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 ⇒ 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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   - Magnons in the elk code (frozen magnon approach)
1\textsuperscript{st} Part

Non Collinear Ground States
Given a ground state $|\Psi_0\rangle$ of a system the ground state magnetic moment $m_0(r)$ is:

$$m_0(r) = \sum_{\alpha\beta=1}^{2} \langle \Psi_0 | \hat{\Psi}_\alpha(r) \tilde{\sigma}_{\alpha\beta} \hat{\Psi}_\beta(r) | \Psi_0 \rangle.$$ 

The $N$ particle problem can not be solved, so a different approach is needed to find the magnetic ground state of a system.
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- $m(r)=0$ everywhere (Non magnetic)
- $m(r) \parallel e_z$ everywhere (Collinear system)
- 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 $m_0(r)$ of a system.

**Green’s Function**

$$m_0(r) = \bar{\sigma}_{\alpha\beta} G_{\alpha\beta} (\mathbf{x}\mathbf{x}^+)$$

$$G(12) = G_0 (\mathbf{x}_1\mathbf{x}_2) \delta_{\alpha\beta}$$

$$+ \iiint d3d4 G_0 (13) M (34) G (42)$$

$$M_{\alpha\beta} = \begin{cases} 
\delta_{\alpha\beta} M & \text{non magnetic solution} \\
\delta_{\alpha\beta} M_{\alpha} & \text{collinear } m_0 (r) \\
M_{\alpha\beta} & \text{non collinear } m_0 (r) 
\end{cases}$$

**The Kohn-Sham Scheme (DFT)**

No external magnetic field.

$$m_0(r) = \sum_j^{\text{occ.}} \varphi_j^{KS*} \cdot \bar{\sigma}_{2\times2} \cdot \varphi_j^{KS}$$

$$\epsilon_j \varphi_j^{KS} = \left[ \hat{h}_0 1_{2\times2} + v_{xc}^{2\times2} [\rho, m] (r) \right] \cdot \varphi_j^{KS}$$

$$\hat{h}_0 = \left( -\frac{\Delta r}{2} + v_0 (r) + v_H [\rho] (r) \right)$$

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A non diagonal potential is necessary to get non collinear magnetism.
Using Green’s function or density functional theory (DFT) one can find the $m_0 (r)$ of a system.

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Using Green’s function or density functional theory (DFT) one can find the \( m_0 (r) \) of a system.

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**

\[
\nu_{\alpha\beta}^{xc} [\rho \mathbf{m}] (\mathbf{r}) = \delta_{\alpha\beta} \left[ \nu_{xc} [\rho \mathbf{m}] (\mathbf{r}) + z_\alpha B_{xc}^z [\rho \mathbf{m}] (\mathbf{r}) \right] \quad \text{diagonal}
\]

\[
+ \sigma_x^{\alpha\beta} \cdot B_{xc}^x [\rho \mathbf{m}] (\mathbf{r}) + \sigma_y^{\alpha\beta} \cdot B_{xc}^y [\rho \mathbf{m}] (\mathbf{r}) \quad \text{off diagonal}
\]

\[
\nu_{xc} [\rho \mathbf{m}] (\mathbf{r}) := \frac{\delta E^{xc} [\rho \mathbf{m}]}{\delta \rho (\mathbf{r})} \quad \text{and} \quad B_{xc} [\rho \mathbf{m}] (\mathbf{r}) := \frac{\delta E^{xc} [\rho \mathbf{m}]}{\delta \mathbf{m} (\mathbf{r})}
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Functionals like LSDA and GGA depend only on \( \rho \) and \( m_z \).
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**Exchange Correlation Potential**

$$v^{xc}_{\alpha\beta} [\rho \mathbf{m}] (\mathbf{r}) = \delta_{\alpha\beta} [v^{xc} [\rho \mathbf{m}] (\mathbf{r}) + z_{\alpha} B_{xc}^{z} [\rho \mathbf{m}] (\mathbf{r})] \quad \text{diagonal}$$

$$+ \sigma_{\alpha\beta}^{x} \cdot B_{xc}^{x} [\rho \mathbf{m}] (\mathbf{r}) + \sigma_{\alpha\beta}^{y} \cdot B_{xc}^{y} [\rho \mathbf{m}] (\mathbf{r}) \quad \text{off diagonal}$$

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Functionals like LSDA and GGA depend only on $\rho$ and $m_{z}$.
To save these functionals you can use the Kübler trick:

