Magnetic Diffraction

Roger Johnson

Part 1: Magnetic scattering

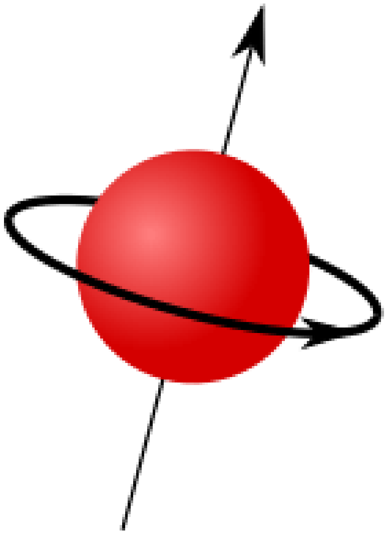
Part 2: Types of magnetic structure

Part 3: Magnetic diffraction

Electron’s magnetic moment

The classical moment from a current loop

$$\boldsymbol{\mu} = IA\hat{\boldsymbol{n}}$$



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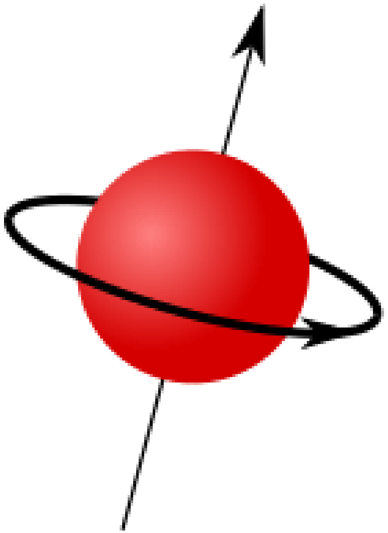

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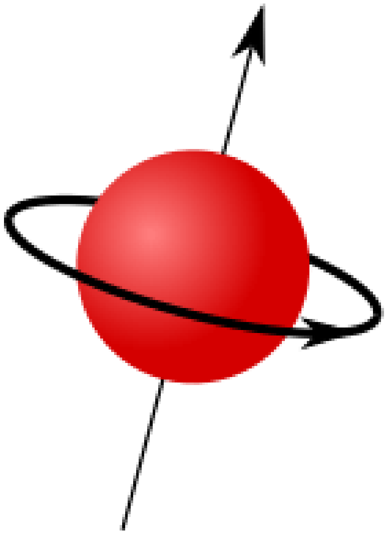
$$\boldsymbol{\mu} = -\frac{ev_\mathrm{e}}{2}r = -\frac{\mu_\mathrm{B}}{\hbar}\boldsymbol{L}$$

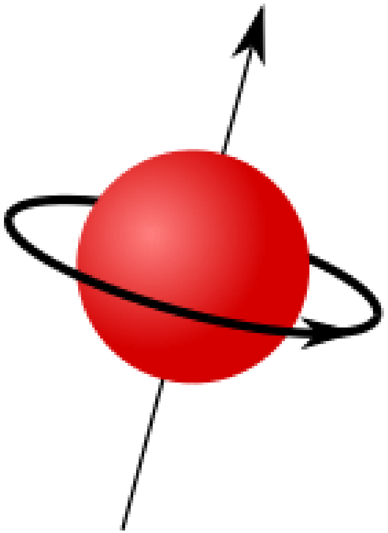
where $\mu_\mathrm{B} = \frac{e\hbar}{2m_\mathrm{e}}$, and $\boldsymbol{L} = v_\mathrm{e} r m_\mathrm{e}$



Electron's magnetic moment

The quantum moment: dimensionless g-factor

$$\boldsymbol{\mu_s} = -g_s \frac{\mu_\mathrm{B}}{\hbar}\boldsymbol{s} \qquad \boldsymbol{\mu_l} = -g_l \frac{\mu_\mathrm{B}}{\hbar}\boldsymbol{l} \qquad g_s \sim 2, \quad g_l = 1$$

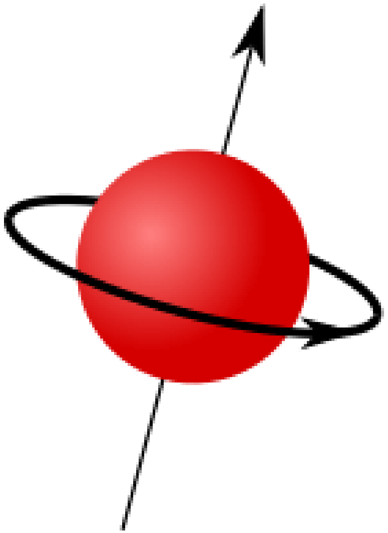


Atom’s magnetic moment

$$\boldsymbol{\mu_s} = -g_s \frac{\mu_\mathrm{B}}{\hbar} \boldsymbol{s} \qquad \boldsymbol{\mu_l} = -g_l \frac{\mu_\mathrm{B}}{\hbar} \boldsymbol{l} \qquad g_s \sim 2, \quad g_l = 1$$

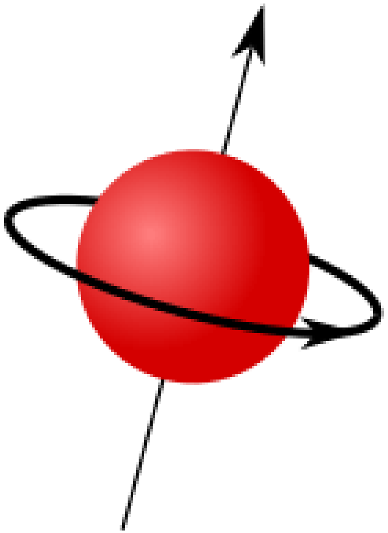
$$\boldsymbol{S} = \sum_i \boldsymbol{s}_i \qquad \boldsymbol{L} = \sum_i \boldsymbol{l}_i$$

$$\boldsymbol{\mu_S} = -g_s \frac{\mu_\mathrm{B}}{\hbar} \boldsymbol{S} \qquad \boldsymbol{\mu_L} = -g_l \frac{\mu_\mathrm{B}}{\hbar} \boldsymbol{L}$$



Atom's magnetic moment

$$\boldsymbol{\mu}_{\boldsymbol{S}} = -g_S \frac{\mu_{\mathrm{B}}}{\hbar} \boldsymbol{S} \qquad \boldsymbol{\mu}_{\boldsymbol{L}} = -g_L \frac{\mu_{\mathrm{B}}}{\hbar} \boldsymbol{L} \qquad g_S \sim 2, \quad g_L = 1$$



From LS coupling $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, and

$$\boldsymbol{\mu}_{\boldsymbol{J}} = -g_J \boldsymbol{J} \qquad g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

Neutron’s magnetic moment

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e}$$

From experiment $|\boldsymbol{\mu}_n| = -1.913\mu_{\mathrm{N},}$

where $\mu_{\mathrm{N}} = \frac{e\hbar}{2m_{\mathrm{p}}} = 5.051 \times 10^{-27}\mathrm{JT}^{-1}$ is the nuclear magneton

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$$\boldsymbol{\mu}_n = -g_n \frac{\mu_{\mathrm{N}}}{\hbar} \boldsymbol{I}$$

$\langle \boldsymbol{I} \rangle = \boldsymbol{s}_n \hbar$, where $\boldsymbol{s}_n = \pm \frac{1}{2}$. Hence $g_n = 3.826$

Born approximation (elastic scattering)

We will assume that the perturbation *V* does not act on the target's eigenstates (*i.e.* the state of the target is not changed by the interaction with a neutron)

Will consider only elastic scattering of neutrons

A central result of the Born approximation is that the differential scattering cross-section depends upon the Fourier transform, $V(\boldsymbol{Q})$, of the interaction potential $V(\boldsymbol{r})$.

$$\boxed{\frac{d\sigma}{d\Omega} = \left(\frac{m_\mathrm{n}}{2\pi\hbar^2}\right)^2 |\langle\sigma_f|V(\boldsymbol{Q})|\sigma_i\rangle|^2}$$

Magnetic interaction potential

- The neutron’s spin couples to microscopic electromagnetic fields in the sample
- The strongest, and hence good approximation, is the dipole-dipole interaction

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$$V(\boldsymbol{r}) = -\boldsymbol{\mu}_{\mathrm{N}} \cdot \boldsymbol{B}(\boldsymbol{r})$$

- $\boldsymbol{B}(\boldsymbol{r})$ is a local magnetic flux density due to unpaired electrons in the sample

$$\boldsymbol{B}(\boldsymbol{r}) = \boldsymbol{B}_S(\boldsymbol{r}) + \boldsymbol{B}_L(\boldsymbol{r})$$

$$\boldsymbol{B}_S(\boldsymbol{r}) = -2\mu_{\mathrm{B}}\frac{\mu_0}{4\pi}\nabla \times \left(\frac{\boldsymbol{s} \times \boldsymbol{r}}{r^3}\right) \qquad \boldsymbol{B}_L(\boldsymbol{r}) = -2\mu_{\mathrm{B}}\frac{\mu_0}{4\pi}\frac{1}{\hbar}\left(\frac{\boldsymbol{p} \times \boldsymbol{r}}{r^3}\right) \qquad (g_e = 2)$$

where $\boldsymbol{s}$ is the electron's spin and $\boldsymbol{p}$ the electron's momentum

