow} + 2e_g^{\uparrow} + 3t_{2g}^{\downarrow}$
CuO	$3t_{2g}^{\uparrow} + 2e_g^{\uparrow} + 3t_{2g}^{\downarrow} + 1e_g^{\downarrow}$

M Däne et al, J. Phys. Condens. Matter **21**, 045604 (2009)







- Fermi surface sonar

S. Lounis et al, Phys. Rev. B **83**, 035427 (2011)

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Magnetic interactions I

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Localized magnetic moments (?)

- Gedankenexperiment: freeze the system in some magnetic configuration.

  If we rotate the moment on site *i* only: $\vec{M}_i(\hat{e}_i) \equiv \int_{V_i} \mathrm{d}\vec{r}\, \vec{m}_i(\vec{r}) = M_i^{\parallel}(\hat{e}_i)\, \hat{e}_i + \vec{M}_i^{\perp}$

- Local moment – approximate Hund's rule: $M_i^{\perp} \ll M_i^{\parallel}(\hat{e}_i)\ , \quad M_i^{\parallel}(\hat{e}_i) \approx M_i^{\parallel}$

- Good candidates: narrow band systems (3d, 4f…); band gap systems

- Other electrons in the system may be polarized by the local moments

- Rigid spin approximation: the xc field depends on the orientation only trivially

$$\vec{B}_i^{\mathrm{xc}}(\vec{r}) \approx B_i^{\mathrm{xc}}(\vec{r})\, \hat{e}_i \implies \underline{t}_i(\varepsilon; \hat{e}_i) \approx \underline{\mathcal{R}}_i(\hat{e}_i)\, \underline{t}_i(\varepsilon; \hat{z})\, \underline{\mathcal{R}}_i(\hat{e}_i)^{-1}$$

Constrained LDA: P. H. Dederichs et al, Phys. Rev. Lett. **53**, 2512 (1984)

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Heisenberg model from DFT

- Dependence of the total energy on the magnetic configuration:

$$E(\{\hat{e}\}) = E_0 + \sum_i E_i^{(1)}(\hat{e}_i) + \sum_{ij} E_{ij}^{(2)}(\hat{e}_i, \hat{e}_j) + \sum_{ijk} E_{ijk}^{(3)}(\hat{e}_i, \hat{e}_j, \hat{e}_k) + \dots$$

- Magnetic force theorem: $E(\{\hat{e}+\delta\hat{e}\}) - E(\{\hat{e}\}) \approx E_{\text{band}}(\{\hat{e}+\delta\hat{e}\}) - E_{\text{band}}(\{\hat{e}\})$

- Liechtenstein formula: follows directly from Lloyd's formula in KKR

$$\delta E_{\text{band}}(\delta\hat{e}_i, \delta\hat{e}_j) \approx \frac{1}{\pi}\text{Im}\,\text{Tr}\int^{\varepsilon_F} \mathrm{d}\varepsilon\, \delta\underline{t}_i^{-1}(\varepsilon)\,\underline{\tau}_{ij}(\varepsilon)\,\delta\underline{t}_j^{-1}(\varepsilon)\,\underline{\tau}_{ji}(\varepsilon) = J_{ij}\,\delta\hat{e}_i \cdot \delta\hat{e}_j$$

- Heisenberg model (great leap of faith): $E_{\text{iso}}(\{\hat{e}\}) = -\frac{1}{2}\sum_{ij} J_{ij}\,\hat{e}_i \cdot \hat{e}_j$

- From a single calculation the energy of a whole class of magnetic states can be estimated – spin spirals

Magnetic force theorem: A. I. Liechtenstein et al, J. Mag. Magn. Mater. **67**, 65 (1987)

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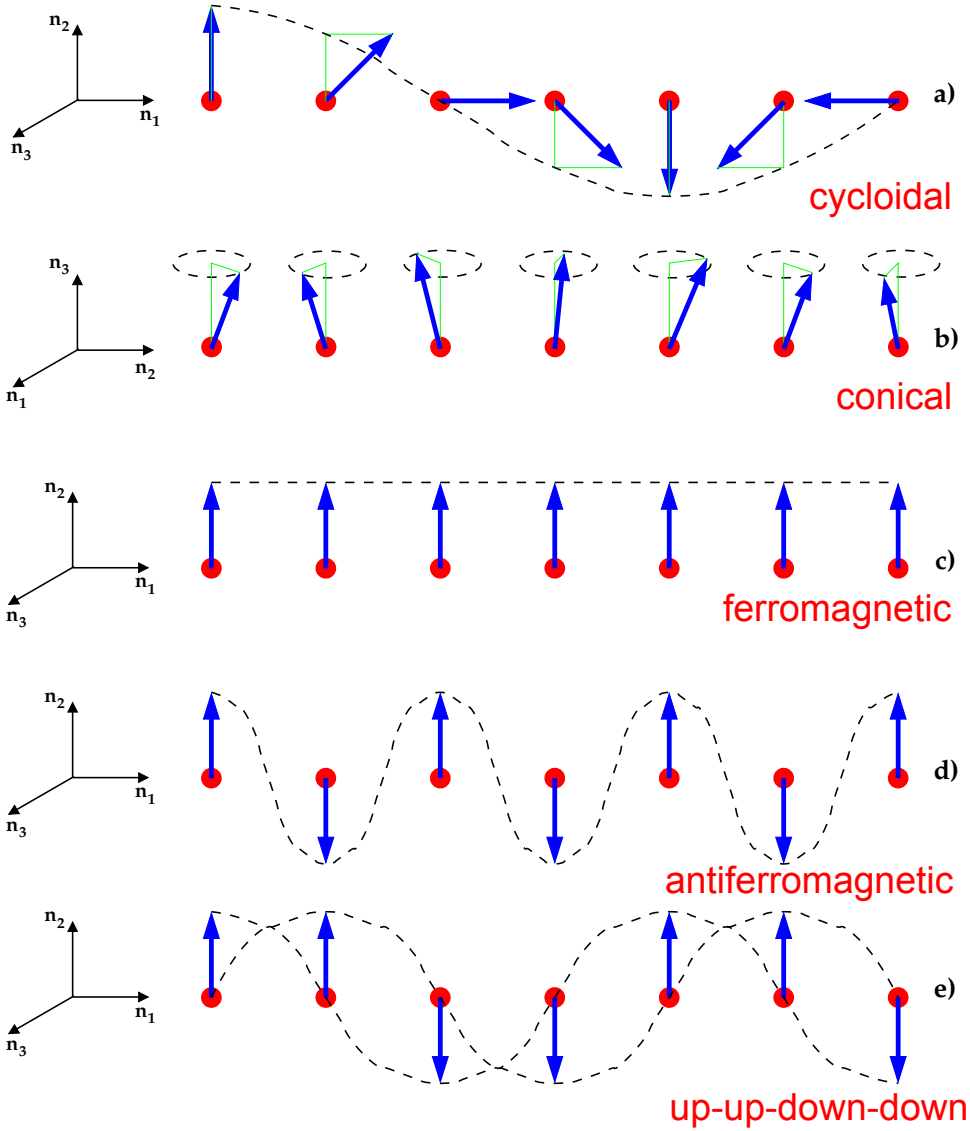
Magnetic groundstates and spin spirals