1. Starting point is a $\rho_{2\times2}(r)$ density:
   $$\rho_{2\times2}(r) := \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} \rho + m_z & m_x - im_y \\ m_x + im_y & \rho - m_z \end{pmatrix}.$$

2. A unitary transformation is used to diagonalize $\rho_{2\times2}(r)$:
   $$\begin{pmatrix} \tilde{\rho}_\uparrow & 0 \\ 0 & \tilde{\rho}_\downarrow \end{pmatrix} = U(r) \rho_{2\times2}(r) U^\dagger(r) \text{ with } \tilde{\rho} = \tilde{\rho}_\uparrow + \tilde{\rho}_\downarrow \text{ and } \tilde{m}_z = \tilde{\rho}_\uparrow - \tilde{\rho}_\downarrow.$$

3. The $\tilde{\rho}$ and $\tilde{m}_z$ are inserted in $\tilde{\nu}_{xc}^{\text{Dia}} [\tilde{\rho}\tilde{m}_z](r)$.

4. The inverse unitary transformation is used to transform the diagonal potential:
   $$\begin{pmatrix} \tilde{\nu}_{xc}^{\uparrow\uparrow} & \tilde{\nu}_{xc}^{\uparrow\downarrow} \\ \tilde{\nu}_{xc}^{\downarrow\uparrow} & \tilde{\nu}_{xc}^{\downarrow\downarrow} \end{pmatrix} = U^\dagger(r) \nu_{xc}^{\text{Dia}} [\tilde{\rho}\tilde{m}_z](r) U(r).$$

We have a non diagonal potential in hand, how NCM ground state calculations are practically done?
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Properties of $B_{xc}$

\[
B_{xc}^{(n)} := B_{xc} \left[ \rho^{(n-1)}, m^{(n-1)} \right] \parallel m^{(n-1)} \iff \text{Kübler trick} \quad (A)
\]

\[
B_{tot}^{(n)} := (B_{MT}^{\text{ext}} + B_{xc}^{(n)}) \parallel m^{(n)} \iff E = -m^{(n)} \cdot B_{tot}^{(n)} \quad (B)
\]

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

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m^{(n)} \parallel B_{MT}^{\text{ext}} \quad \xrightarrow{(A)} \quad B_{xc}^{(n+1)} \parallel m^{(n)}
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\[
m^{(n+1)} \parallel B_{MT}^{\text{ext}} \quad \xrightarrow{(B)} \quad m^{(n+1)} \parallel m^{(n)}
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m^{(\text{final})} \parallel B_{MT}^{\text{ext}} \Rightarrow \text{The external fields can be used to guide the code towards a desired magnetic structure.}
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Properties of $B_{\text{xc}}$

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

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$m^{(\text{final})} \parallel B_{ext}^{MT} \Rightarrow$ The external fields can be used to guide the code towards a desired magnetic structure.
Complicated magnetic structure $\iff$ Larger unit cells

If one gets $m_{MT}^{(\text{final})} \neq 0$ within the self consistent cycles depends on the topology of the energy surface.
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If the system is pushed towards one magnetic structure
- It may converge in that structure
- or go back to the NM state

The ground state is $E_0 = \min\{\text{All structures}\}$

$E_0 \approx \min\{E_{\text{NC2}}, E_{\text{NC1}}, E_{\text{FM}}, E_{\text{AFM}}, E_{\text{NM}}\}$. 
If the system is pushed towards one magnetic structure

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Ground State Calculation

Excitations

Definition of CM and NCM

NC Magnetic Ground State Calculation

The Spin Spiral Ansatz

Summary - Non Collinear Magnetic Ground States

Bloch State

$$\vec{\phi}_{nk}(r) = \begin{pmatrix} u_{nk}(1, r) e^{ikr} \\ u_{nk}(2, r) e^{ikr} \end{pmatrix}$$

$$u_{nk}(\alpha, r + T) = u_{nk}(\alpha, r)$$

$$\Rightarrow m_0(r + T) = m_0(r)$$

Spin Spiral Ansatz

$$\vec{\phi}_{nk}(r) = \begin{pmatrix} u_{nk}(1, r) e^{i(k - \frac{q}{2})r} \\ u_{nk}(2, r) e^{i(k + \frac{q}{2})r} \end{pmatrix}$$

Moment is rotating with

$$\phi = q \cdot r.$$
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\tilde{\varphi}_{nk}(r) = \begin{pmatrix}
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**Spin Spiral - Magnetic Moment**

\[
m_q(r) = M(\theta_0) \begin{pmatrix}
    \cos(\phi_0 + q \cdot r) \sin(\theta_0) \\
    \sin(\phi_0 + q \cdot r) \sin(\theta_0) \\
    \cos(\theta_0)
\end{pmatrix}
\]
The angles $\theta_0$ and $\phi_0$ are controlled via $B^\text{ext}_{\text{MT}}$.