Magnetic interaction potential

Consider a system of many electrons, each labeled *j*. Calculating the Fourier transform of $\boldsymbol{B}(\boldsymbol{r})$ one finds:

$$\{\boldsymbol{B}_S(\boldsymbol{Q})\}_j = -2\mu_B\mu_0 \left\{\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{s}_j \times \widehat{\boldsymbol{Q}}\right)\right\} \exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)$$

$$\{\boldsymbol{B}_L(\boldsymbol{Q})\}_j = -2\mu_B\mu_0 \frac{i}{\hbar Q}\left(\boldsymbol{p}_j \times \widehat{\boldsymbol{Q}}\right) \exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)$$

Taking $\boldsymbol{\mu}_{\mathrm{n}} = -g_{\mathrm{n}}\mu_{\mathrm{N}}\boldsymbol{s}_{\mathrm{n}}$,

$$V(\boldsymbol{Q}) = -\boldsymbol{\mu}_{\mathrm{N}}\cdot\boldsymbol{B}(\boldsymbol{Q}) = -2g_{\mathrm{n}}\mu_B\mu_0\mu_{\mathrm{N}}\boldsymbol{s}_{\mathrm{n}}\cdot\sum_j\left\{\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{s}_j \times \widehat{\boldsymbol{Q}}\right) + \frac{i}{\hbar Q}\left(\boldsymbol{p}_j \times \widehat{\boldsymbol{Q}}\right)\right\}\exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)$$

Magnetic interaction potential (strength of interaction)

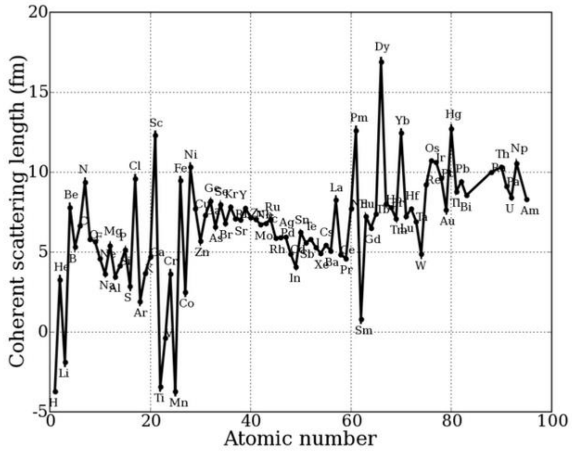
$$\frac{d\sigma}{d\Omega} = \left(\frac{m_{\mathrm{N}}}{2\pi\hbar^2}\right)^2 |\langle\sigma_f|V(\boldsymbol{Q})|\sigma_i\rangle|^2$$

$$V(\boldsymbol{Q}) = -2g_{\mathrm{n}}\mu_B\mu_0\mu_{\mathrm{N}}\boldsymbol{s}_{\mathrm{n}} \cdot \sum_j \left\{\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{s}_j \times \widehat{\boldsymbol{Q}}\right) + \frac{i}{\hbar Q}\left(\boldsymbol{p}_j \times \widehat{\boldsymbol{Q}}\right)\right\} \exp(i\boldsymbol{Q} \cdot \boldsymbol{r}_j)$$

$$\frac{d\sigma}{d\Omega} \propto \left(\frac{2g_{\mathrm{n}}\mu_{\mathrm{B}}\mu_0\mu_{\mathrm{N}}|\boldsymbol{s}_{\mathrm{n}}|m_{\mathrm{N}}}{2\pi\hbar^2}\right)^2 = \left(\frac{g_{\mathrm{n}}r_0}{2}\right)^2 = (5.39)^2\ \mathrm{fm}^2$$

where $\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e}$, $\mu_{\mathrm{N}} = \frac{e\hbar}{2m_{\mathrm{n}}}$, $r_0 = \frac{\mu_0 e^2}{4\pi m_e}$

For nuclear scattering $\frac{d\sigma}{d\Omega} \propto b^2$



Magnetic interaction potential

Consider a spatially varying magnetization, $\boldsymbol{M}(\boldsymbol{r}) = \boldsymbol{M}_S(\boldsymbol{r}) + \boldsymbol{M}_L(\boldsymbol{r})$

Magnetic interaction potential

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$$\boldsymbol{M}_S(\boldsymbol{r}) = -2\mu_{\mathrm{B}} \sum_j \delta(\boldsymbol{r} - \boldsymbol{r}_j)\boldsymbol{s}_j$$ (sum over localized spins)

$$\boldsymbol{M}_S(\boldsymbol{Q}) = -2\mu_{\mathrm{B}} \sum_j \boldsymbol{s}_j \exp(i\boldsymbol{Q}.\boldsymbol{r}_j)$$

Magnetic interaction potential

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$$\boldsymbol{M}_S(\boldsymbol{Q}) = -2\mu_\mathrm{B}\sum_j \boldsymbol{s}_j \exp(i\boldsymbol{Q}.\boldsymbol{r}_j)$$

$$V(\boldsymbol{Q}) = -2g_\mathrm{n}\mu_B\mu_0\mu_\mathrm{N}\boldsymbol{s}_\mathrm{n}\cdot\sum_j\left\{\widehat{\boldsymbol{Q}}\times\left(\boldsymbol{s}_j\times\widehat{\boldsymbol{Q}}\right)+\frac{i}{\hbar Q}\left(\boldsymbol{p}_j\times\widehat{\boldsymbol{Q}}\right)\right\}\exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)$$

$$= 2g_\mathrm{n}\mu_B\mu_0\mu_\mathrm{N}\boldsymbol{s}_\mathrm{n}\cdot\left[\frac{1}{2\mu_\mathrm{B}}\widehat{\boldsymbol{Q}}\times\left(\boldsymbol{M}_S(\boldsymbol{Q})\times\widehat{\boldsymbol{Q}}\right)-\sum_j\frac{i}{\hbar Q}\left(\boldsymbol{p}_j\times\widehat{\boldsymbol{Q}}\right)\exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)\right]$$

Magnetic interaction potential

One can similarly show that

$$\sum_j \frac{i}{\hbar Q}\left(\boldsymbol{p}_j \times \widehat{\boldsymbol{Q}}\right)\exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j) = -\frac{1}{2\mu_\mathrm{B}}\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_L(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right)$$

$$V(\boldsymbol{Q}) = 2g_\mathrm{n}\mu_B\mu_0\mu_\mathrm{N}\boldsymbol{s}_\mathrm{n}\cdot\left[\frac{1}{2\mu_\mathrm{B}}\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_S(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right) - \sum_j \frac{i}{\hbar Q}\left(\boldsymbol{p}_j \times \widehat{\boldsymbol{Q}}\right)\exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)\right]$$

$$= g_\mathrm{n}\mu_0\mu_\mathrm{N}\boldsymbol{s}_\mathrm{n}\cdot\left[\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_S(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right) + \widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_L(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right)\right]$$

Magnetic interaction potential

$$V(\boldsymbol{Q}) = g_{\mathrm{n}}\mu_0\mu_{\mathrm{N}}\boldsymbol{s}_{\mathrm{n}} \cdot \left[\widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_S(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right) + \widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_L(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right)\right]$$

$$= g_{\mathrm{n}}\mu_0\mu_{\mathrm{N}}\boldsymbol{s}_{\mathrm{n}} \cdot \boldsymbol{M}_{\perp}(\boldsymbol{Q})$$

where $\boldsymbol{M}(\boldsymbol{Q}) = \boldsymbol{M}_S(\boldsymbol{Q}) + \boldsymbol{M}_L(\boldsymbol{Q})$

and $\boldsymbol{M}_{\perp}(\boldsymbol{Q}) = \widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right)$

Magnetic differential scattering cross-section

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e},\ \mu_{\mathrm{N}} = \frac{e\hbar}{2m_{\mathrm{n}}},\ r_0 = \frac{\mu_0 e^2}{4\pi m e}$$

$$V(\boldsymbol{Q}) = g_{\mathrm{n}}\mu_0\mu_{\mathrm{N}}\boldsymbol{s}_{\mathrm{n}} \cdot \boldsymbol{M}_{\perp}(\boldsymbol{Q}) = \left(\frac{2\pi\hbar^2}{m_{\mathrm{N}}}\right)\left(\frac{g_{\mathrm{n}} r_0}{2\mu_{\mathrm{B}}}\right)\boldsymbol{s}_{\mathrm{n}} \cdot \boldsymbol{M}_{\perp}(\boldsymbol{Q})$$

