Non Collinear Magnetism in the Elk Code

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Cecam Workshop 2011

1. Magnetic Ground State Structure
    - What is collinear magnetism (CM) and non collinear magnetism (NCM) ?
    - Calculation of NCM using the elk code.
    - A special form of NCM $\Rightarrow$ spin spirals (SS).

2. Excitation of the Magnetic Structure
    - The low lying collective excitations (magnons)
    - Different approaches to calculate magnons
    - Magnons in the elk code (frozen magnon approach)

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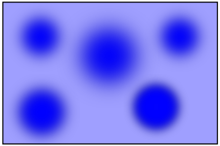
1^{st} Part

Non Collinear Ground States

- Given a ground state $|\Psi_0\rangle$ of a system the ground state magnetic moment $\mathbf{m}_0(\mathbf{r})$ is:

$$\mathbf{m}_0(\mathbf{r}) = \sum_{\alpha\beta=1}^{2} \left\langle \Psi_0 \left| \hat{\Psi}^{\dagger}_{\alpha}(\mathbf{r}) \vec{\sigma}_{\alpha\beta} \hat{\Psi}_{\beta}(\mathbf{r}) \right| \Psi_0 \right\rangle .$$



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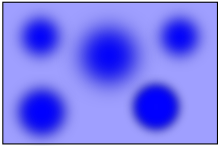

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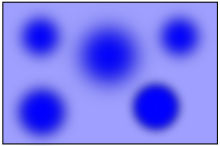

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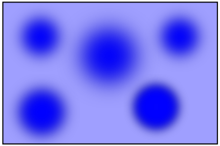

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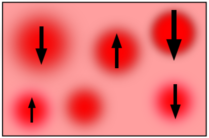

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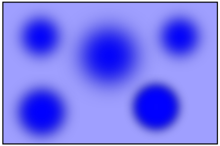

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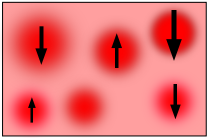

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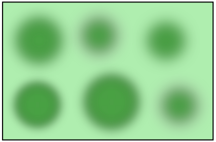

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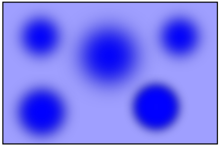

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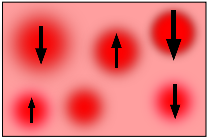

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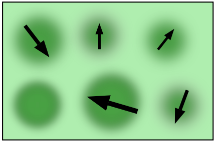

no restriction to **m**(**r**)
(Non collinear system)

- The *N* particle problem can not be solved, so a different approach is needed to find the magnetic ground state of a system.

- Using Green's function or density functional theory (DFT) one can find the $\mathbf{m}_0(\mathbf{r})$ of a system.

Green's Function

$$\mathbf{m}_0(\mathbf{r}) = \vec{\sigma}_{\alpha\beta} G_{\alpha\beta}(\mathbf{x}\mathbf{x}^+)$$

$$G(12) = G_0(\mathbf{x}_1\mathbf{x}_2)\,\delta_{\alpha\beta} + \iint d3d4\,G_0(13)\,\mathcal{M}(34)\,G(42)$$

$$\mathcal{M}_{\alpha\beta} = \begin{cases} \delta_{\alpha\beta}\mathcal{M} & \text{non magnetic solution} \\ \delta_{\alpha\beta}\mathcal{M}_\alpha & \text{collinear } \mathrm{m}_0(\mathbf{r}) \\ \mathcal{M}_{\alpha\beta} & \text{non collinear } \mathrm{m}_0(\mathbf{r}) \end{cases}$$

The Kohn-Sham Scheme (DFT)

No external magnetic field.

$$\mathbf{m}_0(\mathbf{r}) = \sum_j^{\text{occ.}} \vec{\varphi}_j^{\text{KS}*} \cdot \vec{\sigma}_{2\times 2} \cdot \overleftarrow{\varphi}_j^{\text{KS}}$$

$$\epsilon_j \vec{\varphi}_j^{\text{KS}} = \left[\hat{h}_0 \mathbf{1}_{2\times 2} + v^{\text{xc}}_{2\times 2}[\rho, \mathbf{m}](\mathbf{r})\right] \cdot \vec{\varphi}_j^{\text{KS}}$$

$$\hat{h}_0 = \left(-\frac{\triangle_{\mathbf{r}}}{2} + v_0(\mathbf{r}) + v_{\text{H}}[\rho](\mathbf{r})\right)$$

$$v^{\text{xc}}_{\alpha\beta} = \begin{cases} \delta_{\alpha\beta} v^{\text{xc}} & \text{non magnetic solution} \\ \delta_{\alpha\beta} v^{\text{xc}}_\alpha & \text{collinear } \mathrm{m}_0(\mathbf{r}) \\ v^{\text{xc}}_{\alpha\beta} & \text{non collinear } \mathrm{m}_0(\mathbf{r}) \end{cases}$$

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- A non diagonal potential is **necessary** to get non collinear magnetism.

- The potential can be decomposed in a diagonal and off diagonal part.