- Spin spirals:

$$\vec{M}_i(\vec{q}) = M(\vec{q}) \left(\cos(\vec{q}\cdot\vec{R}_i + \phi) \sin\theta\, \hat{n}_1 + \sin(\vec{q}\cdot\vec{R}_i + \phi) \sin\theta\, \hat{n}_2 + \cos\theta\, \hat{n}_3 \right)$$

- Generalized Bloch theorem
- May need constraining fields
- Comparison of total energies of spin spirals with force theorem calculations checks assumptions



Noncollinear magnetism: L.M. Sandratskii, Adv. Phys. **47**, 91 (1998)

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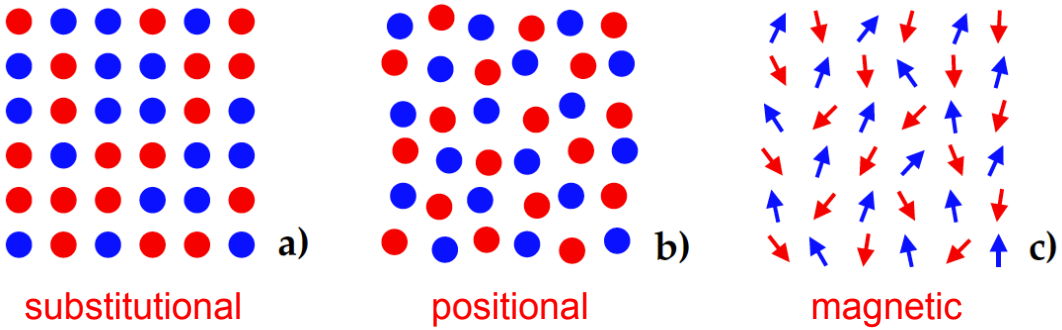
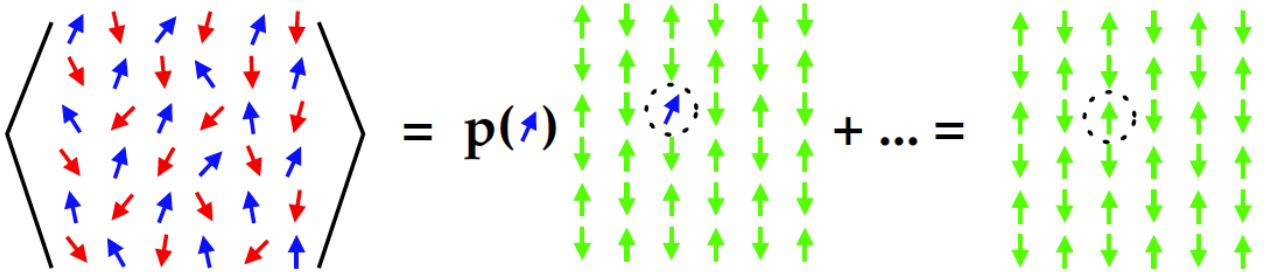
Disordered Local Moment (DLM) state

- Disorder types:



- Effective medium (CPA): $\langle G_{ii} \rangle = \int \mathrm{d}\hat{e}_i \, P_i(\hat{e}_i) \, G_{ii}(\hat{e}_i; \{\vec{m}\}) \quad \vec{m}_i = \int \mathrm{d}\hat{e}_i \, P_i(\hat{e}_i) \, \hat{e}_i$



- Each local moment sees average magnetic medium set up by all other moments

- Paramagnetic instabilities estimate stable magnetic states, transition temperature

B.L. Gyorffy et al, J. Phys. F: Met. Phys. **15**, 1337 (1985)