Periodic magnetic structures are constructed using a planar spiral:

- $\theta_0$ is set to $90^\circ$
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2nd Part
Magnetic Excitations
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The quantized modes of the spin waves are called "magnons".

Magnons are bosonic quasi-particles (QP) carrying $1\mu_B$.

The energies and lifetimes are $\omega_q^{\text{Max}} \approx \text{few} \ 100 \ \text{meV}$ and $\tau_q \in [10^{-4} \text{s}, 10^{-14} \text{s}]$.

A Magnon ranges over the whole crystal
⇒ "Collective excitation"

Dispersion $\lim_{q \to 0} \omega_q^{\text{FM}} \propto |q|^2$ and $\lim_{q \to 0} \omega_q^{\text{AFM}} \propto |q|$
⇒ "Low lying excitation"

Two approaches to obtain magnon spectra:
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$\chi$ with Green’s functions

\[ \chi = P + P v \chi \]

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\[ \chi = \chi_{KS} + \chi_{KS} (v + f_{xc}) \chi \]

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$P \begin{align*}
&= \begin{array}{c}
\text{Diagram 1} \\
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![3D plot of Imχ(qω)]
Starting point is the Heisenberg Hamiltonian:

$$\hat{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \hat{M}_i(t) \cdot \hat{M}_j(t).$$

The equations of motion reads:

$$\dot{\hat{M}}_j(t) = [\hat{H}, \hat{M}_j] (t) = \sum_{i(\neq j)} J_{ij} \left( \hat{M}_j(t) \times \hat{M}_i(t) \right)$$

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\[ \left\langle \hat{M}_j(t) \right\rangle \approx \sum_{i(\neq j)} J_{ij} \left( \left\langle \hat{M}_j(t) \right\rangle \times \left\langle \hat{M}_i(t) \right\rangle \right). \]

• The times scales of electron hopping (fast) and the magnon movement (slow) justifies an adiabatic approximation:

\[ \left\langle \hat{M}_j(t) \right\rangle \approx \left\langle \hat{M}_j \right\rangle(t). \]
Starting point is the Heisenberg Hamiltonian:

\[ \hat{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \hat{\mathbf{M}}_i(t) \cdot \hat{\mathbf{M}}_j(t). \]

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Spin Wave Moment

\[
\langle \hat{M}_i \rangle (t) := M_i(t) = M_i \left( \begin{array}{c}
\cos (\phi_i(t)) \sin (\theta_i) \\
\sin (\phi_i(t)) \sin (\theta_i) \\
\cos \theta_i
\end{array} \right)
\]

\[
\theta_i \approx 0
\]

The angle \( \phi \) is time dependent:

\[
\phi_i(t) = \phi_0 + q \cdot R_i + \omega_q t.
\]

- \( M_i(t) \) has no damping, so the magnons have infinite lifetime.
- Insert \( M_i(t) \) in the equation of motion, linearize \( \sin \theta_i \approx \theta_i \) to get an eigen value problem in real space:

\[
\theta_k \omega_q = \sum_{i(\neq k)} J_{ki} (\delta_{ik} - \cos (\phi_k - \phi_i)) M_i \theta_i.
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Spin Wave Moment

\[ \langle \hat{M}_i \rangle (t) := M_i(t) = M_i \begin{pmatrix} \cos (\phi_i(t)) \sin (\theta_i) \\ \sin (\phi_i(t)) \sin (\theta_i) \\ \cos \theta_i \end{pmatrix} \]

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The eigen value problem is transformed to inverse space:

$$\sqrt{M_\mu} \theta_\mu \omega_q = \sum_\nu \sqrt{M_\mu M_\nu} \text{Re} \left[ J_q^{\mu \nu} \right] \sqrt{M_\nu} \theta_\nu.$$

$$\Rightarrow 0 = \det \left[ \delta_{\mu \nu} \omega_q - \sqrt{M_\mu M_\nu} \text{Re} \left[ J_q^{\mu \nu} \right] \right]$$

The indices $\mu$ and $\nu$ run over all $m_{MT}$ in the unit cell.