Exchange Correlation Potential

$$v^{xc}_{\alpha\beta}[\rho\mathbf{m}](\mathbf{r}) = \delta_{\alpha\beta}\left[v_{xc}[\rho\mathbf{m}](\mathbf{r}) + z_\alpha B^z_{xc}[\rho\mathbf{m}](\mathbf{r})\right] \text{ diagonal}$$
$$+ \sigma^x_{\alpha\beta}\cdot B^x_{xc}[\rho\mathbf{m}](\mathbf{r}) + \sigma^y_{\alpha\beta}\cdot B^y_{xc}[\rho\mathbf{m}](\mathbf{r}) \text{ off diagonal}$$

$$v_{xc}[\rho\mathbf{m}](\mathbf{r}) := \frac{\delta E^{xc}[\rho\mathbf{m}]}{\delta\rho(\mathbf{r})} \text{ and } \mathbf{B}_{xc}[\rho\mathbf{m}](\mathbf{r}) := \frac{\delta E^{xc}[\rho\mathbf{m}]}{\delta\mathbf{m}(\mathbf{r})}$$

- Functionals like LSDA and GGA depend only on ρ and $\mathbf{m}_z$.

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- To save these functionals you can use the Kübler trick:
  1. Starting point is a $\rho_{2\times 2}(\mathbf{r})$ density:
  $$\rho_{2\times 2}(\mathbf{r}) := \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} \rho + m_z & m_x - im_y \\ m_x + im_y & \rho - m_z \end{pmatrix}.$$
  2. A unitary transformation is used to diagonalize $\rho_{2\times 2}(\mathbf{r})$:
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Properties of $\mathbf{B}_{xc}$

$$\mathbf{B}_{xc}^{(n)} := \mathbf{B}_{xc}\left[\rho^{(n-1)}, \mathbf{m}^{(n-1)}\right] \parallel \mathbf{m}^{(n-1)} \quad \Leftrightarrow \quad \text{Kübler trick} \quad (A)$$

$$\mathbf{B}_{tot}^{(n)} := \left(\mathbf{B}_{MT}^{ext} + \mathbf{B}_{xc}^{(n)}\right) \parallel \mathbf{m}^{(n)} \quad \Leftrightarrow \quad E = -\mathbf{m}^{(n)} \cdot \mathbf{B}_{tot}^{(n)} \quad (B)$$

- Starting point: $(\mathbf{m}^{(0)} = 0, \rho^{(0)} = \rho_{\text{Atom}})$ with $\mathbf{B}_{xc}\left[\rho^{(0)}, \mathbf{m}^{(0)} = 0\right] = 0$
- An external field $\mathbf{B}_{MT}^{ext}$ is applied in the muffin tin (MT). (not physical!)
- The $\mathbf{m}^{(1)} \parallel \mathbf{B}_{MT}^{ext}$ since $\mathbf{B}_{xc}^{(0)} = 0$
- This is conserved in the self consistent solution:

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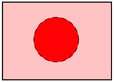

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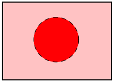

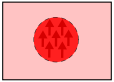

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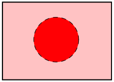

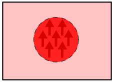

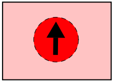

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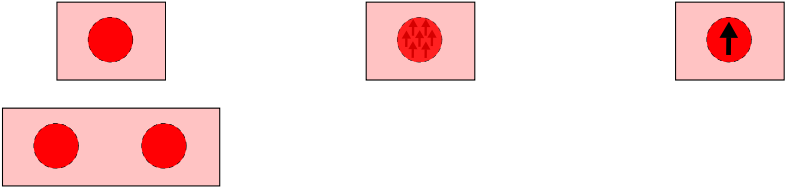

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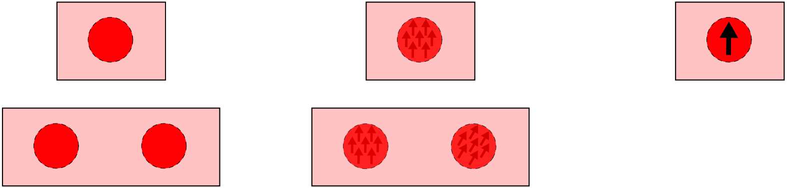

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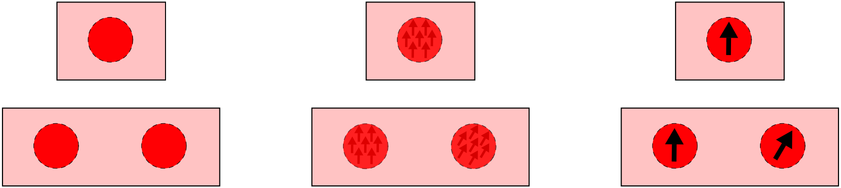

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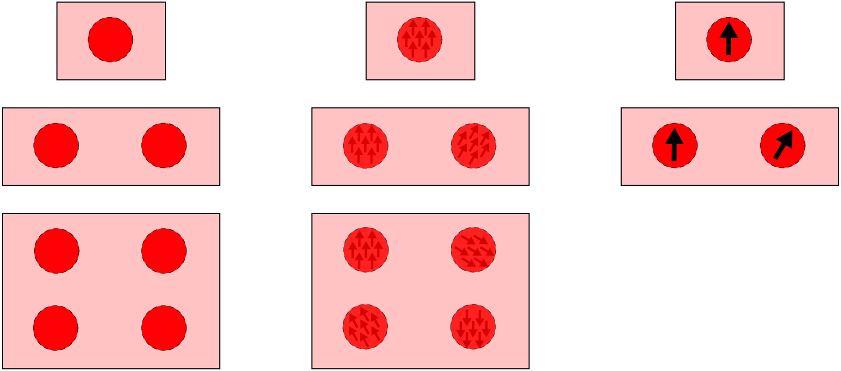