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$$\frac{d\sigma}{d\Omega} = \left(\frac{m_{\mathrm{N}}}{2\pi\hbar^2}\right)^2 |\langle\sigma_f|V(\boldsymbol{Q})|\sigma_i\rangle|^2 = \left(\frac{g_{\mathrm{n}}r_0}{2\mu_{\mathrm{B}}}\right)^2 |\langle\sigma_f|\boldsymbol{s}_n|\sigma_i\rangle\langle\boldsymbol{M}_{\perp}(\boldsymbol{Q})\rangle|^2$$

For unpolarized neutrons, we evaluate $\langle\sigma_f|\boldsymbol{s}_n|\sigma_i\rangle$, averaged over σ_i and σ_f, giving $\frac{1}{2}$

$$\boxed{\frac{d\sigma}{d\Omega} = \left(\frac{g_{\mathrm{n}}r_0}{4\mu_{\mathrm{B}}}\right)^2 |\langle\boldsymbol{M}_{\perp}(\boldsymbol{Q})\rangle|^2}$$

M(*Q*) of an atom: Magnetic form factors

- Ignore filled shells
- Assume atomic-like orbitals for unpaired electrons
- To good approximation:

$$\boldsymbol{M}(Q) \simeq -2\mu_{\mathrm{B}}\left[\langle j_0(Q)\rangle \boldsymbol{S} + \tfrac{1}{2}\{\langle j_0(Q)\rangle + \langle j_2(Q)\rangle\}\boldsymbol{L}\right] = -g_J\mu_{\mathrm{B}}\boldsymbol{J}f(\mathrm{Q}) = \boldsymbol{\mu}f(Q)$$

where $f(Q) = \langle j_0(Q)\rangle + \left(\frac{2-g_J}{g_J}\right)\langle j_2(Q)\rangle$

and $\langle j_n(Q)\rangle = \int_0^\infty j_n(Qr)r^2R^2(r)\mathrm{d}r$, where $j_n(Qr)$ is a spherical Bessel function

M(*Q*) of an atom: Magnetic form factors

$$\boldsymbol{M}(Q) \simeq \boldsymbol{\mu} f(Q)$$

$$f(Q) = \langle j_0(Q) \rangle + \left(\frac{2-g_J}{g_J}\right) \langle j_2(Q) \rangle$$

When $Q = 0$, $\langle j_0 \rangle = 1$, $\langle j_2 \rangle = 0$, and $\boldsymbol{M}(Q) \simeq \boldsymbol{\mu}$

Hence this approximation is known as *the dipole approximation*

Penelope Jane Brown

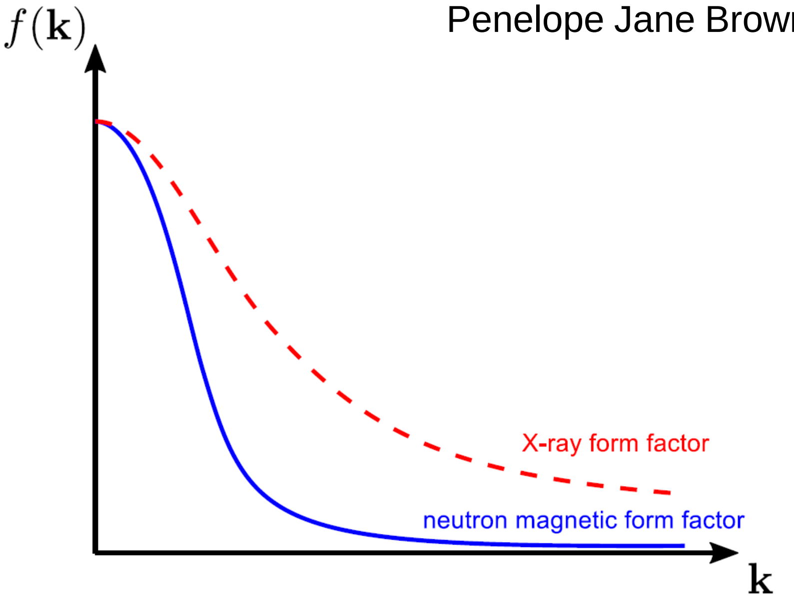
M(*Q*) of an atom: Magnetic form factors

$$\langle j_0(s)\rangle = A\exp(-as^2) + B\exp(-bs^2) + C\exp(-cs^2) + D$$

$$\langle j_2(s)\rangle = [A\exp(-as^2) + B\exp(-bs^2) + C\exp(-cs^2) + D]s^2$$

$$s = \frac{\sin\theta}{\lambda}$$

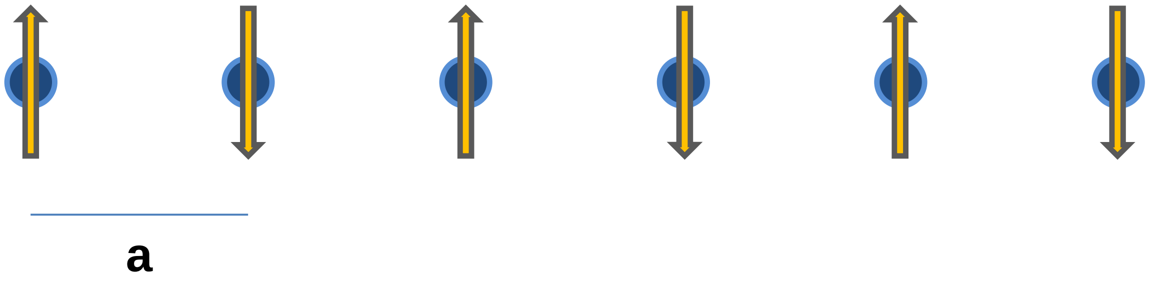
https://www.ill.eu/sites/ccsl/ffacts/ffachtml.html



Part 2: Types of magnetic structure

- The propagation vector
- Ferromagnets
- Collinear commensurate antiferromagnets
- Canted commensurate antiferromagnets / weak ferromagnets
- Incommensurate spin density waves
- Incommensurate cycloids and helices

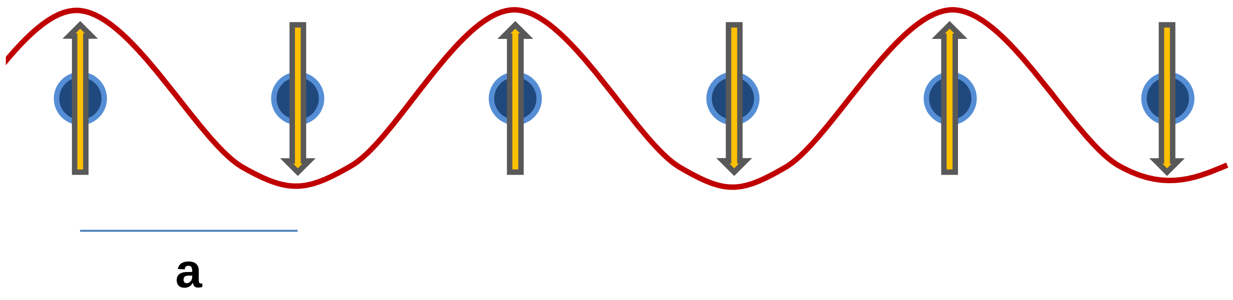
The propagation vector



The propagation vector

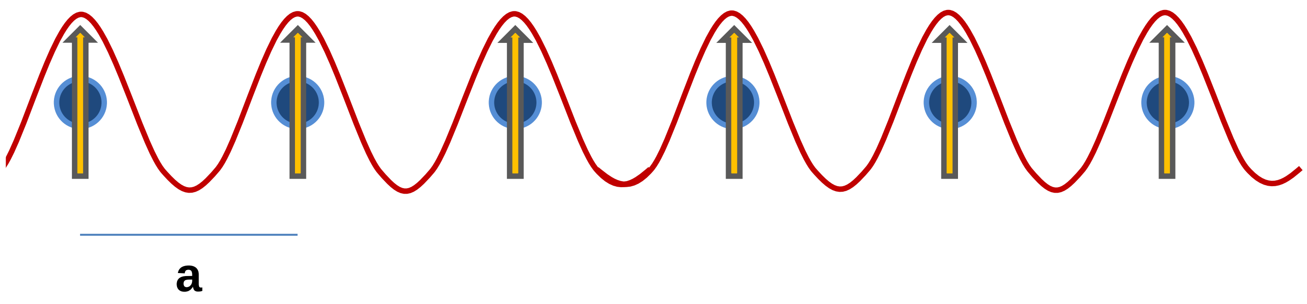
$$\boldsymbol{q} = \left(\frac{1}{2}, 0{,}0\right)$$