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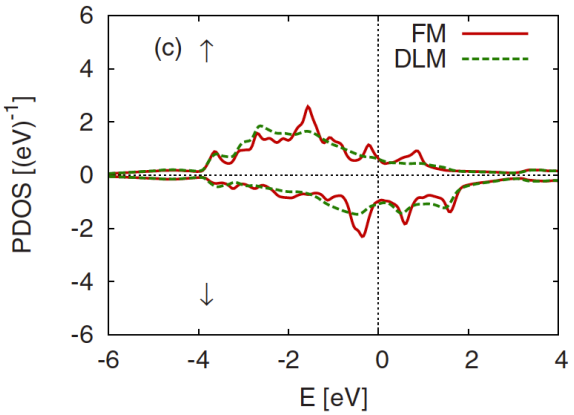
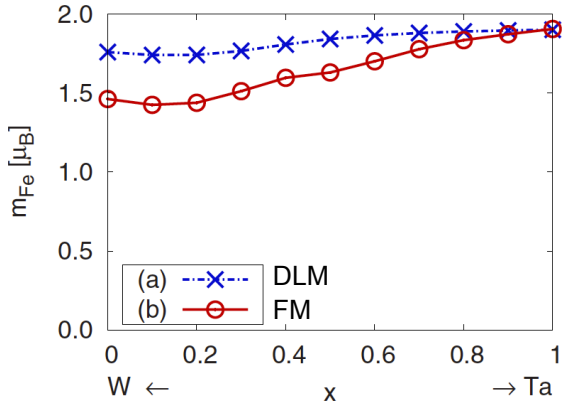
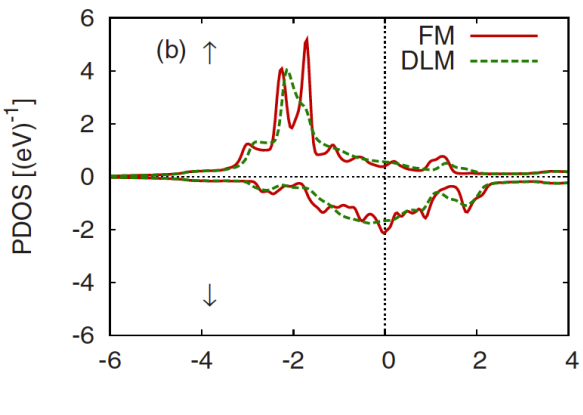
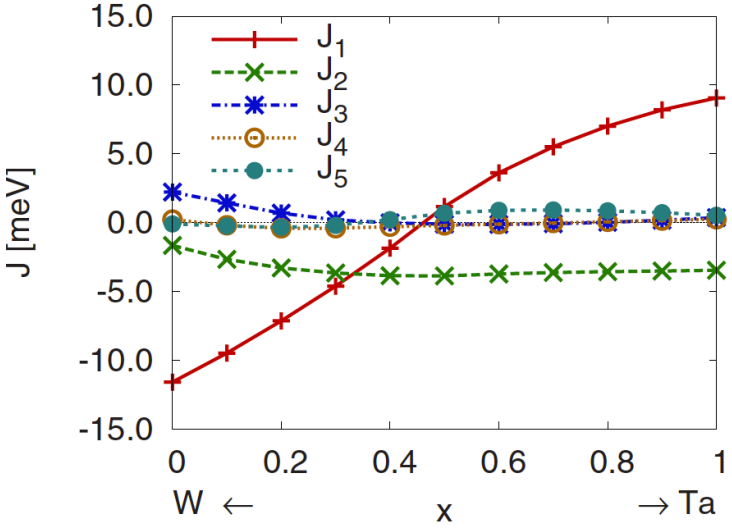
Fe monolayer on (W,Ta) substrate

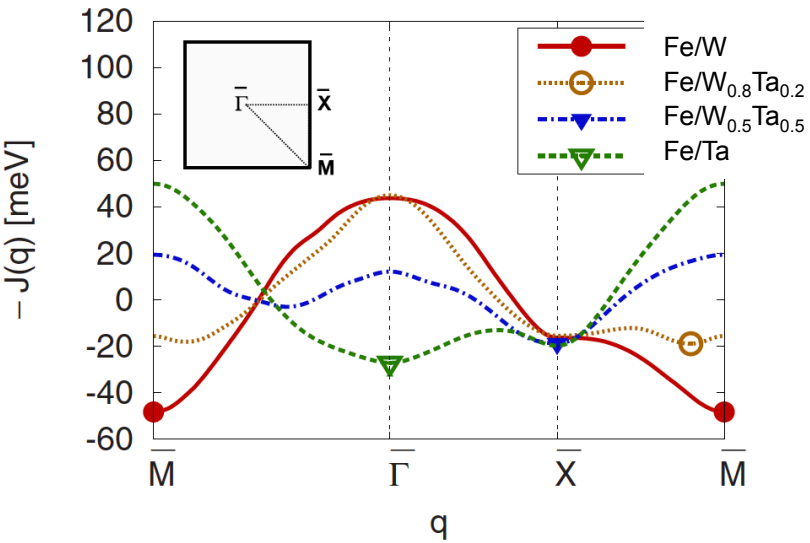
- Electronic structure for ferromagnetic and disordered local moment states:











LMTO CPA+DLM: M. Ondracek et al, Phys. Rev. B **81**, 064410 (2010)

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Magnetic interactions II

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Magnetic anisotropy and stability

- Goldstone theorem: it costs no energy to rotate all the magnetic moments by the same angle

$$E_{\text{iso}}(\{\hat{e}\}) = -\frac{1}{2}\sum_{ij} J_{ij}\,\hat{e}_i \cdot \hat{e}_j$$

- Spin-orbit coupling – coupling of spin and orbital angular momentum; energy now depends on how the moments point with respect to the lattice