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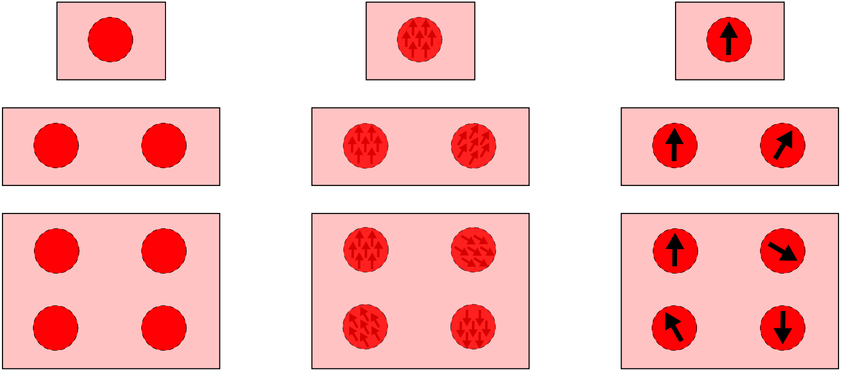

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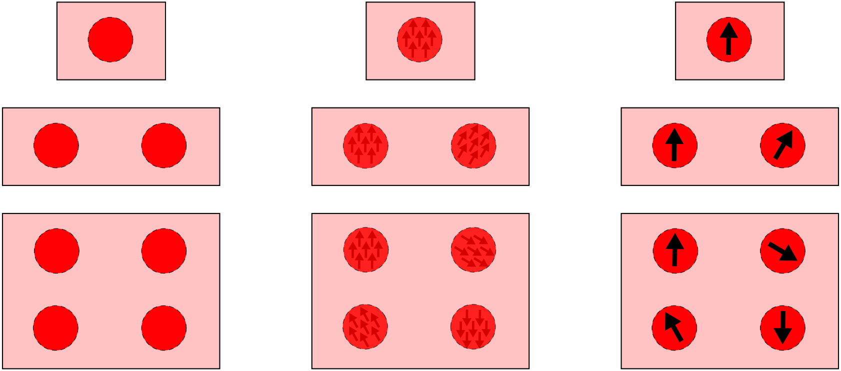

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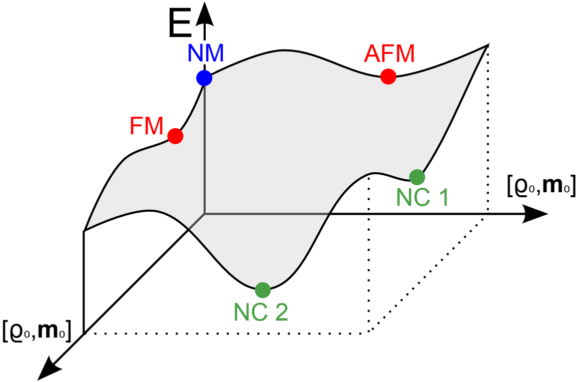

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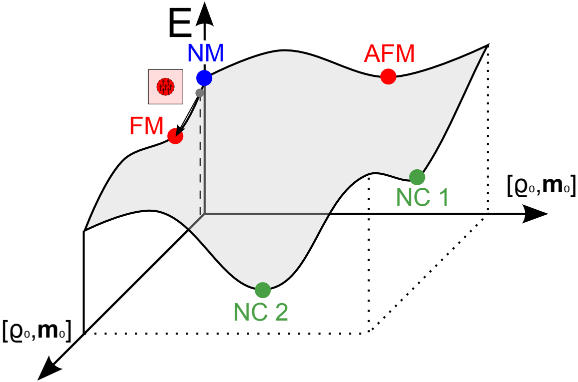

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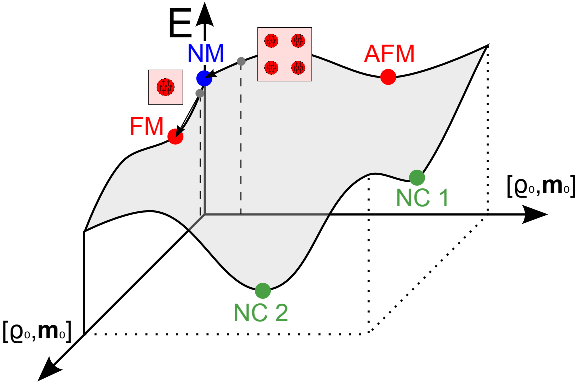

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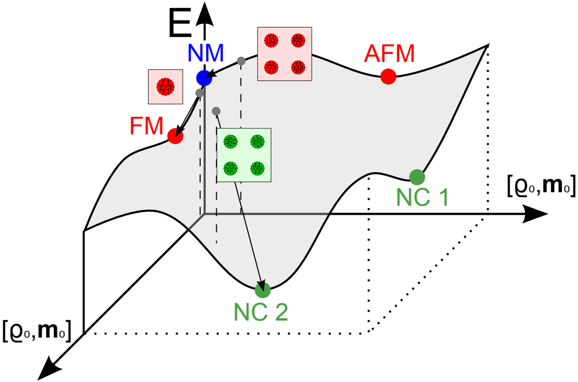

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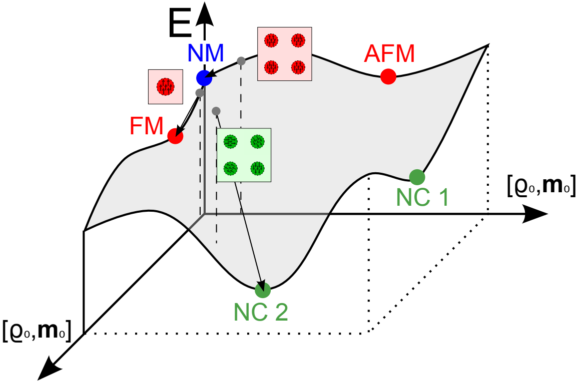