$\cos(2\pi\boldsymbol{q}\cdot\boldsymbol{R})$



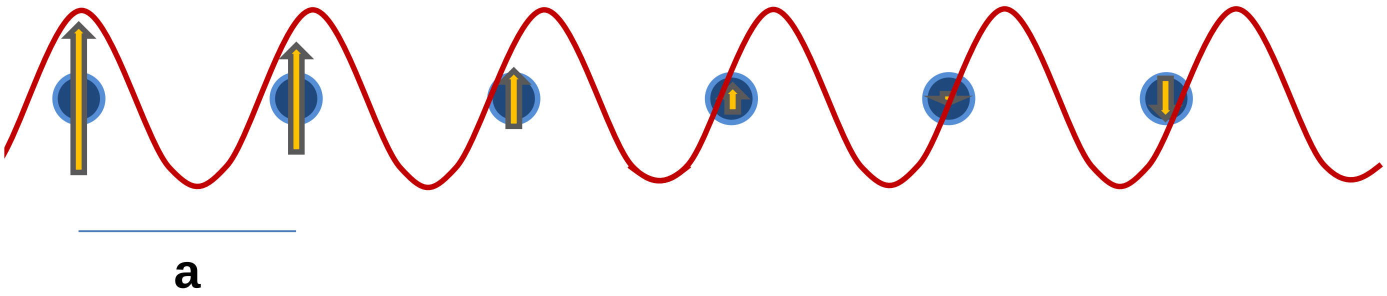
The propagation vector

$$\boldsymbol{q} = (0,0,0)$$



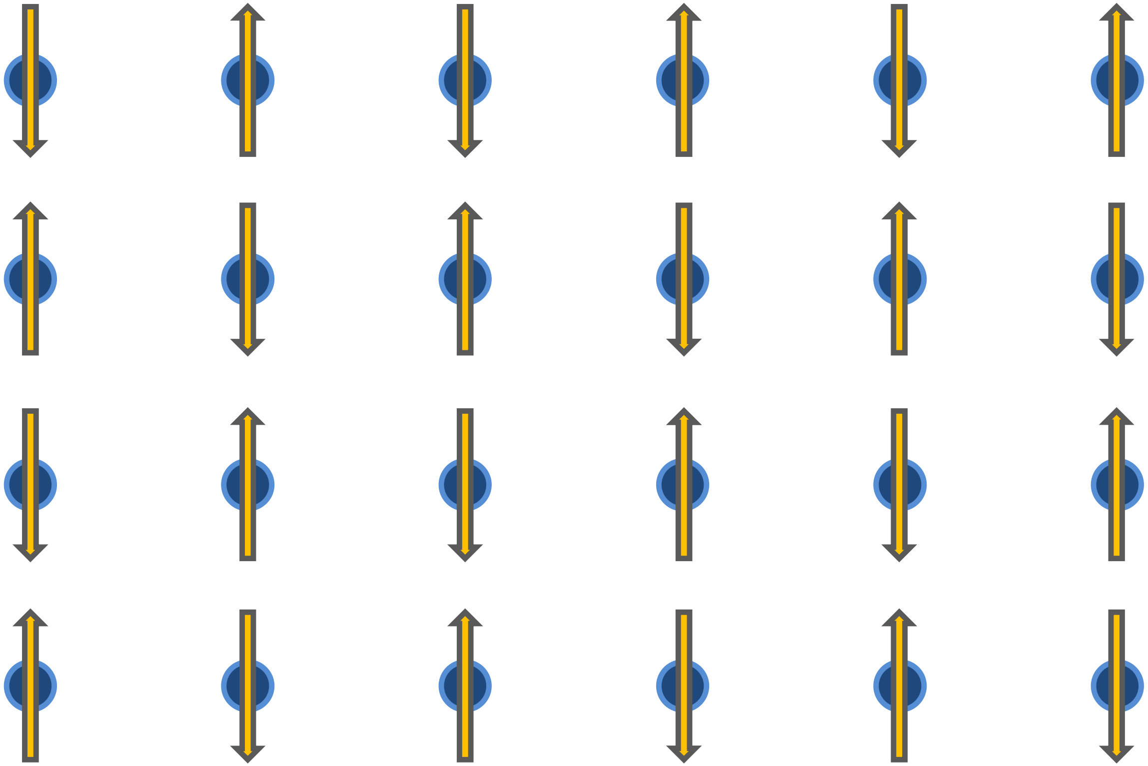
The propagation vector

$$\boldsymbol{q} = (\delta, 0,0)$$



The propagation vector

$$\boldsymbol{q} = \left(\frac{1}{2}, \frac{1}{2}, 0\right)$$



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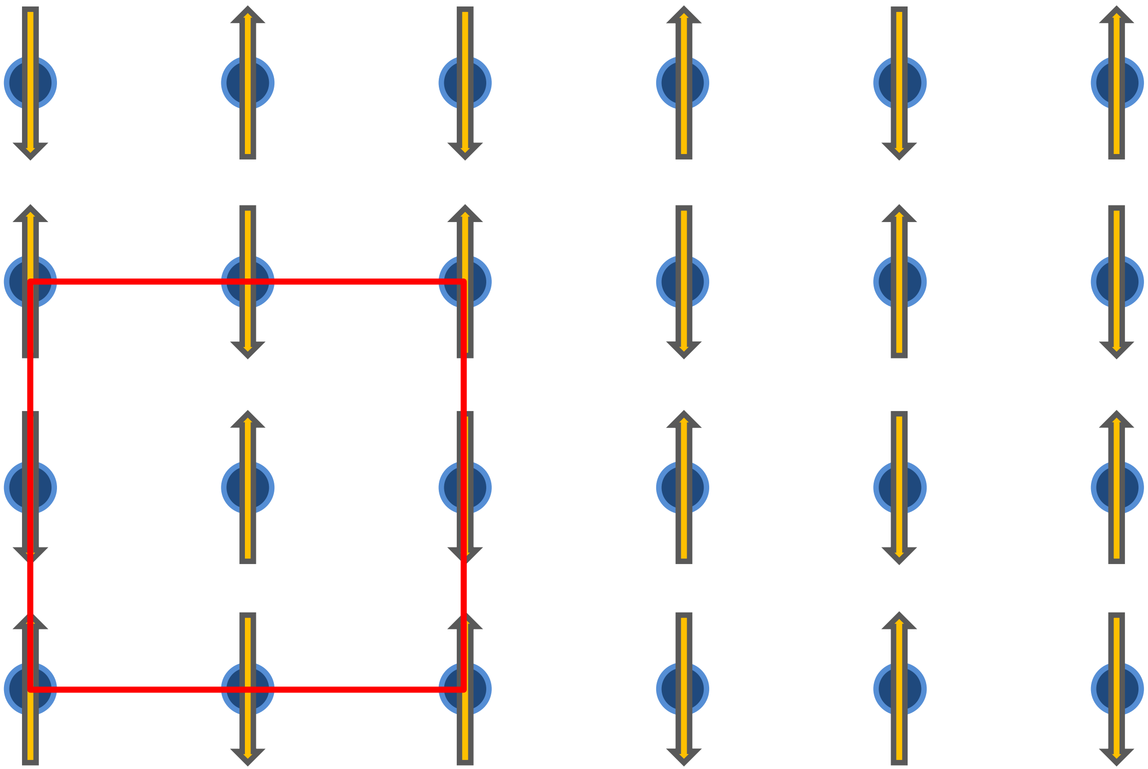

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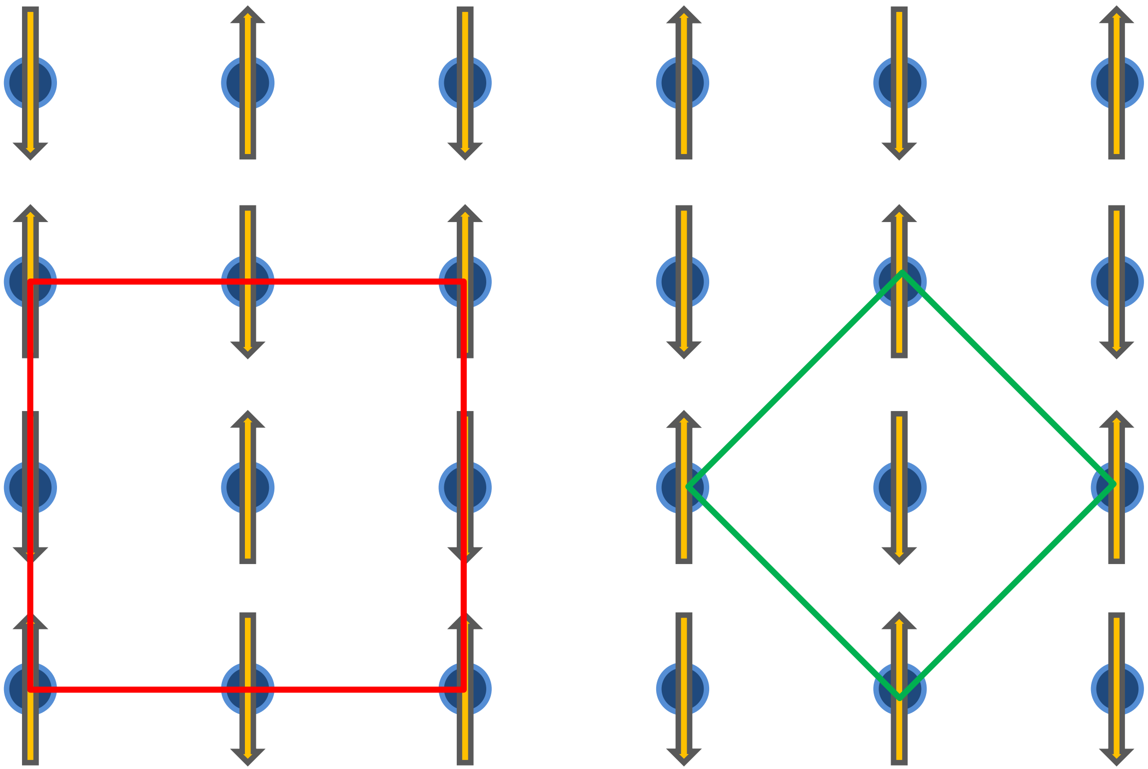