- Magnetic anisotropy energy – can be magnetocrystalline or magnetostatic

$$E_{\text{dd}}(\{\hat{e}\}) = \frac{1}{2}\sum_{ij}\left[\frac{3}{R_{ij}^3}\,\vec{M}_i \cdot \vec{M}_j - \frac{1}{R_{ij}^5}(\vec{M}_i \cdot \vec{R}_{ij})(\vec{M}_j \cdot \vec{R}_{ij})\right]$$

$$E_{\text{a}}^{(1)}(\{\hat{e}\}) = \sum_i K_i(\hat{e}_i) = \sum_i \left[K_{1i}\sin^2\theta_i + (K_{2i} + K'_{2i}\cos 4\phi_i)\sin^4\theta_i + \ldots\right] \quad (C_{4v})$$

- The last expression is for the onsite anisotropy, tetragonal symmetry.

  The pair interaction will also become anisotropic…

R. Skomski, *Simple Models of Magnetism*, OUP (2008)

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Anisotropic pair interactions

- Bilinear pair interaction tensor: $E^{(2)}(\{\hat{e}\}) = -\frac{1}{2}\sum_{ij} \hat{e}_i \cdot \underline{J}_{ij} \cdot \hat{e}_j$

- Isotropic part:

$$J_{ij}^{\mathrm{iso}} = \frac{1}{3}\,\mathrm{Tr}\,\underline{J}_{ij} \longrightarrow J_{ij}^{\mathrm{iso}}\,\hat{e}_i \cdot \hat{e}_j$$

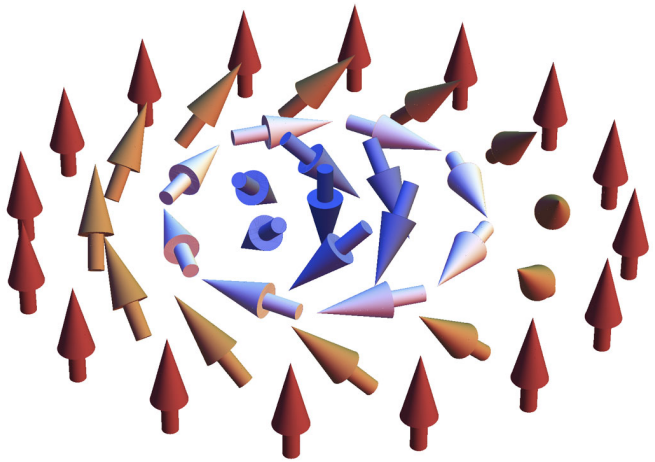
- Dzyaloshinskii-Moriya (DM) part:

$$\underline{J}_{ij}^{\mathrm{anti}} = \frac{1}{2}\left(\underline{J}_{ij} - \underline{J}_{ij}^{\mathrm{T}}\right) \longrightarrow \vec{D}_{ij} \cdot (\hat{e}_i \times \hat{e}_j)$$

- Symmetric traceless part similar to dipole-dipole term

- DM term needs broken inversion symmetry

- This leads to chirality – meet the skyrmion:



- Anisotropic terms on same energy scale as higher order isotropic terms…

R. Skomski, *Simple Models of Magnetism*, OUP (2008)

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$Mn_1/W(001)$ as detailed case study – I

- Mn monolayer on W(001) has a chiral spin spiral as groundstate –

  P. Ferriani et al, Phys. Rev. Lett. **101**, 027201 (2008) – why?

- Spin spiral energy:

$$E_{\mathrm{iso}}(\vec{q};\theta) = -\frac{1}{2N}\sum_{ij} J_{ij}\,\vec{m}_i(\vec{q})\cdot\vec{m}_j(\vec{q}) = \frac{J(0)-J(\vec{q})}{2}\sin^2\theta - \frac{J(0)}{2}$$

$$J(\vec{q}) = \sum_j J_{0j}\cos(\vec{q}\cdot\vec{R}_{0j}) = 2J_1\left[\cos(\pi q_x)+\cos(\pi q_y)\right] + 4J_2\cos(\pi q_x)\cos(\pi q_y)$$

- Extremal values of the energy:

$$\sin(\pi q_x)\left(1+\frac{2J_2}{J_1}\cos(\pi q_y)\right) = 0$$

$$\sin(\pi q_y)\left(1+\frac{2J_2}{J_1}\cos(\pi q_x)\right) = 0$$

$$\left(J(0)-J(\vec{q})\right)\sin 2\theta = 0$$

  - Ferromagnetic: (0,0)
  - Row-wise antiferromagnetic: (1,0), etc.
  - Checkerboard antiferromagnetic: (1,1), etc.
  - Spiral if J_2 sufficiently large w.r.t. J_1…
  - … which it isn't.

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$Mn_1/W(001)$ as detailed case study – II

- DM energy depends on the orientation of the spin spiral:

$$E_{\mathrm{DM}}(\vec{q};\theta;\hat{n}_3) = -\frac{1}{2N}\sum_{ij}\vec{D}_{ij}\cdot(\vec{m}_i\times\vec{m}_j) = -\frac{1}{2N}\sum_{ij}\vec{D}_{ij}\cdot\hat{n}_3\,\sin(\vec{q}\cdot\vec{R}_{ij})\sin^2\theta$$

- Chirality: DM energy is not the same for *q* and -*q* – rotational sense matters

$$\begin{aligned} E_{\mathrm{DM}}(\vec{q};\theta;\hat{n}_3) &= D\left[(\hat{e}_x\cdot\hat{n}_3)\sin(\pi q_y) - (\hat{e}_y\cdot\hat{n}_3)\sin(\pi q_x)\right]\sin^2\theta \\ &= D\left[\cos\alpha\sin(\pi q_y) - \sin\alpha\sin(\pi q_x)\right]\sin^2\theta \end{aligned}$$