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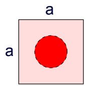

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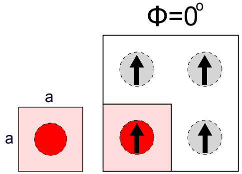

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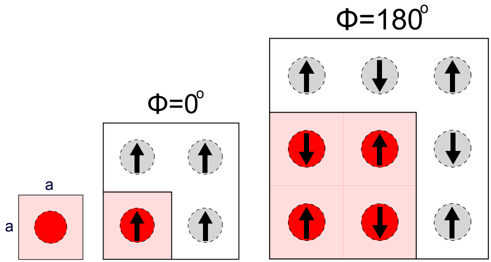

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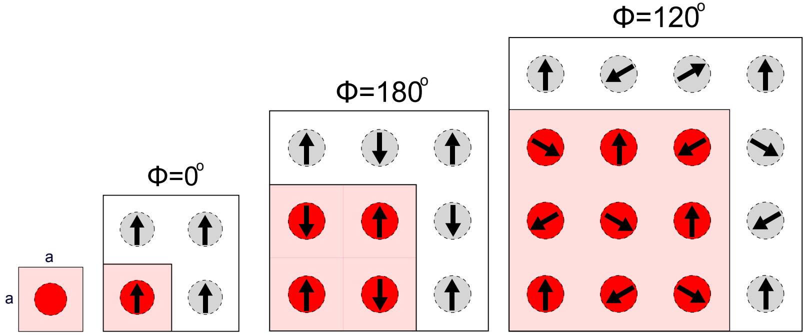

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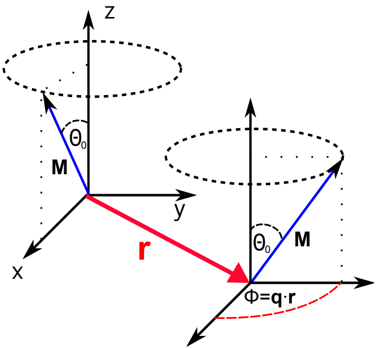

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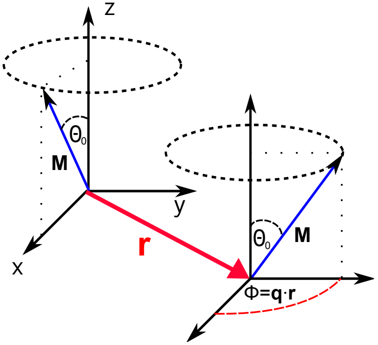

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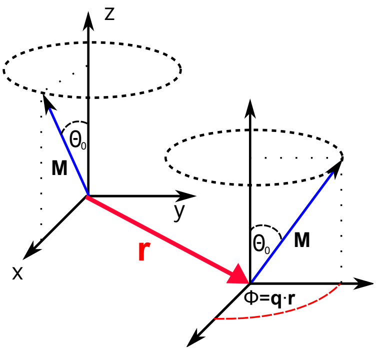

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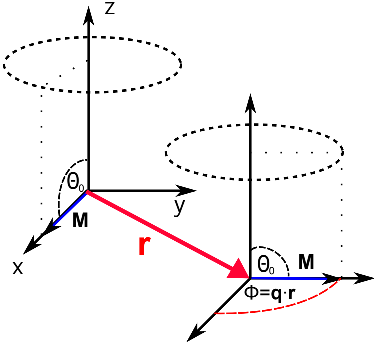

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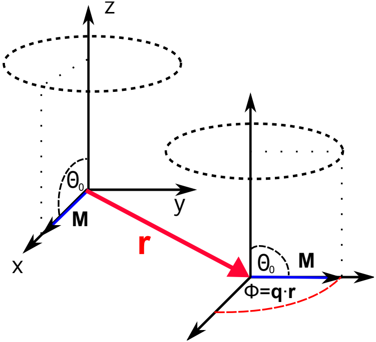

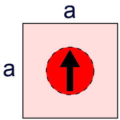

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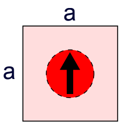

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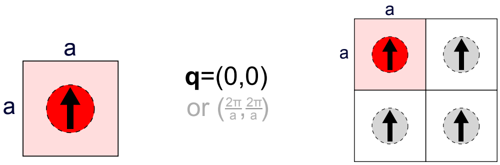

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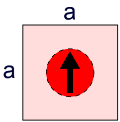

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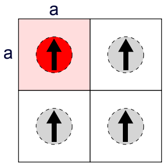

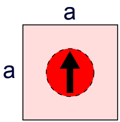

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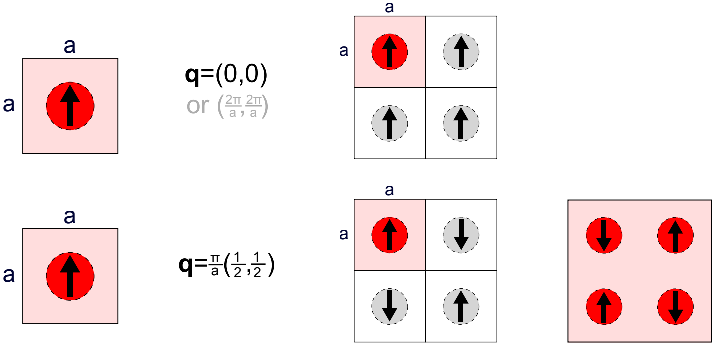