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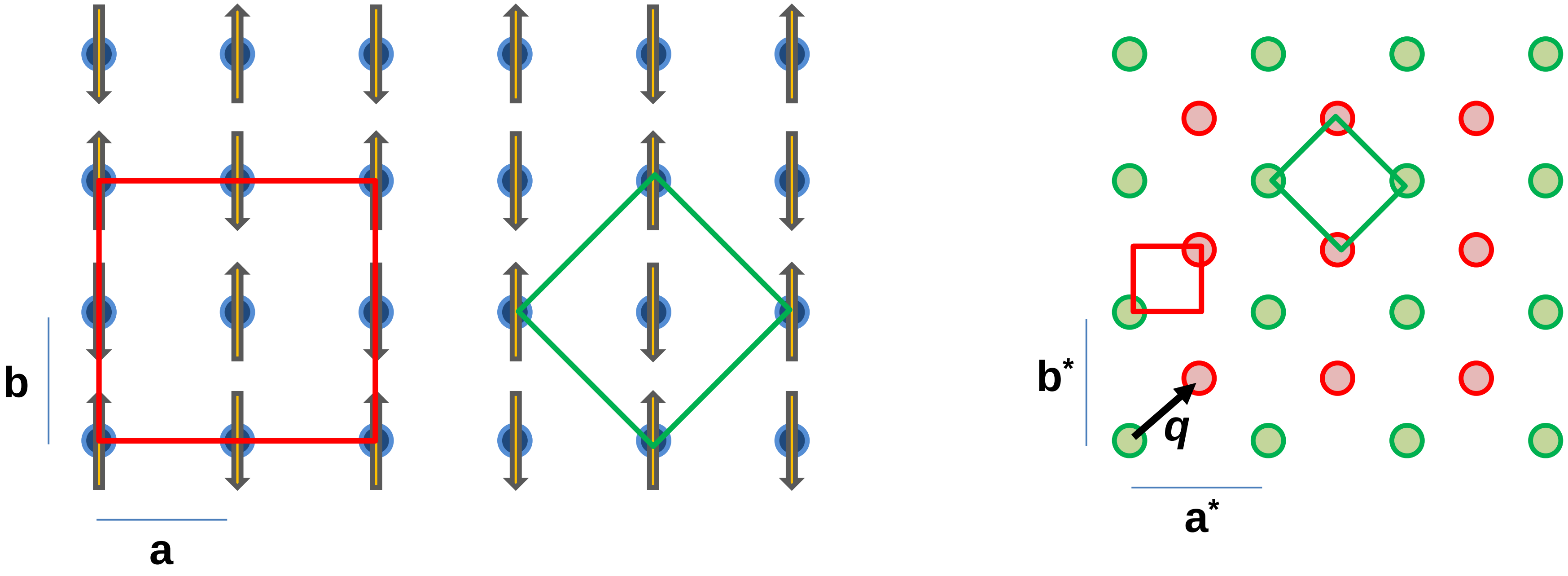


Fourier description of magnetic structures

- Describe magnetic structure as a Fourier series

$$\boldsymbol{\mu}_{\boldsymbol{l}d} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

- $\boldsymbol{\mu}_{\boldsymbol{l}d}$ is the ordered moment at the *d*th site in the unit cell reached by ***l***

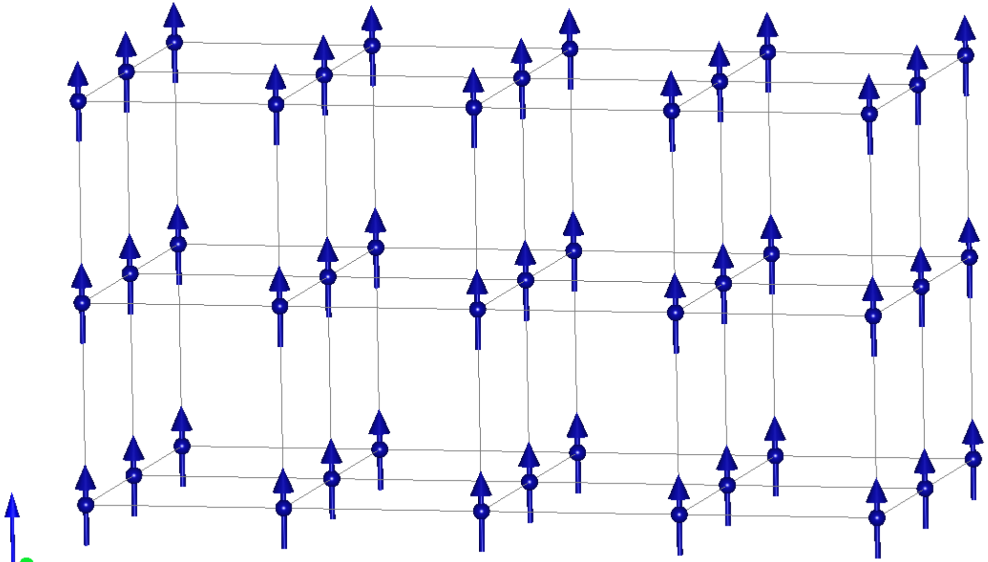
- $\boldsymbol{m}_{\boldsymbol{q}d}^{(n)}$ is the *n*th complex Fourier amplitude containing phase and amplitude of the wave

- $\boldsymbol{m}_{\boldsymbol{q}d} = \boldsymbol{m}_{(\boldsymbol{q}+\boldsymbol{G})d}$, hence summation over 1st Brilluoin zone

- Magnetic moments are real: $\boldsymbol{\mu}_{\boldsymbol{l}d} = \boldsymbol{\mu}_{\boldsymbol{l}d}^{*}$, -***q*** always present, $\boldsymbol{m}_{-\boldsymbol{q}d} = \boldsymbol{m}_{\boldsymbol{q}d}^{*}$

- $\boldsymbol{m}_{\boldsymbol{q}d}$ related to basis functions derived by representation theory

Ferromagnets

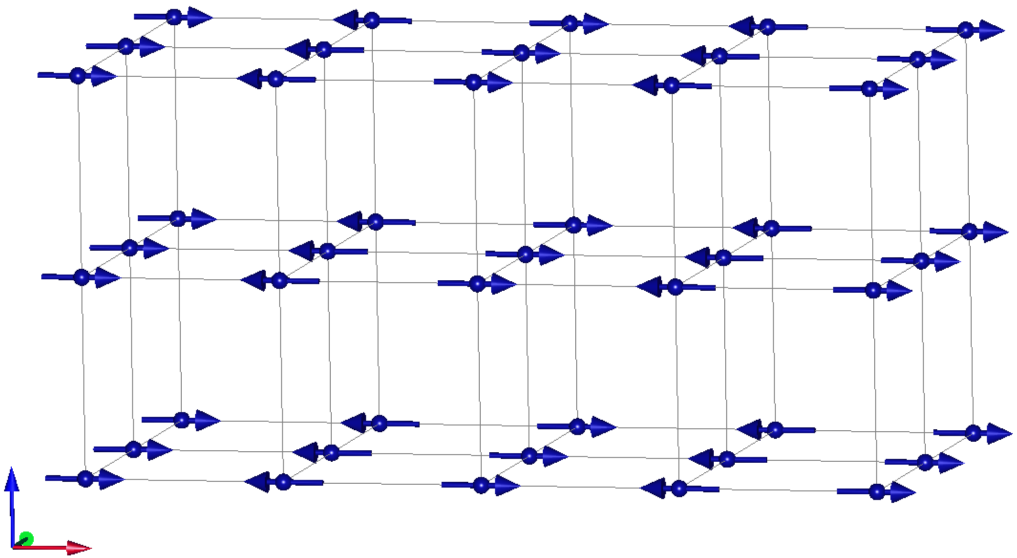


$$\boldsymbol{\mu}_{ld} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

$$\boldsymbol{m}_{\boldsymbol{q}} = \tfrac{1}{2}[0,0,\mu],\ \boldsymbol{q} = (0,0,0)$$