- Extremal values of the energy:

$$\sin(\pi q_x)\left[1+\frac{2J_2}{J_1}\cos(\pi q_y) \pm \frac{D}{J_1}\frac{\cos(\pi q_x)}{\sqrt{\sin^2(\pi q_x)+\sin^2(\pi q_y)}}\right] = 0$$

$$\sin(\pi q_y)\left[1+\frac{2J_2}{J_1}\cos(\pi q_x) \pm \frac{D}{J_1}\frac{\cos(\pi q_y)}{\sqrt{\sin^2(\pi q_x)+\sin^2(\pi q_y)}}\right] = 0$$

- Spiral also possible if J_2 zero; cycloidal spirals: $\hat{n}_3\cdot\vec{q} = 0$

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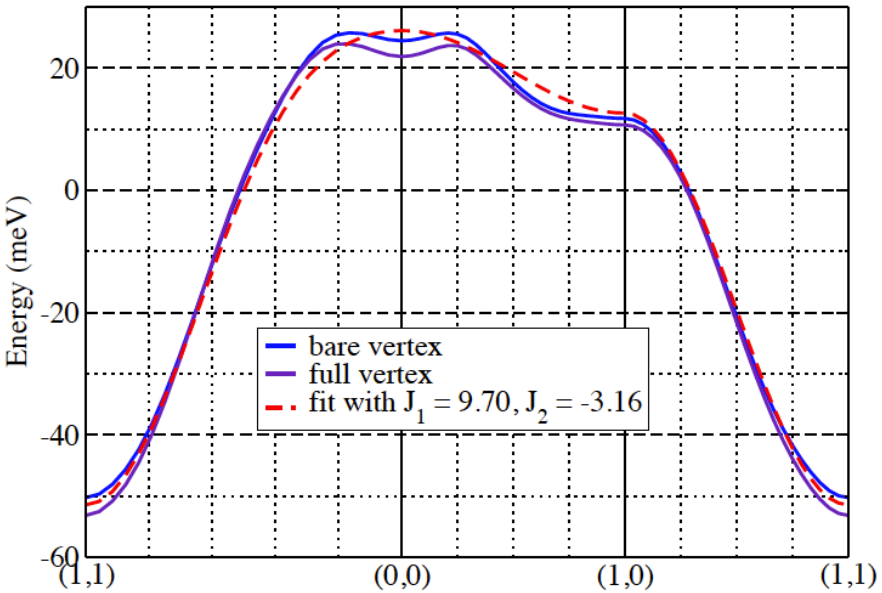
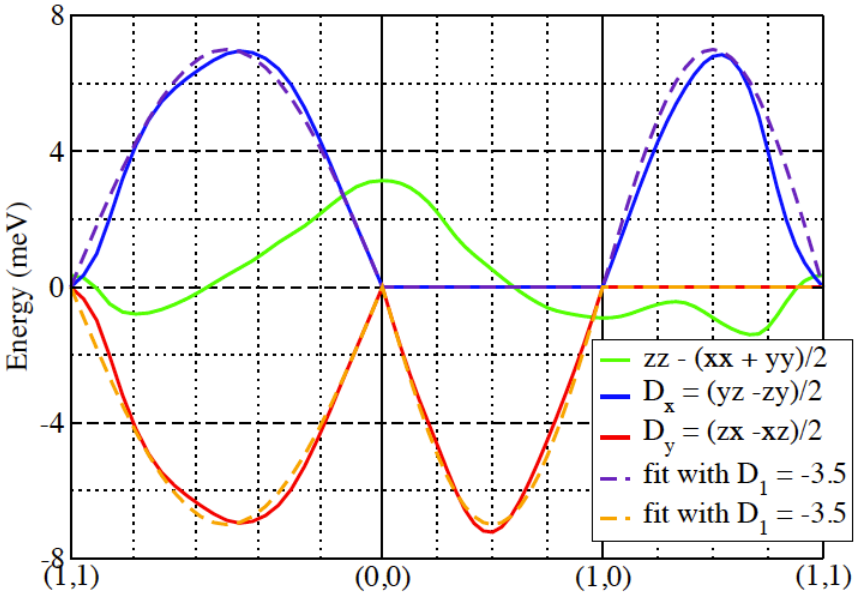
$Mn_1/W(001)$ as detailed case study – III

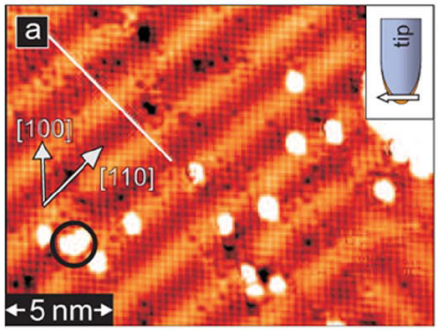
Isotropic part of J(q):

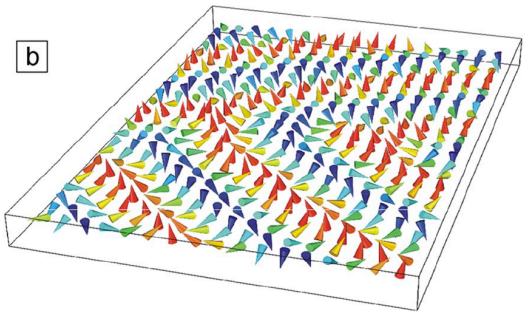


Anisotropic part of J(q):



- Maximum in isotropic part of J(q) is a Fermi surface effect
- Min energy for q = (0.17,0.17) good agreement with experiment





- For relativistic DLM formalism, see M. dos Santos Dias et al, Phys. Rev. B 83, 054435 (2011)

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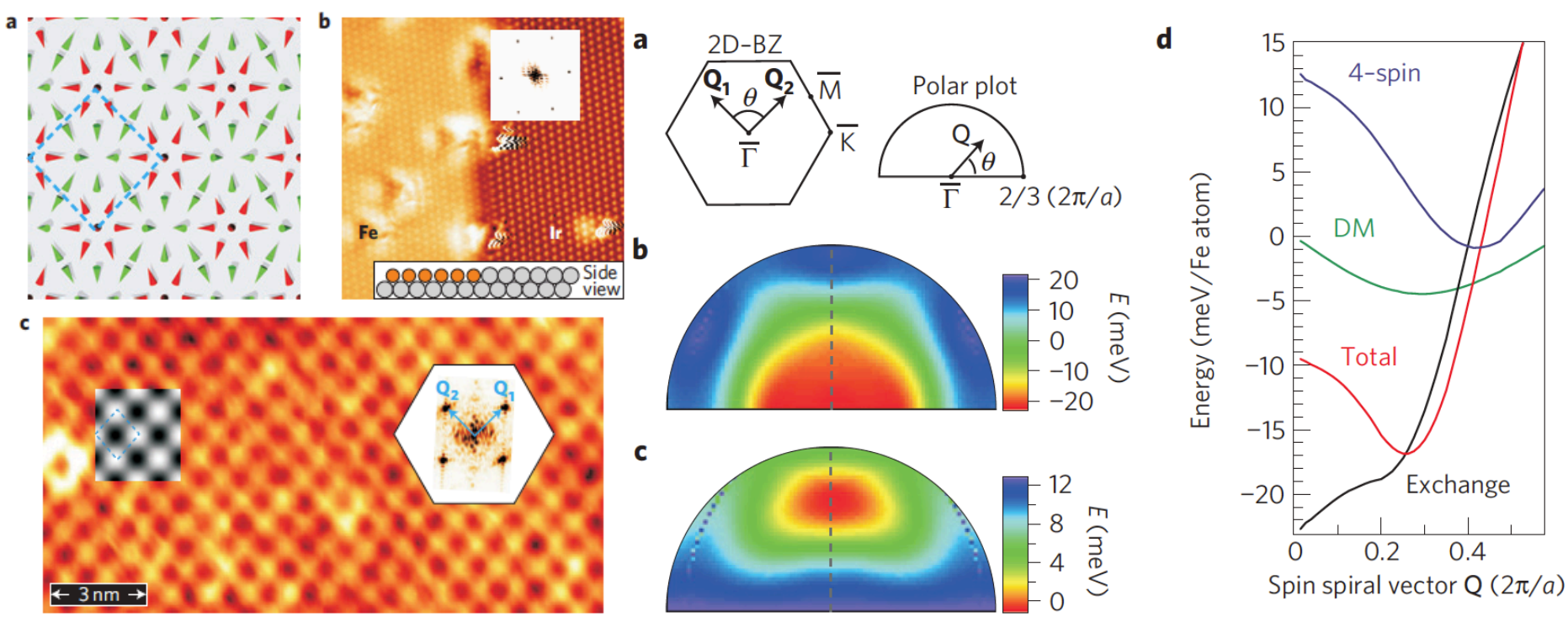
Higher order interactions – $Fe_1/Ir(111)$

- Biquadratic and four-spin interactions:

$$E_{\text{more}}(\{\hat{e}\}) = \sum_{ij} B_{ij}(\hat{e}_i \cdot \hat{e}_j)^2 + \sum_{ijkl} Q_{ijkl}\left[(\hat{e}_i \cdot \hat{e}_j)(\hat{e}_k \cdot \hat{e}_l) - (\hat{e}_i \cdot \hat{e}_k)(\hat{e}_j \cdot \hat{e}_l) + (\hat{e}_i \cdot \hat{e}_l)(\hat{e}_j \cdot \hat{e}_k)\right]$$



- Squarish skyrmion lattice out of an hexagonal magnetic monolayer

S. Heinze et al, Nature Phys. **7**, 713 (2011)

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Beyond the groundstate

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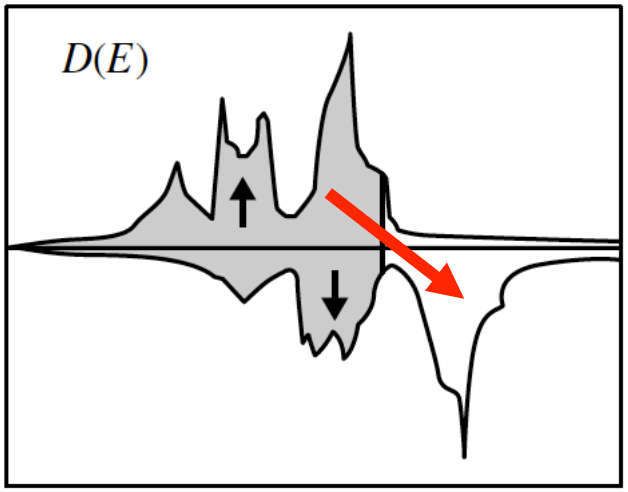
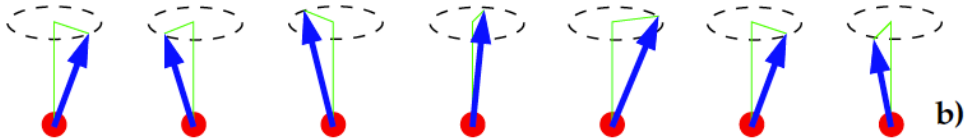
Spin waves and spin flips

- Stoner excitations:

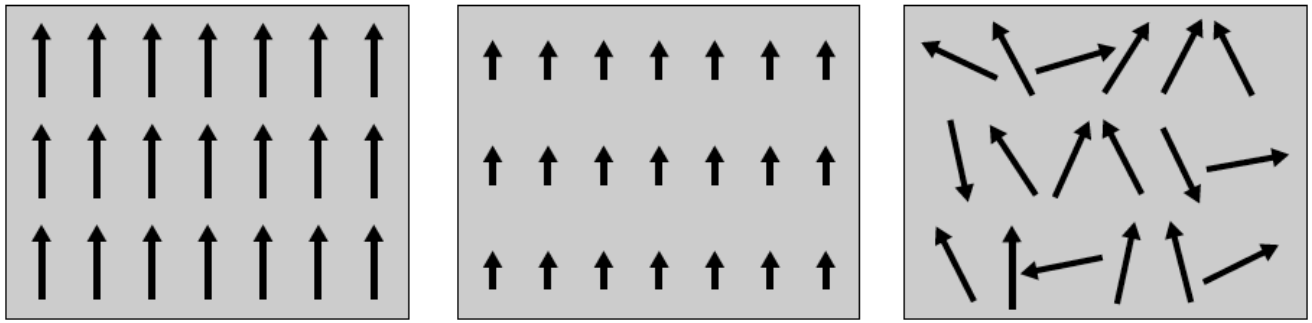


- Spin waves:



  - Spin spirals also called frozen magnons
  - Spin spiral energies approximate spin wave energies?
  - Adiabatic approximation

- What does the high temperature magnetic state look like?



T = 0: ferromagnet (DFT) | T > 0: Stoner | T > 0: Heisenberg

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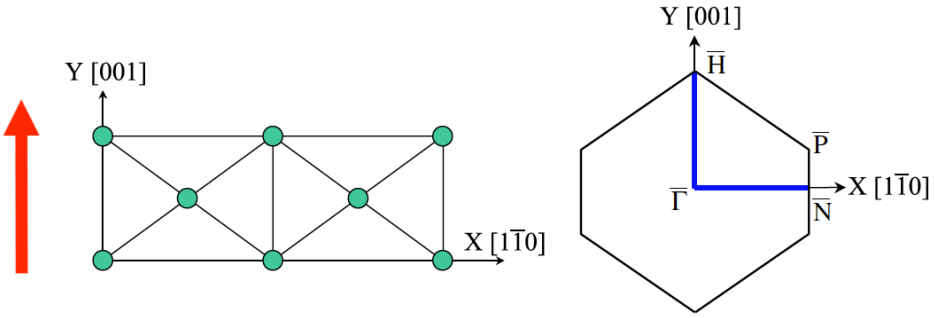
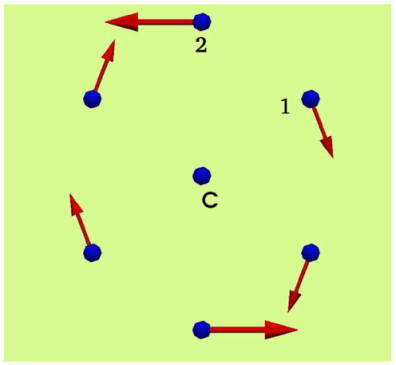
Spin wave spectra in adiabatic approx

- Landau-Lifshitz equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{M}_i \approx M_i \frac{\mathrm{d}\hat{e}_i}{\mathrm{d}t} = -\gamma\,\vec{M}_i \times \frac{\delta\mathcal{F}}{\delta\hat{e}_i} = -\gamma\,\vec{M}_i \times \vec{B}_i$$

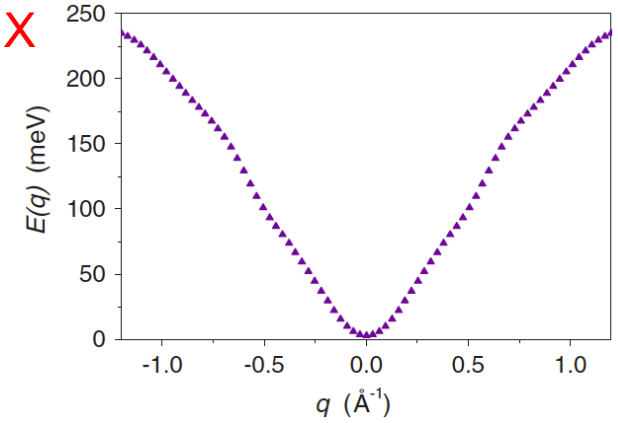
- $Fe_1/W(110)$: magnetization in-plane, along Y axis



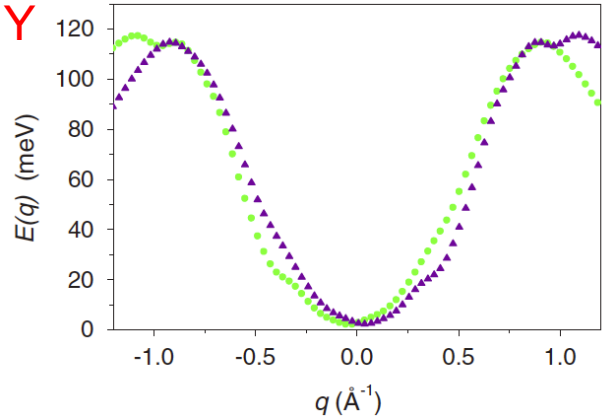


➢ DM vectors, nn and nnn

➢ q along X



➢ q along Y



L. Udvardi and L. Szunyogh, Phys. Rev. Lett. **102**, 207204 (2009)

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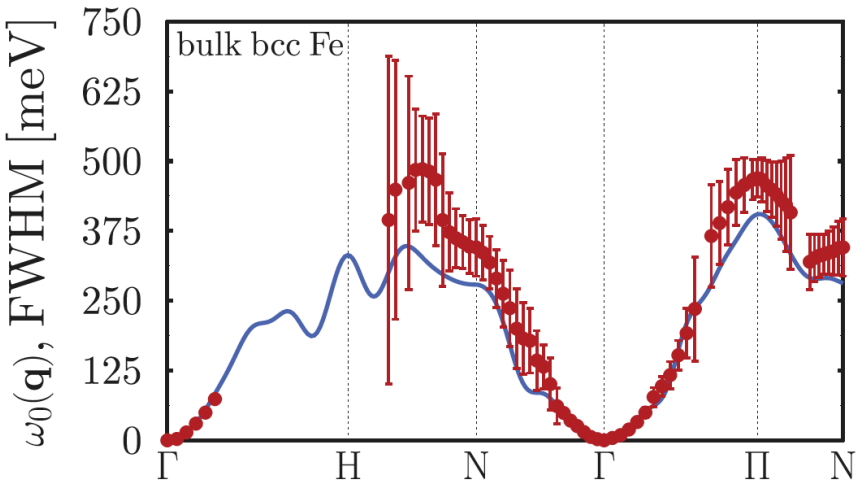
Spin waves from TD-DFT

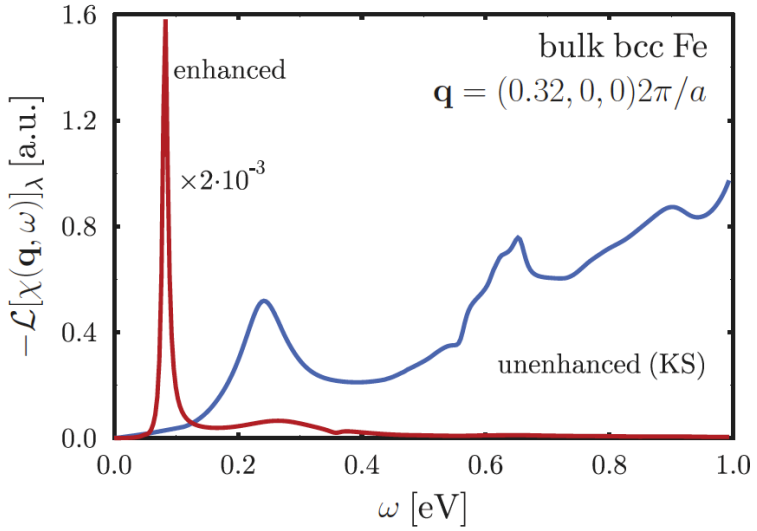
- Dynamical magnetic susceptibility:

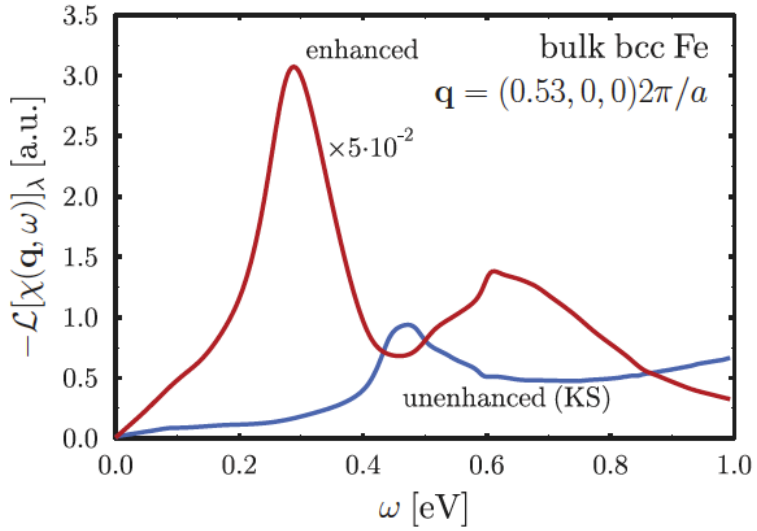
$$\chi(\omega) = \chi^{\mathrm{KS}}(\omega) + \chi^{\mathrm{KS}}(\omega)\,\mathcal{K}^{\mathrm{xc}}\,\chi(\omega)$$

- Example: beloved bcc Fe

- What is a spin wave peak and what isn't?







P. Buczek et al, Phys. Rev. B **84**, 174418 (2011)

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Comments and books

- DFT-KKR as powerful and versatile tool for magnetic properties
- Magnetic hamiltonians: how many terms do we need and make sense to include?
- Check calculations are converged before writing the PRL – k-points!

- Start here: S. Blundell, *Magnetism in Condensed Matter*, OUP (2001)
- Overview: R. Skomski, *Simple Models of Magnetism*, OUP (2008)
- DFT: J. Kübler, *Theory of Itinerant Electron Magnetism*, OUP (2000)
- Many other nice books around, lots of KKR references also – ask me

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