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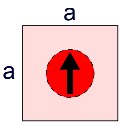
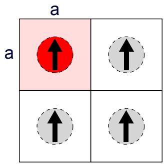
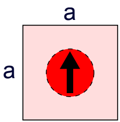


$\mathbf{q}=(0,0)$ or $(\frac{2\pi}{a},\frac{2\pi}{a})$





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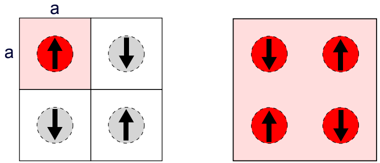

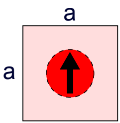

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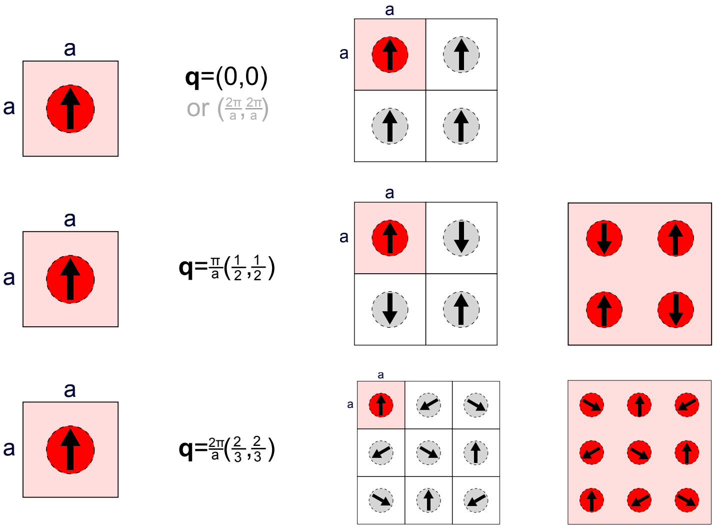

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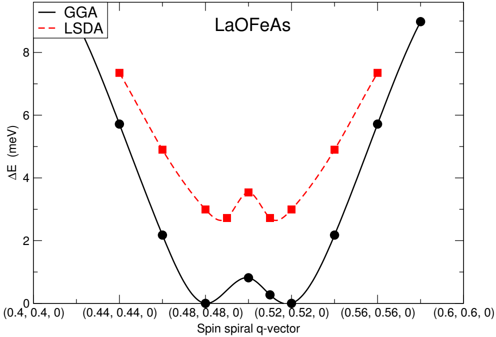

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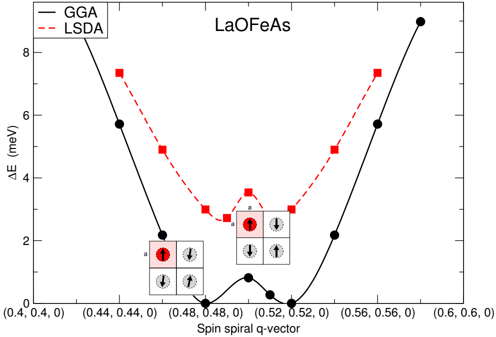

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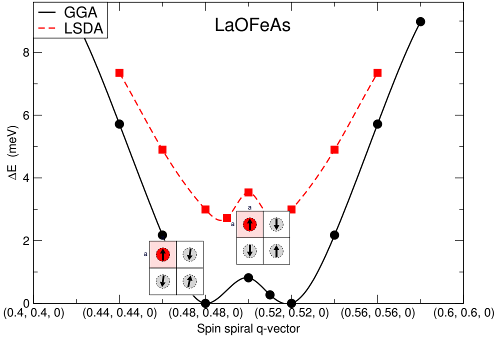

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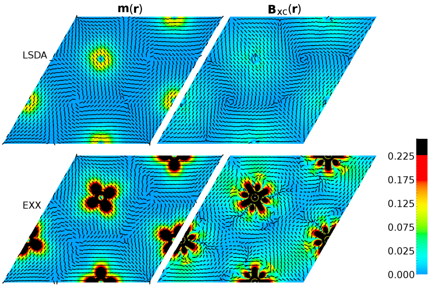

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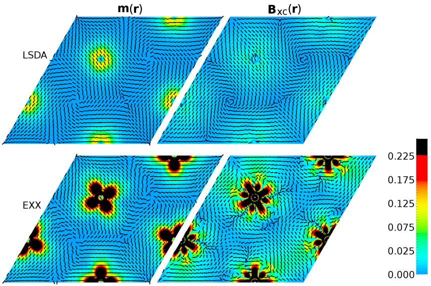

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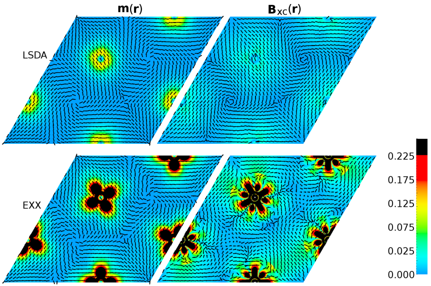

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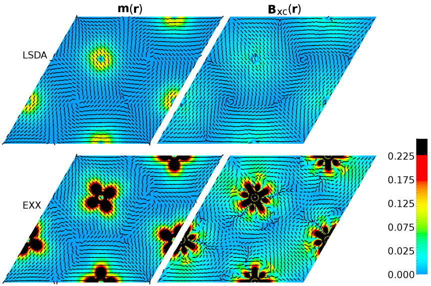
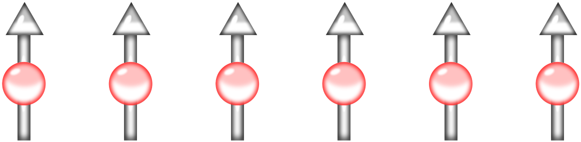


2^{nd} Part

Magnetic Excitations

- Spin waves are excitations on top of a (collinear) magnetic ordering.
- The moments are distorted by small θ and start to turn with $\phi = \mathbf{q} \cdot \mathbf{r}$ from cell to cell.