$$\boldsymbol{\mu}_{\boldsymbol{l}} = [0,0,\mu]$$

Collinear commensurate antiferromagnets

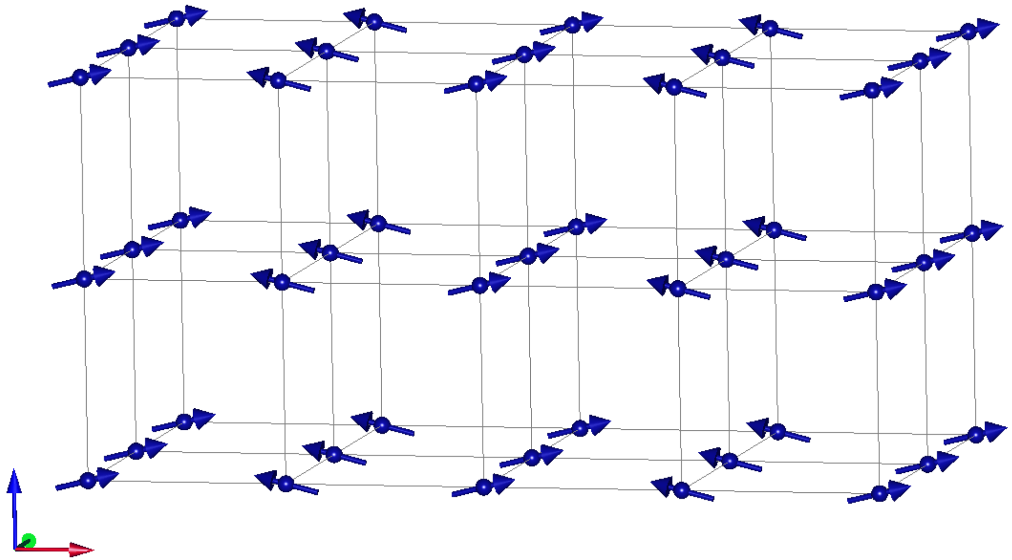


$$\boldsymbol{\mu}_{ld} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

$$\boldsymbol{m}_{\boldsymbol{q}} = \tfrac{1}{2}[\mu, 0,0],\ \boldsymbol{q} = \left(\tfrac{1}{2}, 0,0\right)$$

$$\begin{aligned}\boldsymbol{\mu}_{\boldsymbol{l}} &= \boldsymbol{m}_{\boldsymbol{q}}\big(\exp(-\pi l_x) + \exp(\pi l_x)\big) \\ &= 2\boldsymbol{m}_{\boldsymbol{q}} \cos(\pi l_x) \\ &= [(-1)^{l_x}\mu, 0,0]\end{aligned}$$

Canted commensurate antiferromagnets



$$\boldsymbol{\mu}_{\boldsymbol{l}d} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

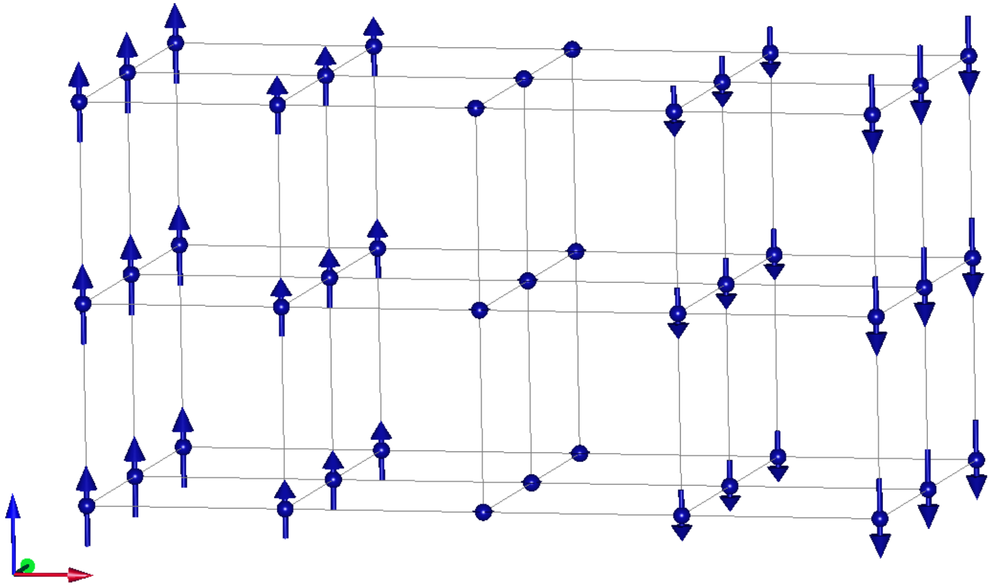
$$\boldsymbol{m}_{\boldsymbol{q}}^{(1)} = \tfrac{1}{2}[0,0,\mu^{(1)}],\ \boldsymbol{q}^{(\mathbf{1})} = (0,0,0)$$

$$\boldsymbol{m}_{\boldsymbol{q}}^{(2)} = \tfrac{1}{2}[\mu^{(2)},0,0],\ \boldsymbol{q}^{(\mathbf{2})} = \left(\frac{1}{2},0,0\right)$$

$$\begin{aligned}\boldsymbol{\mu}_{\boldsymbol{l}} &= \left[(-1)^{l_x}\mu^{(2)},0,0\right] + \left[0,0,\mu^{(1)}\right] \\ &= m[(-1)^{l_x}\cos\theta, 0, \sin\theta]\end{aligned}$$

where $\tan(\theta) = \frac{\mu^{(1)}}{\mu^{(2)}}$

Incommensurate spin density waves

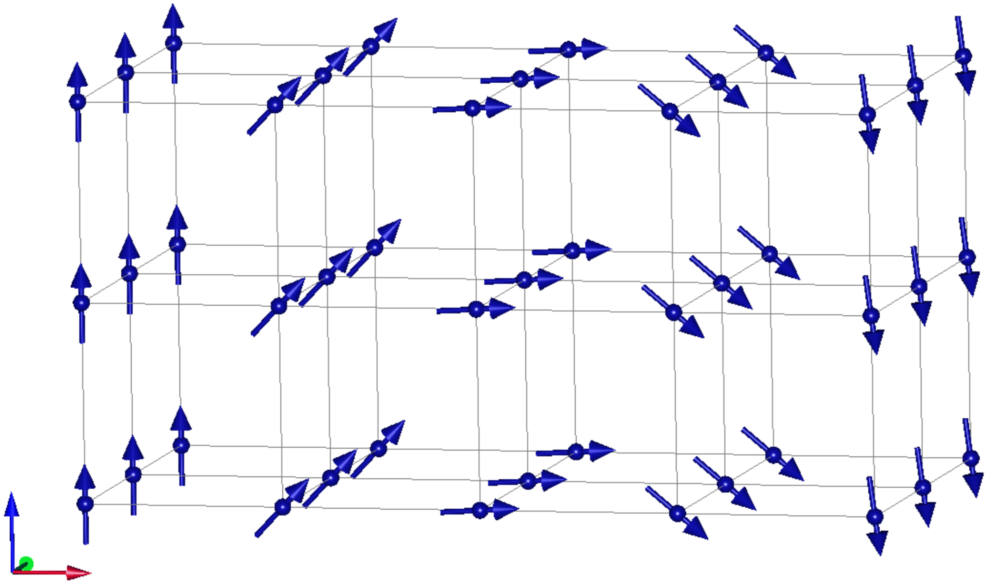


$$\boldsymbol{\mu}_{\boldsymbol{l}d} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

$$\boldsymbol{m}_{\boldsymbol{q}} = \tfrac{1}{2}(0,0,\mu),\ \boldsymbol{q} = (\delta,0,0)$$

$$\begin{aligned}\boldsymbol{\mu}_{\boldsymbol{l}} &= \boldsymbol{m}_{\boldsymbol{q}}\big(\exp(-2\pi\delta l_x) + \exp(2\pi\delta l_x)\big)\\ &= 2\boldsymbol{m}_{\boldsymbol{q}}\cos(2\pi\delta l_x)\\ &= [0,0,\mu\cos(2\pi\delta l_x)]\end{aligned}$$

Incommensurate cycloids and helices



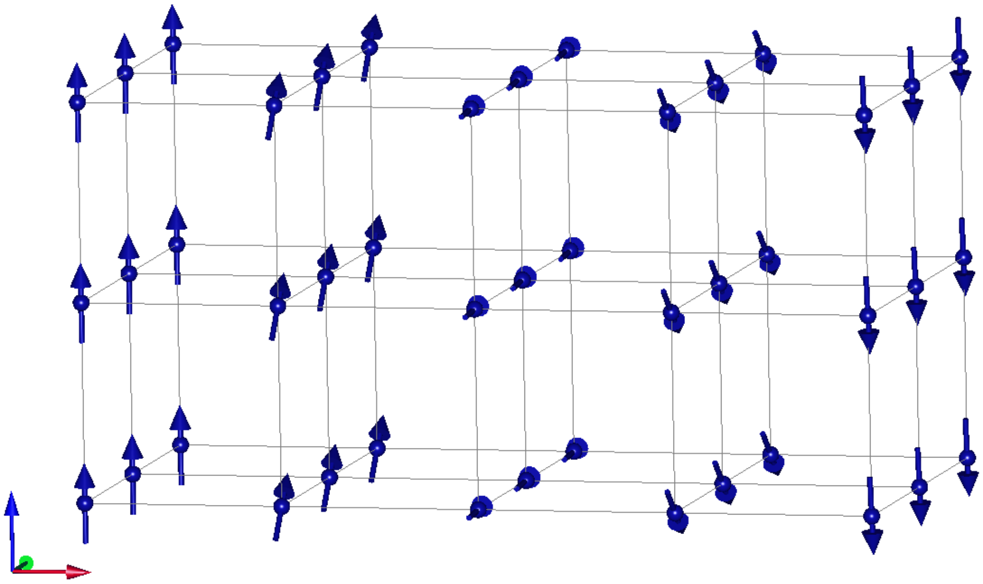
$$\boldsymbol{\mu}_{ld} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

$$\boldsymbol{m}_{\boldsymbol{q}}^{(1)} = \tfrac{1}{2}[0,0,\mu],\ \boldsymbol{q}^{(\mathbf{1})} = (\delta,0,0)$$

$$\boldsymbol{m}_{\boldsymbol{q}}^{(2)} = \tfrac{1}{2}[i\mu,0,0],\ \boldsymbol{q}^{(\mathbf{2})} = (\delta,0,0)$$

$$\begin{aligned}\boldsymbol{\mu}_{\boldsymbol{l}} &= \boldsymbol{m}_{\boldsymbol{q}}^{(1)}\big(\exp(-2\pi\delta l_x) + \exp(2\pi\delta l_x)\big) \\ &\quad + \boldsymbol{m}_{\boldsymbol{q}}^{(2)}\big(\exp(-2\pi\delta l_x) - \exp(2\pi\delta l_x)\big) \\ &= 2\boldsymbol{m}_{\boldsymbol{q}}^{(1)} \cos(2\pi\delta lx) - 2i\boldsymbol{m}_{\boldsymbol{q}}^{(2)} \sin(2\pi\delta l_x) \\ &= \mu[\sin(2\pi\delta l_x)\,, 0, \cos(2\pi\delta l_x)]\end{aligned}$$

Incommensurate cycloids and helices



$$\boldsymbol{\mu}_{ld} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

$$\boldsymbol{m}_{\boldsymbol{q}}^{(1)} = \tfrac{1}{2}[0,0,\mu],\ \boldsymbol{q}^{(\mathbf{1})} = (\delta, 0,0)$$

$$\boldsymbol{m}_{\boldsymbol{q}}^{(2)} = \tfrac{1}{2}[0, i\mu, 0],\ \boldsymbol{q}^{(\mathbf{2})} = (\delta, 0,0)$$

$$\begin{aligned}\boldsymbol{\mu}_{\boldsymbol{l}} &= \boldsymbol{m}_{\boldsymbol{q}}^{(1)}\big(\exp(-2\pi\delta l_x) + \exp(2\pi\delta l_x)\big) \\ &\quad + \boldsymbol{m}_{\boldsymbol{q}}^{(2)}\big(\exp(-2\pi\delta l_x) - \exp(2\pi\delta l_x)\big) \\ &= 2\boldsymbol{m}_{\boldsymbol{q}}^{(1)} \cos(2\pi\delta l_x) - 2i\boldsymbol{m}_{\boldsymbol{q}}^{(2)} \sin(2\pi\delta l_x) \\ &= \mu[0, \sin(2\pi\delta l_x), \cos(2\pi\delta l_x)]\end{aligned}$$

Part 3: Magnetic diffraction

- Commensurate magnetic structures
- Incommensurate magnetic structures
- Integrated intensities

Commensurate magnetic structures

$$\frac{d\sigma}{d\Omega} = \left(\frac{g_{\mathrm{n}} r_0}{4\mu_{\mathrm{B}}}\right)^2 |\langle \boldsymbol{M}_{\perp}(\boldsymbol{Q})\rangle|^2 \; = N_m \frac{(2\pi)^3}{v_m} \sum_{\mathbf{G}_m} \left|\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q})\right|^2 \delta(\boldsymbol{Q} - \boldsymbol{G}_m)$$

Where the magnetic unit cell structure factor is:

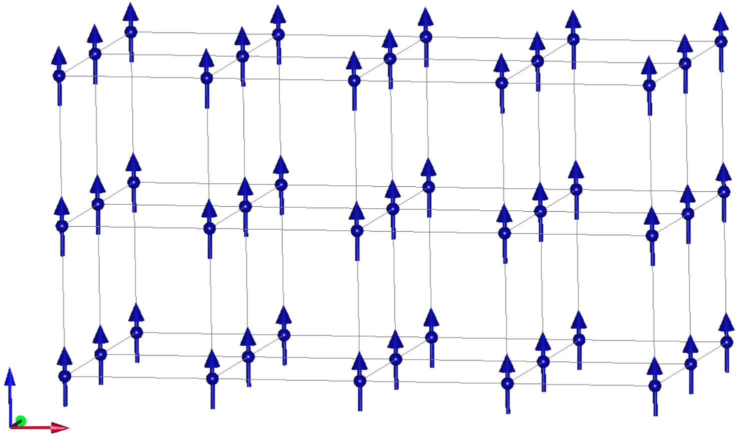
$$\boldsymbol{M}_{uc}(\boldsymbol{Q}) = p \sum_{d} \boldsymbol{\mu}_d f_d(Q) \exp(-W_d) \exp(i\boldsymbol{Q}.\boldsymbol{d}) \qquad\qquad p = \frac{g_{\mathrm{n}} r_0}{4\mu_{\mathrm{B}}}$$

$$\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q}) = \widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_{uc}(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right)$$

Commensurate magnetic structures (simple ferromagnet)

$$\boldsymbol{M}_{uc}(\boldsymbol{Q}) = p\sum_{d} \boldsymbol{\mu}_d f_d(Q)\exp(-W_d)\exp(i\boldsymbol{Q}.\boldsymbol{d}) = pf(Q)\exp(-W)\boldsymbol{\mu}$$

$$\boldsymbol{\mu}_{ld} = [0,0,\mu]$$



$$\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q}) = \widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_{uc}(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right) = pf(Q)\exp(-W)\sin\theta\,\mu$$

where $\sin\theta$ is the tilt of $\boldsymbol{\mu}$ away from $\widehat{\boldsymbol{Q}}$

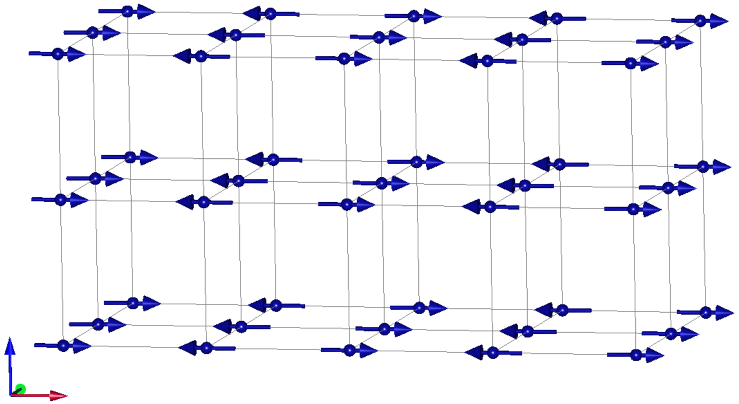
$$\frac{d\sigma}{d\Omega} = N_m\frac{(2\pi)^3}{v_m}\sum_{\mathbf{G}_m}\left|\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q})\right|^2\delta(\boldsymbol{Q}-\boldsymbol{G}_m)$$

$$= N\frac{(2\pi)^3}{v_0}p^2 f^2(Q)\exp(-2W)\sin^2(\theta)\,\mu^2\sum_{\mathbf{G}}\delta(\boldsymbol{Q}-\boldsymbol{G})$$

Commensurate magnetic structures (simple antiferromagnet)

$$\boldsymbol{M}_{\perp}(\boldsymbol{Q}) = pf(Q)\exp(-W)\sin\theta\,\mu(1-\exp(\pi i h_m))$$

$$\boldsymbol{\mu}_{\boldsymbol{l}d} = [(-1)^{l_x}\mu, 0,0]$$



$(1-\exp(\pi i h_m)) = 0$ for $hkl: h_m = 2n$
$(1-\exp(\pi i h_m)) = 2$ for $hkl: h_m = 2n+1$

For $hkl: h_m = 2n+1$

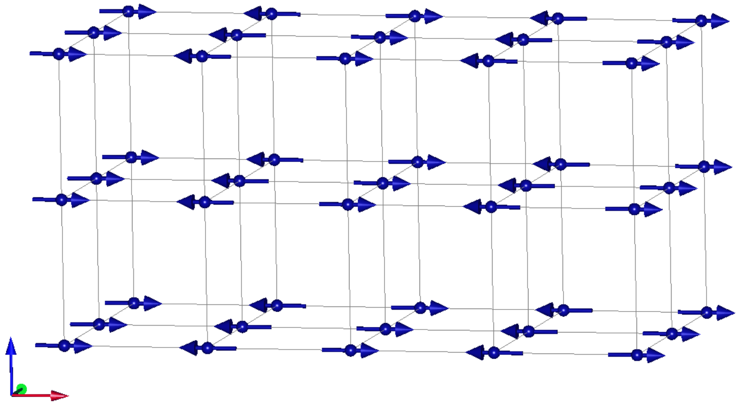
$$\frac{d\sigma}{d\Omega} = N_m \frac{(2\pi)^3}{v_m} \sum_{\mathbf{G}_m} \left|\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q})\right|^2 \delta(\boldsymbol{Q}-\boldsymbol{G}_m)$$

$$= 2N_m \frac{(2\pi)^3}{v_m} p^2 f^2(Q)\exp(-2W)\sin^2\theta\,\mu^2 \sum_{\mathbf{G}_m} \delta(\boldsymbol{Q}-\boldsymbol{G}_m)$$

Commensurate magnetic structures (simple antiferromagnet)

and in the nuclear unit cell…

$$\boldsymbol{\mu}_{\boldsymbol{ld}} = [(-1)^{l_x}\mu, 0,0]$$



$(1 - \exp(\pi i h_m)) = 0$ for $hkl: h_m = 2n$
$(1 - \exp(\pi i h_m)) = 2$ for $hkl: h_m = 2n+1$

$\boldsymbol{a}_m = 2\boldsymbol{a}$ $\quad$ $\boldsymbol{a}_m^* = \frac{1}{2}\boldsymbol{a}^*$

$h_m \boldsymbol{a}_m^* = h\ \boldsymbol{a}$ ➡ $h_m = 2h$

$\boldsymbol{M}_{uc} = 0$ for $hkl: h = n$
$\boldsymbol{M}_{uc} = 2$ for $hkl: h = n + \frac{1}{2}$

Incommensurate magnetic structures

$$\frac{d\sigma}{d\Omega} = N\frac{(2\pi)^3}{v_0}\sum_{\mathbf{G}}\sum_{\boldsymbol{q}}\left|\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q})\right|^2\delta(\boldsymbol{Q}-\boldsymbol{q}-\boldsymbol{G})$$

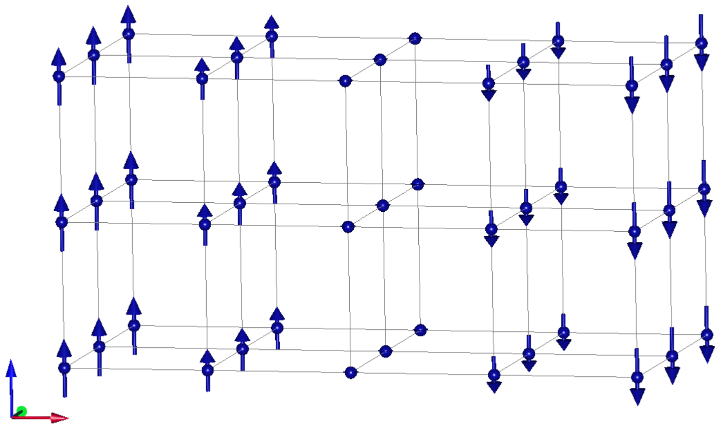
Incommensurate magnetic structures

$$\boldsymbol{m}_{+\boldsymbol{q}d} = \frac{1}{2}(0,0,\mu e^{-i\phi})$$

$$\boldsymbol{m}_{-\boldsymbol{q}d} = \frac{1}{2}(0,0,\mu e^{i\phi})$$

$$\boldsymbol{M}_{uc,+\boldsymbol{q}}(\boldsymbol{Q}) = p\boldsymbol{m}_{+\boldsymbol{q}} f(Q)\exp(-W)$$

$$\boldsymbol{M}_{uc,\perp,+\boldsymbol{q}}(\boldsymbol{Q}) = \frac{1}{2} p \sin\theta\, \mu e^{-i\phi} f(Q)\exp(-W)$$



$$\frac{d\sigma}{d\Omega} = N\frac{(2\pi)^3}{v_0}\sum_{\mathbf{G}}\sum_{\boldsymbol{q}} |\boldsymbol{M}_{uc\perp}(\boldsymbol{Q})|^2 \delta(\boldsymbol{Q}-\boldsymbol{q}-\boldsymbol{G})$$

$$= N\frac{(2\pi)^3}{v_0} p^2 f^2(Q)\exp(-2W)\sin^2\theta\,\mu^2\frac{1}{4}\sum_{\mathbf{G}}\delta(\boldsymbol{Q}-\boldsymbol{G}\pm\boldsymbol{q})$$

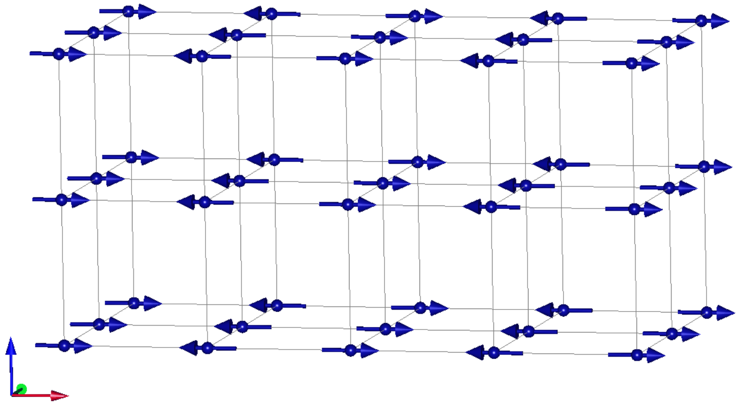
Commensurate magnetic structures (again!)

$$\boldsymbol{m}_{+\boldsymbol{q}d} = \tfrac{1}{2}[\mu, 0,0]$$

$$\boldsymbol{m}_{-\boldsymbol{q}d} = \tfrac{1}{2}[\mu, 0,0] \text{ , } \boldsymbol{q} = \left(\tfrac{1}{2}, 0,0\right)$$

$$\boldsymbol{M}_{uc,+\boldsymbol{q}}(\boldsymbol{Q}) = p\boldsymbol{m}_{+\boldsymbol{q}} f(Q) \exp(-W)$$

$$\boldsymbol{M}_{uc,\perp,+\boldsymbol{q}}(\boldsymbol{Q}) = \frac{1}{2} p \sin\theta \, \mu f(Q) \exp(-W)$$



$$\begin{aligned}\frac{d\sigma}{d\Omega} &= N \frac{(2\pi)^3}{v_0} \sum_{\mathbf{G}} \sum_{\boldsymbol{q}} \left|\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q})\right|^2 \delta(\boldsymbol{Q} - \boldsymbol{q} - \boldsymbol{G}) \\ &= \frac{1}{2} N \frac{(2\pi)^3}{v_0} p^2 f^2(Q) \exp(-2W) \sin^2\theta \, \mu^2 \sum_{\mathbf{G}} \delta\left(\boldsymbol{Q} - \boldsymbol{G} - \frac{1}{2}\right) \\ &= 2N_m \frac{(2\pi)^3}{v_m} p^2 f^2(Q) \exp(-2W) \sin^2\theta \, \mu^2 \sum_{\mathbf{G}_m} \delta(\boldsymbol{Q} - \boldsymbol{G}_m)\end{aligned}$$

Summary

$$\boldsymbol{\mu}_{ld} = \sum_{\boldsymbol{q},n} \boldsymbol{m}_{\boldsymbol{q}d}^{(n)} \exp(-i\boldsymbol{q}.\boldsymbol{l})$$

$$\boldsymbol{M}_{uc}(\boldsymbol{Q}) = p \sum_{d} \boldsymbol{\mu}_d f_d(Q) \exp(-W_d) \exp(i\boldsymbol{Q}.\boldsymbol{d}) \qquad p = \frac{g_\mathrm{n} r_0}{4\mu_\mathrm{B}} = 0.2695 \times 10^{-12}\ \mathrm{cm}\ \mu_\mathrm{B}^{-1}$$

$$\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q}) = \widehat{\boldsymbol{Q}} \times \left(\boldsymbol{M}_{uc}(\boldsymbol{Q}) \times \widehat{\boldsymbol{Q}}\right)$$

$$\frac{d\sigma}{d\Omega} \propto \sum_{\mathbf{G}} \sum_{\boldsymbol{q}} \left|\boldsymbol{M}_{uc,\perp}(\boldsymbol{Q})\right|^2 \delta(\boldsymbol{Q} - \boldsymbol{q} - \boldsymbol{G})$$