The matrix $J_q^{\mu \nu}$ is related to the energy surface $E_q (\{\theta_\lambda\}):$

$$\text{Re} \left[ J_q^{\mu \nu} \right] = \frac{1}{M_\mu M_\nu} \left. \frac{\partial^2 E_q (\{\theta_\lambda\})}{\partial \theta_\mu \partial \theta_\nu} \right|_{\{\theta_\lambda\}=0}.$$

The $E_q (\{\theta_\lambda\})$ can be obtained using static SS calculations with fixed $\{\theta_\lambda\}$ and $q$. 

The Frozen Magnon Approach
The eigen value problem is transformed to inverse space:

$$\sqrt{M_\mu} \theta_\mu \omega_\mathbf{q} = \sum_\nu \sqrt{M_\mu M_\nu} \text{Re} \left[ \tilde{J}^{\mathbf{q}}_{\mu \nu} \right] \sqrt{M_\nu} \theta_\nu. $$

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The Energy $E_q(\theta)$ of an spin spiral state with one magnetic atom per unit cell (for any $\theta$):

$$E_q(\theta) = \frac{1}{2} \text{Re} \left[ \tilde{J}^0 \right] M^2(\theta) + \frac{1}{2} \text{Re} \left[ \tilde{J}_q \right] M^2(\theta) \sin^2(\theta).$$

For small angles $M(\theta) \approx M(\theta = 0) = M_0$ and the eigenvalue equation is also valid:

$$E_q(\theta)^{\text{small}} \approx E_{FM} + \frac{1}{2} \text{Re} \left[ \tilde{J}_q \right] M_0^2 \sin^2(\theta)$$

$$\omega_q = M_0 \text{Re} \left[ \tilde{J}_q \right].$$

**Magnon Energies for one Atom per Unit Cell**

$$\omega_q = \lim_{\theta \to 0} \frac{2 \left[ E_q(\theta) - E_{FM} \right]}{M_0 \sin^2(\theta)}$$

The largest angles for which this equation holds depends on the material.
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Ground State Calculation

Excitations

Magnons: Definition, Properties...

Different Approaches to Calculate the \( \chi^{\pm}(q, \omega) \)

The Frozen Magnon Approach

Summary - Magnons

Energy Difference

\[
\Delta E_q(\theta) = \frac{\omega_q M_0}{2} \sin^2(\theta)
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Let's fit \( \Delta E_q(\theta) \) with \( A_0 \sin^2(\theta) \).

- Extremely good natured behavior for Fe.
- In the afternoon you will do FCC Ni, which shows a bit more 😊.
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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**

$$T_c^{\text{MFA}} = \frac{M}{3k_B N} \sum_{q \in \text{BZ}} \omega_q$$

**Random Phase Approximation**

$$T_c^{\text{RPA}} = \frac{MN}{3k_B} \left[ \sum_{q \in \text{BZ}} \frac{1}{\omega_q} \right]^{-1}$$

● In RPA values close to zero have a strong weight, hence $T_c^{\text{RPA}} < T_c^{\text{MFA}}$.

● The MFA overestimates the critical temperature $T_c^{\text{exp}} < T_c^{\text{MFA}}$.

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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 $\chi(q\omega)$ will be soon in the code giving access to QP lifetimes.

There is a simple connection $T_c \leftrightarrow \omega_q$ within the MFA or RPA.
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Thank you for your attention
Questions:

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

$$\hat{T} \left[ v(r)_{2 \times 2} \varphi_{nk}^{\text{Bloch}}(r) \right] = v(r) \hat{T} \left[ \varphi_{nk}^{\text{Bloch}}(r) \right],$$

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.:

$$\hat{T} \left[ v(r)_{2 \times 2} \varphi_{nk}^{\text{SS}}(r) \right] = v(r)_{2 \times 2} \hat{T} \left[ \varphi_{nk}^{\text{SS}}(r) \right].$$

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

\[ \varphi_{nk}^{SS}(r) = \begin{pmatrix} u_{nk}(1, r) e^{i(k - \frac{q}{2})r} \\ u_{nk}(2, r) e^{i(k + \frac{q}{2})r} \end{pmatrix} \]

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

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