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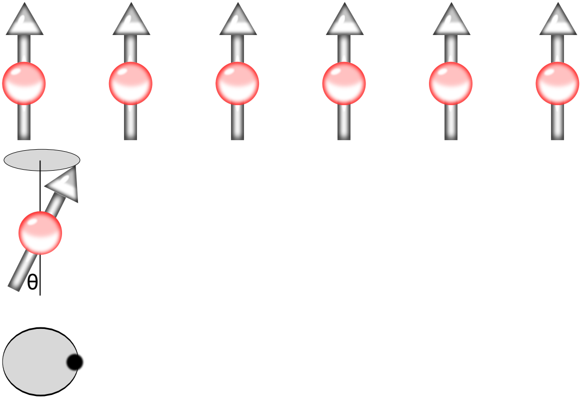

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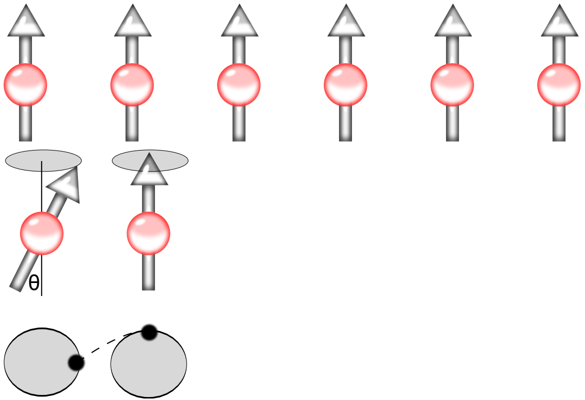

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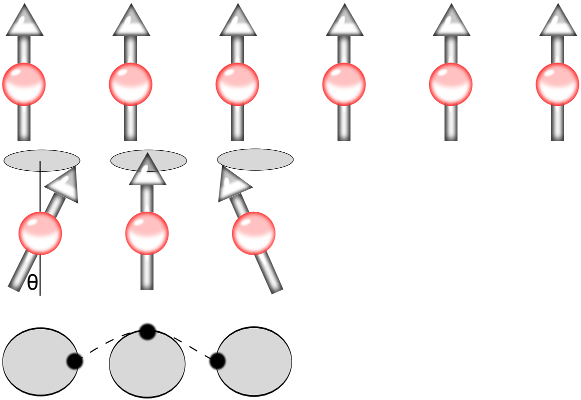

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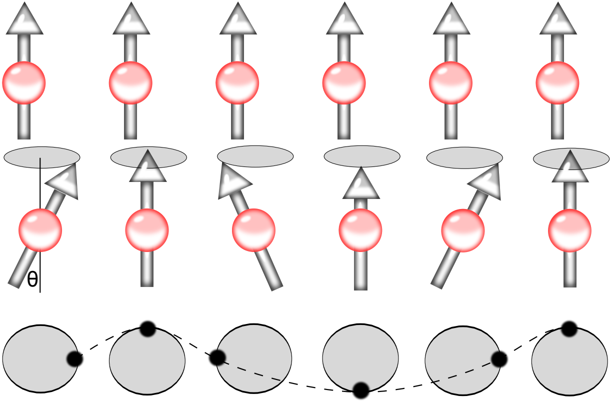

- The quantized modes of the spin waves are called "magnons".
- Magnons are bosonic quasi-particles (QP) carrying $1\mu_{\mathbf{B}}$.
- The energies and lifetimes are $\omega_{\mathbf{q}}^{\text{Max}} \approx$ few 100 meV and $\tau_{\mathbf{q}} \in \left[10^{-4}\text{s}, 10^{-14}\text{s}\right]$.
- A Magnon ranges over the whole crystal
  $\Rightarrow$ "Collective excitation"
- Dispersion $\lim_{\mathbf{q}\to 0} \omega_{\mathbf{q}}^{\text{FM}} \propto |\mathbf{q}|^2$ and $\lim_{\mathbf{q}\to 0} \omega_{\mathbf{q}}^{AFM} \propto |\mathbf{q}|$
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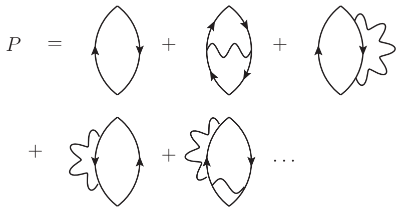

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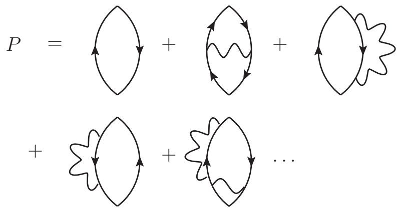

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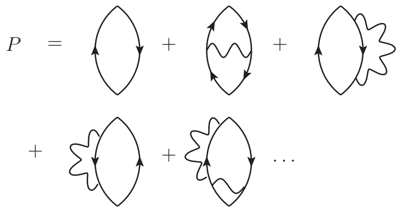

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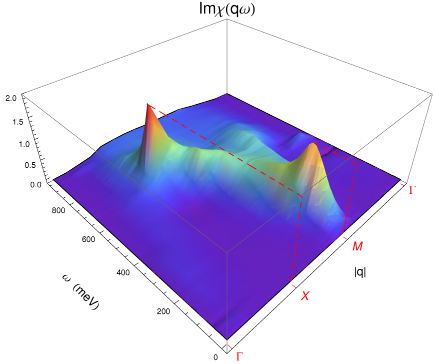

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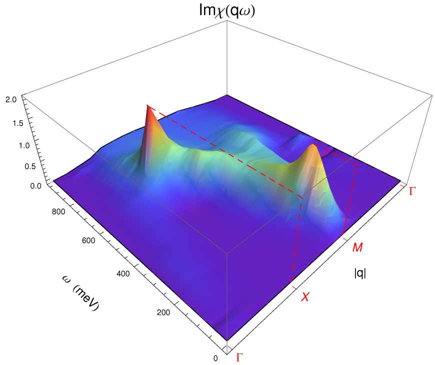

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- Starting point is the Heisenberg Hamiltonian:

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$$\theta_i \approx 0$$

The angle ϕ is time dependent:

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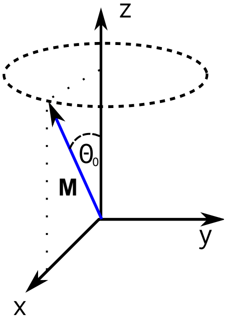

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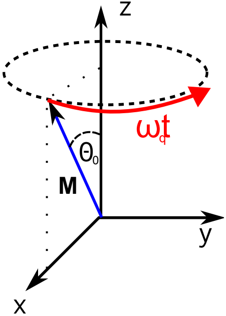

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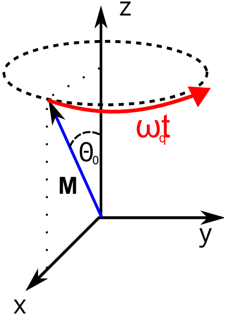

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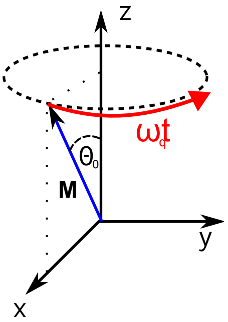

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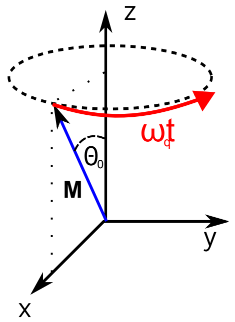

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$$\Rightarrow 0 = \det\left[\delta_{\mu\nu}\omega_{\mathbf{q}} - \sqrt{M_\mu M_\nu}\mathrm{Re}\left[\tilde{J}^{\mathbf{q}}_{\mu\nu}\right]\right]$$

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Magnon Energies for one Atom per Unit Cell

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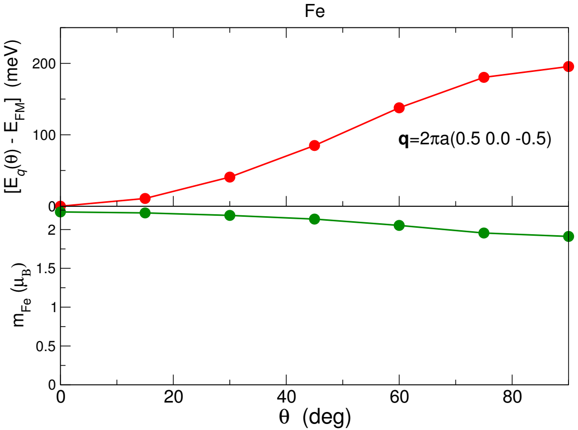

Energy Difference

$$\Delta E_{\mathbf{q}}(\theta) = \frac{\omega_{\mathbf{q}} M_0}{2} \sin^2(\theta)$$

Let's fit $\Delta E_{\mathbf{q}}(\theta)$ with $A_0 \sin^2(\theta)$.

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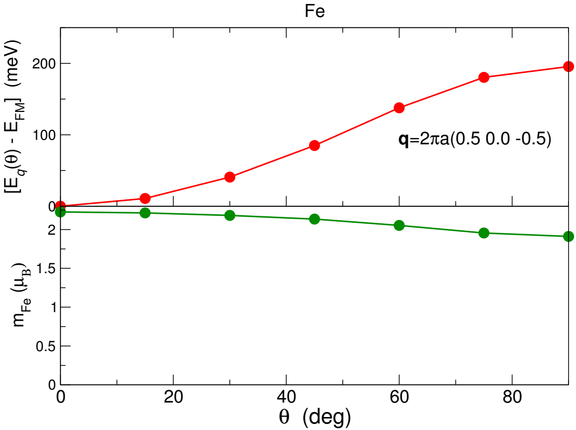

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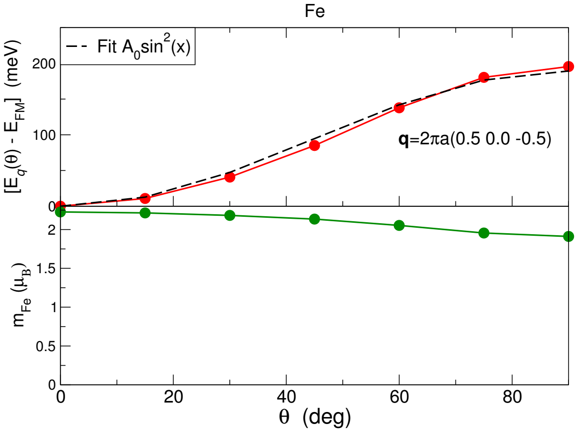

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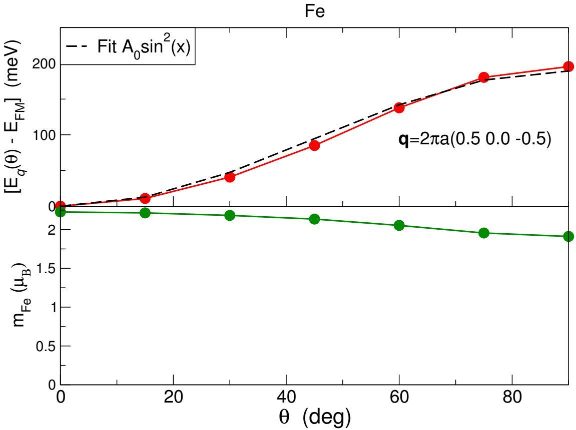

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- The excitation of magnons reduces the magnetic order.
- The energy needed to excite magnons is related to the critical temperature T_c.

Mean Field Approximation

$$T_c^{\mathrm{MFA}} = \frac{M}{3k_\mathrm{B}N} \sum_{\mathbf{q}\in\mathrm{BZ}}^{N} \omega_\mathbf{q}$$

Random Phase Approximation

$$T_c^{\mathrm{RPA}} = \frac{MN}{3k_\mathrm{B}} \left[\sum_{\mathbf{q}\in\mathrm{BZ}}^{N} \frac{1}{\omega_\mathbf{q}} \right]^{-1}$$

- In RPA values close to zero have a strong weight, hence $T_c^{\mathrm{RPA}} < T_c^{\mathrm{MFA}}$.
- The MFA overestimates the critical temperature $T_c^{\mathrm{exp}} < T_c^{\mathrm{MFA}}$.
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- The energy needed to excite magnons is related to the critical temperature T_c.

Mean Field Approximation

$$T_c^{\mathrm{MFA}} = \frac{M}{3k_{\mathrm{B}}N} \sum_{\mathbf{q}\in\mathrm{BZ}}^{N} \omega_{\mathbf{q}}$$

Random Phase Approximation

$$T_c^{\mathrm{RPA}} = \frac{MN}{3k_{\mathrm{B}}} \left[\sum_{\mathbf{q}\in\mathrm{BZ}}^{N} \frac{1}{\omega_{\mathbf{q}}} \right]^{-1}$$

- In RPA values close to zero have a strong weight, hence $T_c^{\mathrm{RPA}} < T_c^{\mathrm{MFA}}$.
- The MFA overestimates the critical temperature $T_c^{\mathrm{exp}} < T_c^{\mathrm{MFA}}$.
- As a rule of thumb one finds $T_c^{\mathrm{RPA}} \lessapprox T_c^{\mathrm{exp}} < T_c^{\mathrm{MFA}}$.

- Magnons are the low lying collective modes of the spin lattice.
- At the moment the elk code can only calculate "frozen magnons".
- The frozen magnon frequencies are obtained by energy differences of ground state calculations (quick).
- The Response function $\chi(\mathbf{q}\omega)$ will be soon in the code giving access to QP lifetimes .
- There is a simple connection $T_c \leftrightarrow \omega_\mathbf{q}$ within the MFA or RPA.

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Thank you for your attention

Questions:

1. For translation invariant potentials $v(\mathbf{r})_{2\times2}$ one finds:

$$\hat{T}\left[v(\mathbf{r})_{2\times2}\,\vec{\varphi}^{\text{Bloch}}_{n\mathbf{k}}(\mathbf{r})\right] = v(\mathbf{r})\,\hat{T}\left[\vec{\varphi}^{\text{Bloch}}_{n\mathbf{k}}(\mathbf{r})\right],$$

which is necessary to reduce the calculation to one unit cell. How a potential must look like in the spin spiral case to obtain the same essential property i.e.:

$$\hat{T}\left[v(\mathbf{r})_{2\times2}\,\vec{\varphi}^{\text{SS}}_{n\mathbf{k}}(\mathbf{r})\right] = v(\mathbf{r})_{2\times2}\,\hat{T}\left[\vec{\varphi}^{\text{SS}}_{n\mathbf{k}}(\mathbf{r})\right].$$

2. When you found the form of the potential, what are contributions to the Hamiltonian that could destroy this symmetry?
3. Look at the susceptibility of FeSe. What is strange?

Things you probably need:

1. The form of the spin spiral wavefunction is

$$\vec{\varphi}^{SS}_{n\mathbf{k}}(\mathbf{r}) = \begin{pmatrix} u_{n\mathbf{k}}(1,\mathbf{r})\, e^{i\left(\mathbf{k}-\frac{\mathbf{q}}{2}\right)\mathbf{r}} \\ u_{n\mathbf{k}}(2,\mathbf{r})\, e^{i\left(\mathbf{k}+\frac{\mathbf{q}}{2}\right)\mathbf{r}} \end{pmatrix}$$

   where the functions $u_{n\mathbf{k}}(1,\mathbf{r})$ and $u_{n\mathbf{k}}(2,\mathbf{r})$ are translation invariant *i.e.* $\hat{T}[u_{n\mathbf{k}}(1,\mathbf{r})] = u_{n\mathbf{k}}(1,\mathbf{r}+\mathbf{T}) = u_{n\mathbf{k}}(1,\mathbf{r})$.

2. The picture of the $\mathrm{Im}\chi^{+-}(\mathbf{q}\omega)$ in FeSe: