X-ray non-resonant and resonant magnetic scattering

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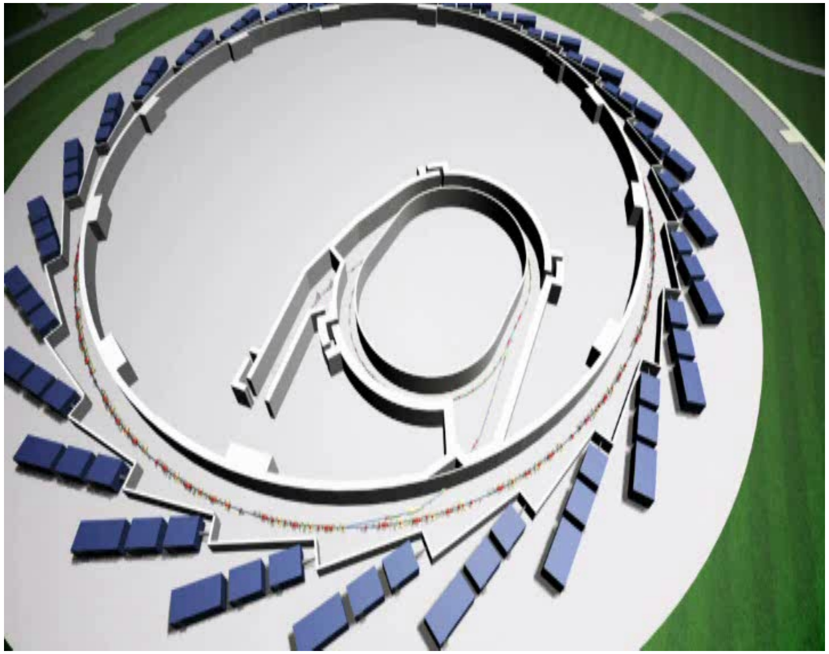
European School on Magnetism

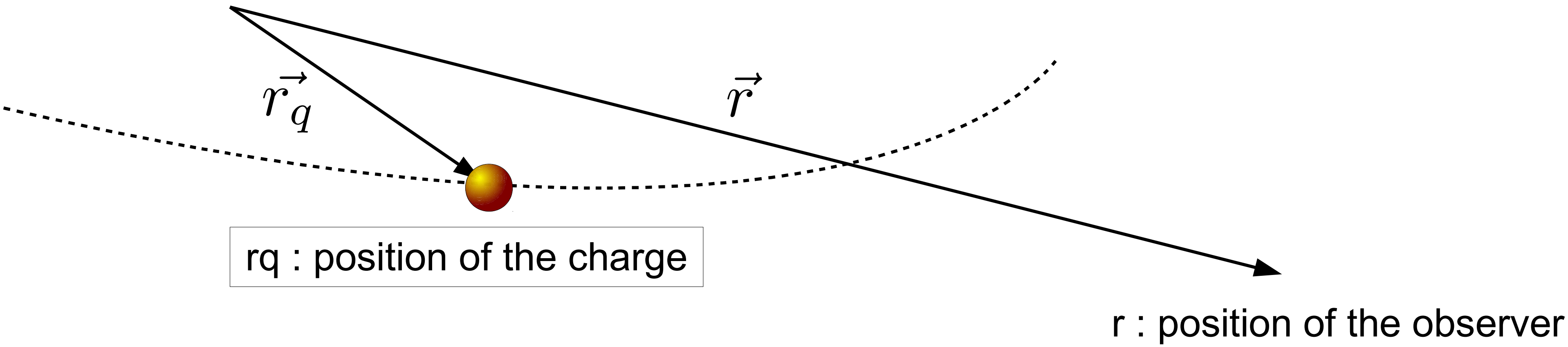
The Diamond synchrotron

3 GeV, 300 mA



Lienard-Wiechert potentials

n.b: Use S.I units throughout.



$$\phi(\vec{r},t) = \frac{q}{4\pi\epsilon_0}\int \frac{\delta(\vec{r'} - \vec{r_q}(t_r))}{|\vec{r} - \vec{r_q}(t_r)|} d^3r'$$

$$\vec{A}(\vec{r},t) = \frac{\mu_0 q c}{4\pi}\int \frac{\delta(\vec{r'} - \vec{r_q}(t_r))\vec{\beta}(t_r)}{|\vec{r} - \vec{r_q}(t_r)|} d^3r'$$

The retarded time t_r:

$$t_r = t - \frac{|\vec{r} - \vec{r_q}(t_r)|}{c}$$

Lienard-Wiechert potentials

By changing variable: $\vec{r}^* = \vec{r} - \vec{r_q}(tr)$ and considering the Jacobian, one finds:

$$\phi(\vec{r},t) = \frac{q}{4\pi\epsilon_0}\left[\frac{1}{R(1-\vec{\beta}.\vec{n})}\right]_{ret}$$

$$\vec{A}(\vec{r},t) = \frac{q}{4\pi\epsilon_0 c}\left[\frac{\vec{\beta}}{R.(1-\vec{\beta}.\vec{n})}\right]_{ret}$$

with

$$\vec{R} = \vec{r} - \vec{r_q}(t_r)$$

$$R = |\vec{r} - \vec{r_q}(t_r)|$$

$$\vec{n} = \frac{\vec{R}}{R}$$

$$\vec{E} = -\vec{\nabla}\Phi - \frac{\partial \vec{A}}{\partial t}$$

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

The difficulty is in evaluating the vector fields at time t.
This involves derivatives with a lot of chain rules.

Fields

$$-\vec{\nabla}\Phi = \frac{q}{4\pi\epsilon_0(1-\vec{\beta}.\vec{n})^3}\left[\frac{1}{R^2}\left(\vec{n}(1-\beta^2)-\vec{\beta}(1-\vec{\beta}.\vec{n})\right)+\frac{1}{R}\frac{(\dot{\vec{\beta}}.\vec{n})}{c}\vec{n}\right]$$

$$-\frac{\partial\vec{A}}{\partial t} = -\frac{q}{4\pi\epsilon_0(1-\vec{\beta}.\vec{n})^3}\left[\frac{(\vec{\beta}.\vec{n}-\beta^2)\vec{\beta}}{R^2}+\frac{(1-\vec{\beta}.\vec{n})\frac{\dot{\vec{\beta}}}{c}+(\dot{\vec{\beta}}.\vec{n})\frac{\vec{\beta}}{c}}{R}\right]$$

The far-field part of the electric field is:

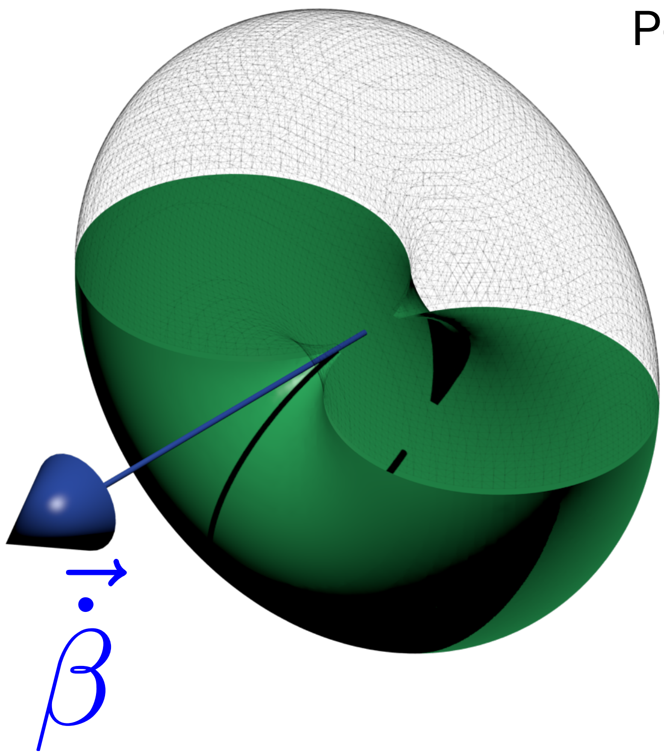
E-field from accelerated charge

$$\vec{E} = \frac{q}{4\pi\epsilon_0 c(1-\vec{\beta}.\vec{n})^3}\frac{\vec{n}\times(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}}{R}$$

These expressions are evaluated at the retarted time t_r.

One can also prove that: $\vec{B} = \frac{\vec{n}}{c}\times\vec{E}$

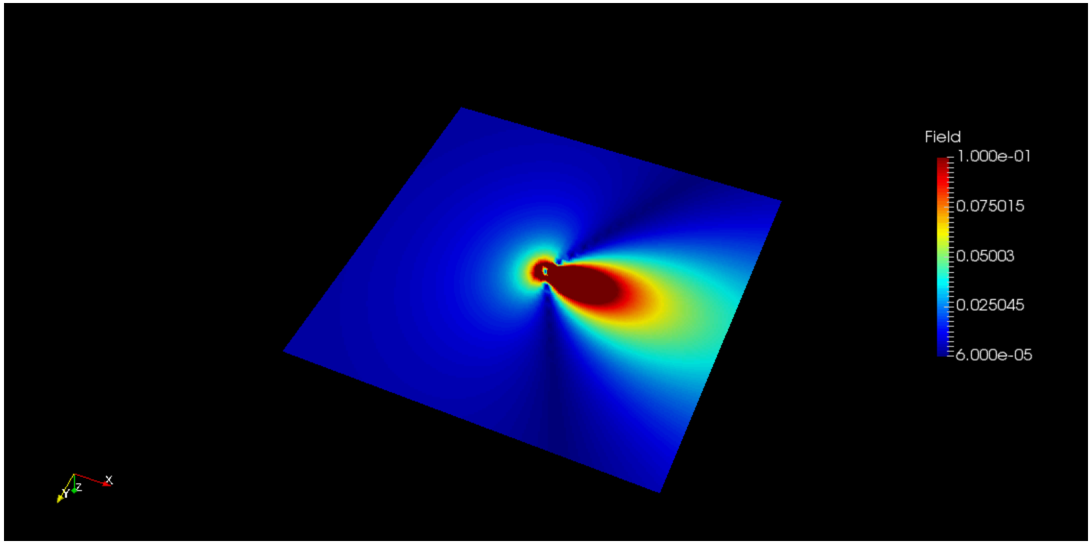
Dipole radiation and forward emitting cone with relativistic e-



Poynting vector:

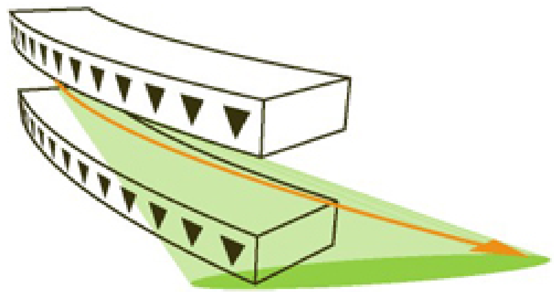
$$\vec{S} = \frac{1}{\mu_0}\vec{E} \times \vec{B}$$

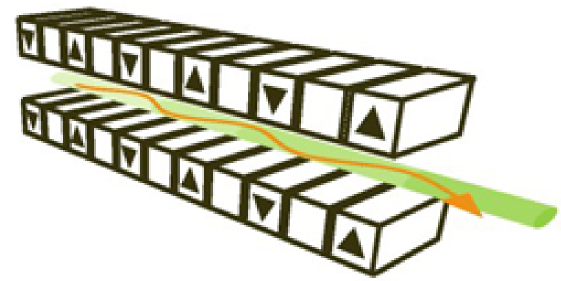
$$\vec{S} = \epsilon_0 c E^2 \vec{n}$$



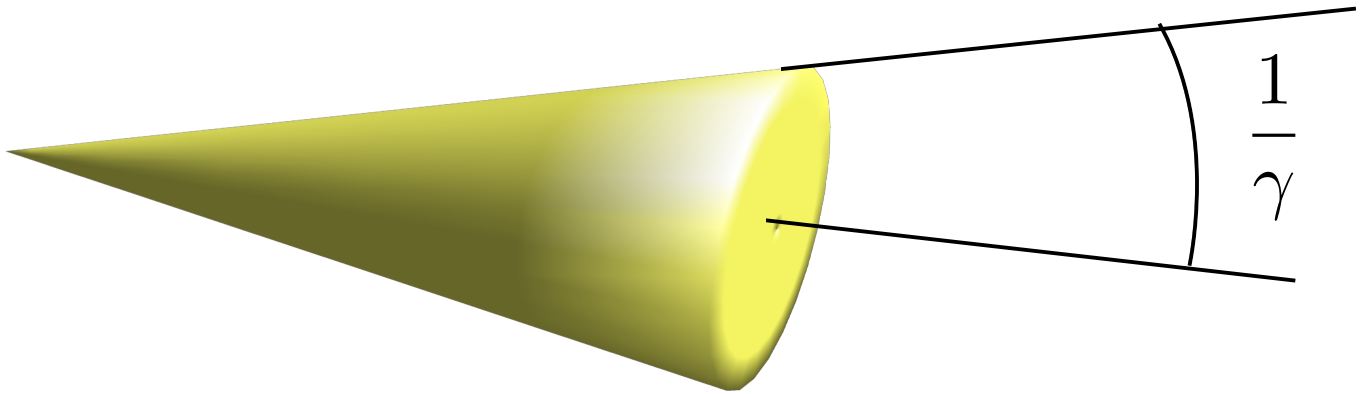
Brilliance and polarisation

Bending Magnet





Insertion Device



$$E = \gamma m_0 c^2$$

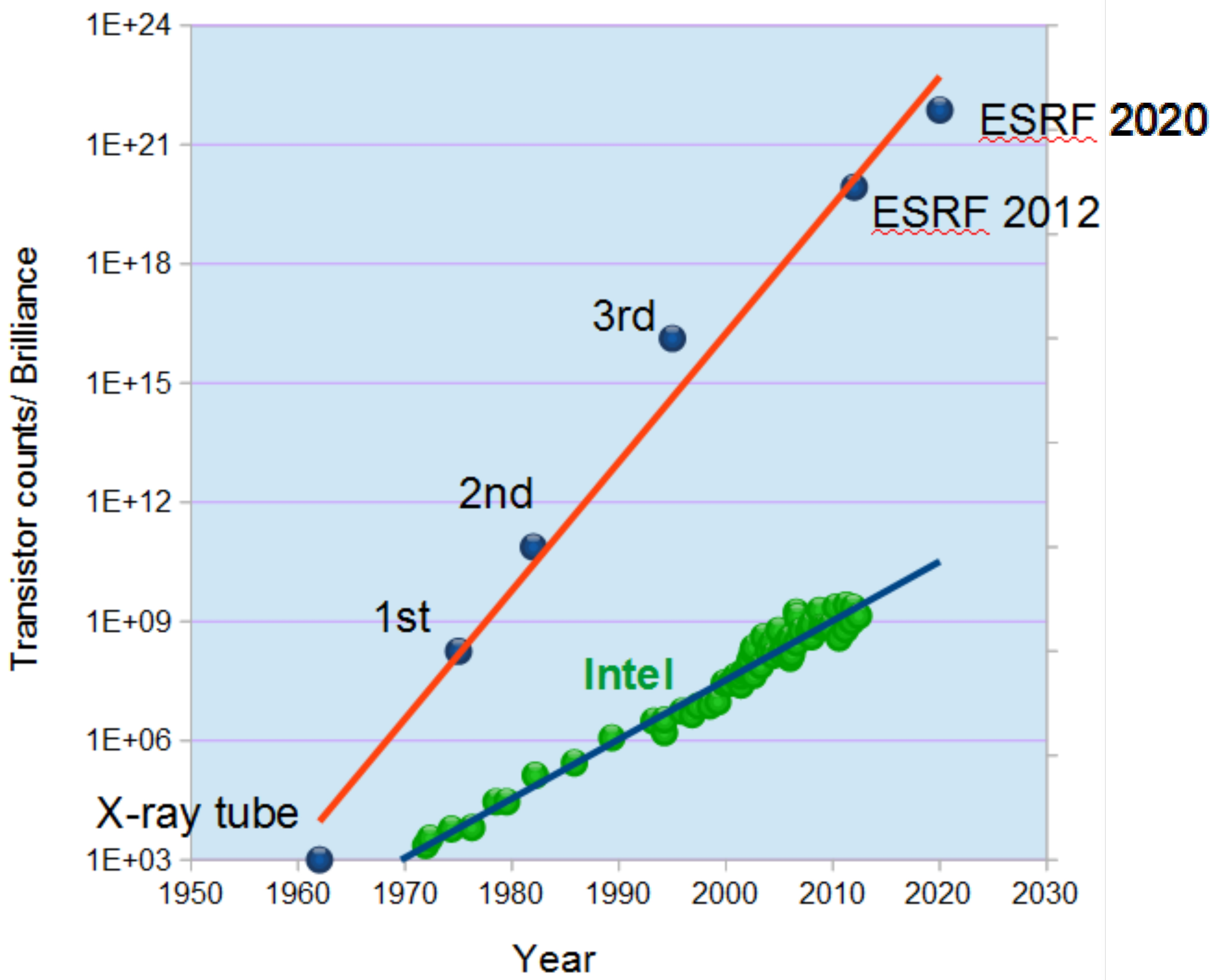
Very small angular opening of the forward emittance cone (fraction of a mrad)

E-field from accelerated charge

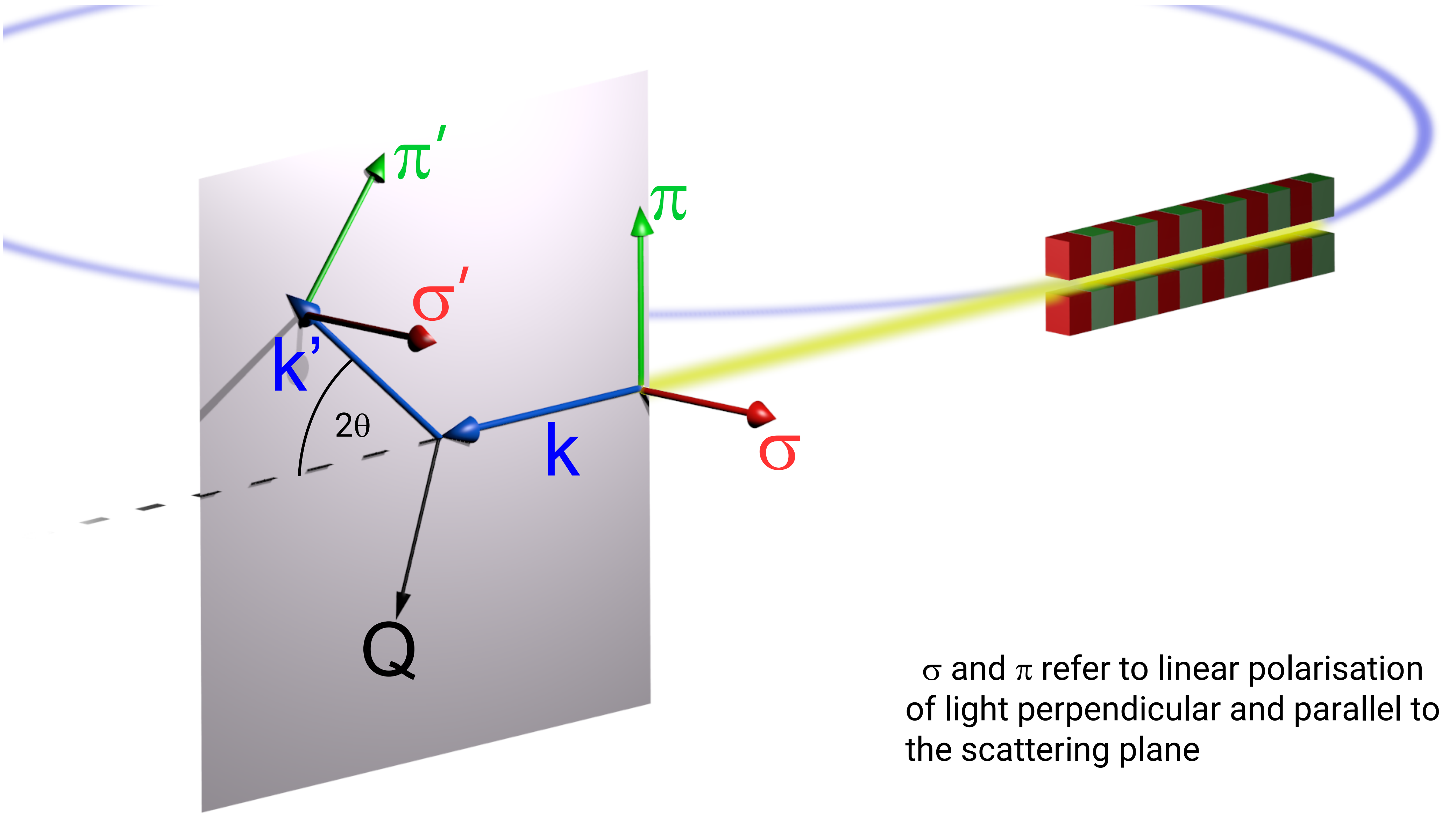
$$\vec{E} = \frac{q}{4\pi\epsilon_0 c(1-\vec{\beta}.\vec{n})^3}\frac{\vec{n}\times(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}}{R}$$

→ Highly polarised radiation in the synchrotron orbit plane

Synchrotron brilliance versus transistor/inch^2

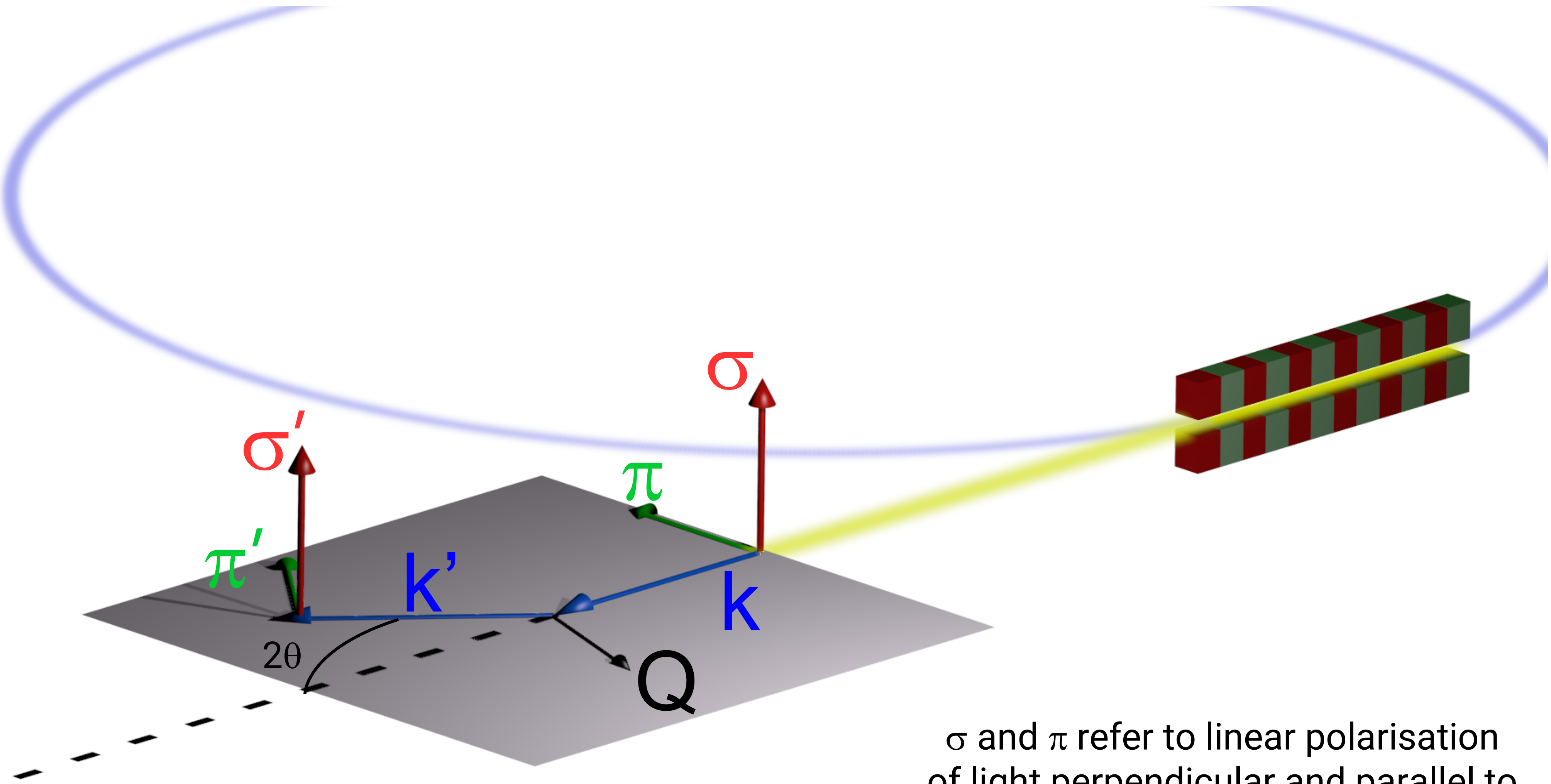


Conventions : Vertical geometry

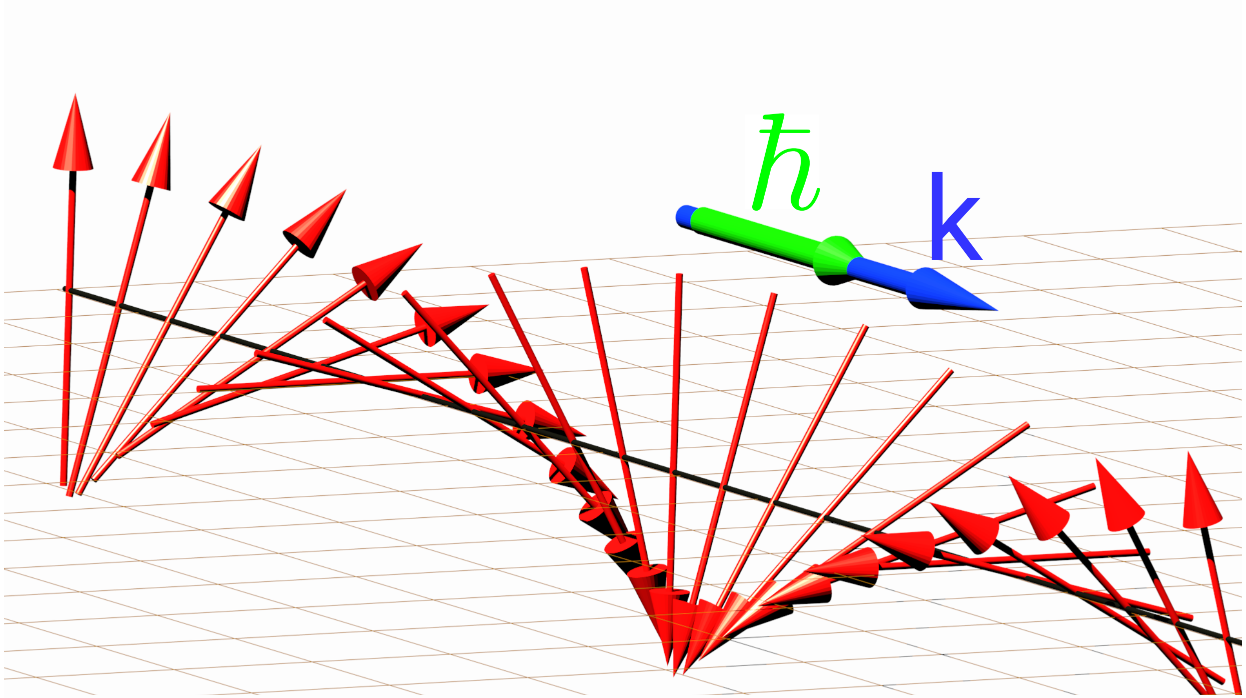


σ and π refer to linear polarisation of light perpendicular and parallel to the scattering plane

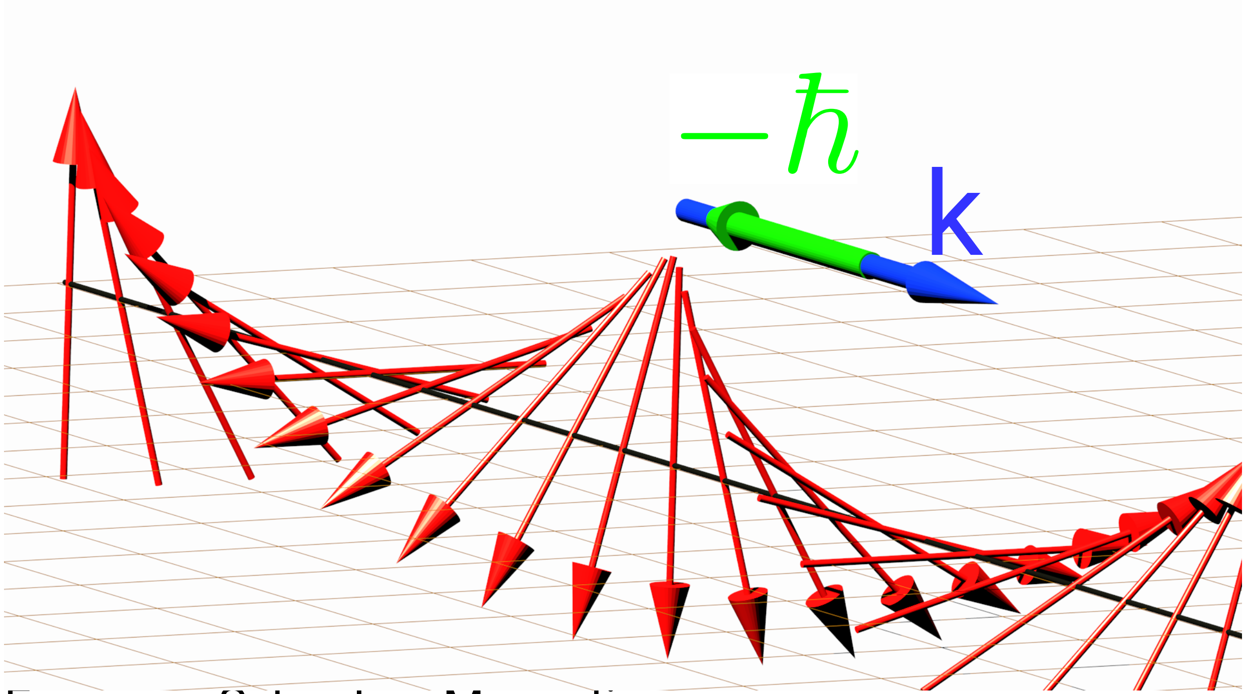
Conventions: Horizontal geometry



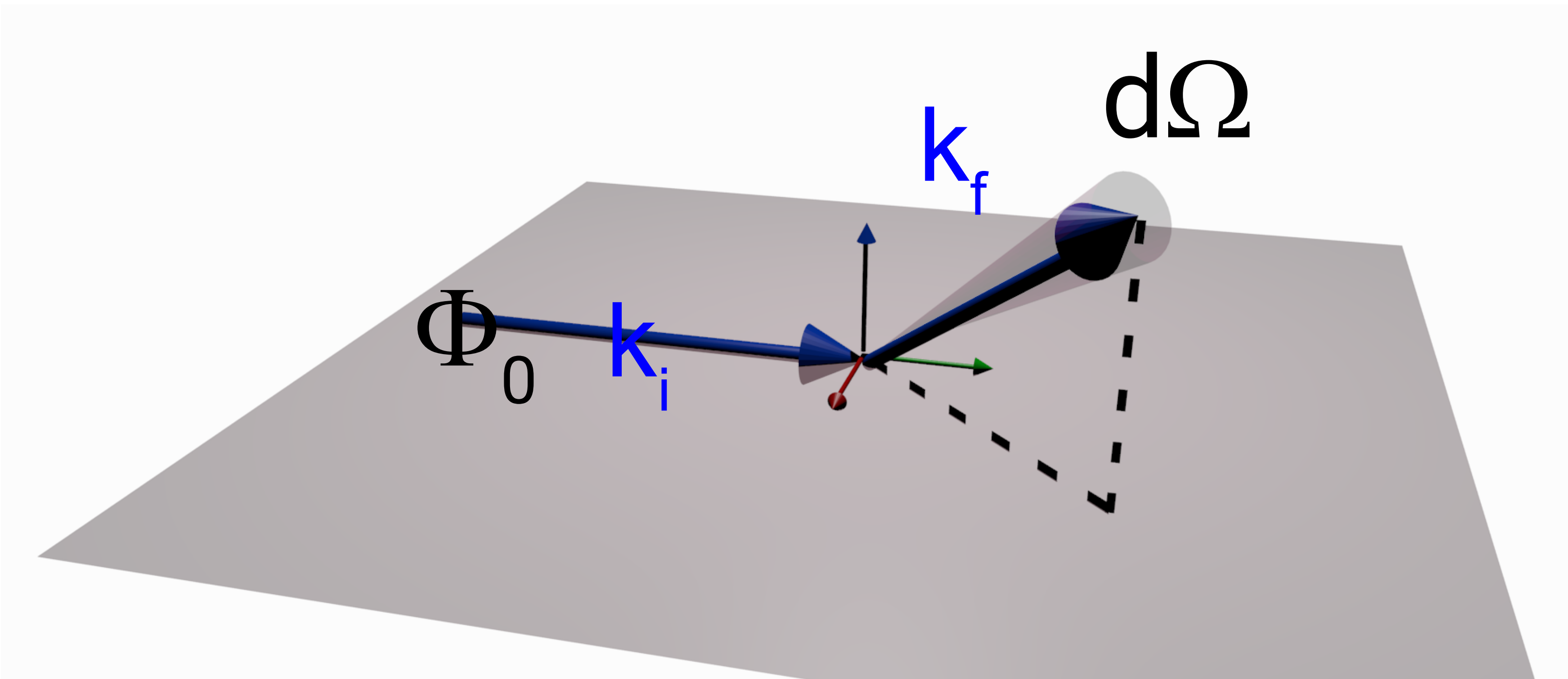
σ and π refer to linear polarisation of light perpendicular and parallel to the scattering plane



$$|\psi\rangle_L = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$$



$$|\psi\rangle_R = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}$$



Transition rate, second order perturbation theory:

Transition rate

$$w_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\,H'\,|i\rangle + \sum_g \frac{\langle f|\,H'\,|g\rangle\,\langle g|\,H'\,|i\rangle}{E_i - E_g}\right|^2 \delta(E_i - E_f)$$

$$|i\rangle = |a; k_i \epsilon_i\rangle \qquad E_i = E_a + \hbar\omega_i$$

$$|f\rangle = |b; k_f \epsilon_f\rangle \qquad E_f = E_b + \hbar\omega_f$$

Maxwell's equations

Maxwell's equations

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{B} = \mu_0(\vec{j} + \epsilon_0 \frac{\partial \vec{E}}{\partial t})$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

In the absences of charges and currents (free space), the solutions are plane-waves:

$$\nabla^2 \vec{E} - \mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \quad \Rightarrow \quad \begin{cases} \vec{E} = \vec{E}_0 e^{i\left(\vec{k}.\vec{R} - \omega t\right)} \\ \omega = kc \end{cases}$$

Quantizing the free electromagnetic field

$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{E} = 0$$

$$\Rightarrow \quad \nabla^2 \phi + \frac{\partial}{\partial t}\left(\vec{\nabla} \cdot \vec{A}\right) = 0$$

$$\vec{\nabla} \times \vec{B} = \vec{\nabla} \times \vec{\nabla} \times \vec{A} = \frac{1}{c^2}\frac{\partial \vec{E}}{\partial t}$$

$$\vec{\nabla}\left(\vec{\nabla} \cdot \vec{A}\right) - \nabla^2 \vec{A} = \frac{1}{c^2}\frac{\partial}{\partial t}\left(-\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t}\right)$$

It is convenient to work in the Coulomb (radiation) Gauge, by setting: $\phi = 0, \vec{\nabla} \cdot \vec{A} = 0$

Free EMF

$$\nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = 0$$

Quantizing the free electromagnetic field

$$\vec{A}(\vec{r},t) = \sum_{k,\alpha=-1,1} a_k^\alpha \varepsilon_k^{\vec{\alpha}} e^{i\left(\vec{k}\cdot\vec{r}-\omega_k t\right)} + c.c = \vec{A^+}(\vec{r},t) + \vec{A^-}(\vec{r},t)$$

The Gauge condition implies: $\vec{k}.\varepsilon_k^{\vec{\alpha}} = 0$ ➡ transverse waves with two orthogonal polarization states.

$$\vec{E}(\vec{r},t) = i\sum_{k,\alpha} \omega_k \left(a_k^\alpha \varepsilon_k^{\vec{\alpha}} e^{i(\vec{k}\cdot\vec{r}-\omega_k t)} - c.c\right)$$

$$\vec{B}(\vec{r},t) = i\sum_{k,\alpha} \vec{k} \times \left(a_k^\alpha \varepsilon_k^{\vec{\alpha}} e^{i(\vec{k}\cdot\vec{r}-\omega_k t)} - c.c\right)$$

Electromagnetic energy:

Electromagnetic energy

$$H = \frac{1}{2}\epsilon_0 \int \left(E^2 + c^2 B^2\right) d^3x = 2\epsilon_0 V \sum_{k,\alpha} \omega_k^2 |a_k^\alpha|^2$$

Quantizing the free electromagnetic field

$$\hat{A} = \sum_{\boldsymbol{k},\boldsymbol{\varepsilon}} \mathcal{N}_k \left(\boldsymbol{\varepsilon} a_{\boldsymbol{k},\boldsymbol{\varepsilon}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{\varepsilon}^* a^\dagger_{\boldsymbol{k},\boldsymbol{\varepsilon}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \right)$$

$$\mathcal{N}_k = \sqrt{\frac{\hbar}{2V\epsilon_0\omega_k}}$$

$$a^\dagger_{\boldsymbol{k},\boldsymbol{\varepsilon}} |0\rangle = |\boldsymbol{k},\boldsymbol{\varepsilon}\rangle$$

$$a_{\boldsymbol{k},\boldsymbol{\varepsilon}} |\boldsymbol{k},\boldsymbol{\varepsilon}\rangle = |0\rangle$$

Lorentz force is not conservative (depends on speed)

$$\vec{F} = -\vec{\nabla} U + \frac{d}{dt}\frac{dU}{d\vec{v}}$$

$$\vec{F} = q\left(\vec{E} + \vec{v} \times \vec{B}\right)$$
$$= q\left(-\vec{\nabla}\phi - \partial_t \vec{A} + \vec{v} \times \vec{\nabla} \times \vec{A}\right)$$
$$= q\left(-\vec{\nabla}\phi - \partial_t \vec{A} + \vec{\nabla}\left(\vec{v} \cdot \vec{A}\right) - \left(\vec{v} \cdot \vec{\nabla}\right)\vec{A}\right)$$

Using : $$\frac{d\vec{A}}{dt} = \frac{\partial \vec{A}}{\partial t} + \vec{v} \cdot \vec{\nabla} \vec{A}$$

$$\vec{F} = q\left(-\vec{\nabla}\left(\phi - \vec{v} \cdot \vec{A}\right) + \frac{d\vec{A}}{dt}\right)$$

EMF potential

$$U = q\left(\phi - \vec{v} \cdot \vec{A}\right)$$

Hamiltonian of a charged particle in an EMF (no spin)

$$\mathcal{L} = T - U = \frac{1}{2}mv^2 - q\phi + q\vec{A}\cdot\vec{v}$$

Generalized momentum: $$\vec{p} = \frac{\partial\mathcal{L}}{\partial\vec{v}} = m\vec{v} + q\vec{A}$$

Hamiltonian

$$\mathcal{H} = \vec{p}\cdot\vec{v} - \mathcal{L} = \frac{\left(\vec{p} - q\vec{A}\right)^2}{2m} + q\phi$$

Zeeman & Spin-orbit coupling terms

$$\mu_e = -g\mu_B \frac{\vec{s}}{\hbar} = -\frac{e\hbar}{2m}.\vec{\sigma}$$

Zeeman

$$V_Z = \frac{e\hbar}{2m}\vec{\sigma}\cdot\vec{\boldsymbol{\nabla}}\times\vec{A}$$

$$\vec{B} = -\frac{\vec{v}\times\vec{E}}{2c^2} = -\frac{\left(\vec{p}+e\vec{A}\right)\times\vec{E}}{2mc^2}$$

See Thomas factor for example
in Jackson “Classical Electromagnetism”

$$V_{SO} = -\vec{\mu_e}\cdot\vec{B} = \frac{e\hbar}{2m}\vec{\sigma}\cdot\vec{B}$$

Spin-orbit

$$V_{SO} = -\frac{e\hbar}{2(2mc)^2}\sigma\cdot(\partial_t\mathbf{A}\times(\mathbf{p}+e\mathbf{A})-(\mathbf{p}+e\mathbf{A})\times\partial_t\mathbf{A})$$

Full Hamiltonian charge in an EMF

$$\mathcal{H} = \sum_j \frac{(\boldsymbol{p_j} + e\boldsymbol{A}(\boldsymbol{r_j}))^2}{2m}$$ Kinetic

$$+ \frac{e\hbar}{2m}\boldsymbol{\sigma_j} \cdot \vec{\boldsymbol{\nabla}} \times \boldsymbol{A}(\boldsymbol{r_j})$$ Zeeman

$$+ \frac{e\hbar}{2(2mc)^2}\boldsymbol{\sigma_j} \cdot [(\boldsymbol{p_j} + \boldsymbol{e}\boldsymbol{A}(\boldsymbol{r_j})) \times \partial_t \mathbf{A_j} - \partial_t \mathbf{A_j} \times (\boldsymbol{p_j} + \boldsymbol{e}\boldsymbol{A}(\boldsymbol{r_j}))]$$ SO coupling

$$+ \sum_n V_{jn}$$ Coulomb

$$+ \sum_{\boldsymbol{k},\epsilon} \hbar\omega_k \left(a^\dagger_{\boldsymbol{k},\epsilon} a_{\boldsymbol{k},\epsilon} + \frac{1}{2} \right)$$ EMF self-energy

Perturbing Hamiltonian

$$\mathcal{H}' = \sum_i \frac{e^2}{2m}\mathbf{A}(\mathbf{r_j})^2 + \frac{e}{m}\mathbf{p_j}\cdot\mathbf{A}(\mathbf{r_j}) + \frac{e\hbar}{2m}\sigma_\mathbf{j}\cdot\vec{\boldsymbol{\nabla}}\times\mathbf{A}(\mathbf{r_j}) + \frac{e^2\hbar}{(2mc)^2}\sigma_j\mathbf{A}(\mathbf{r_j})\times\partial_t\mathbf{A}(\mathbf{r_j})$$

$\mathcal{H}'_1$, $\mathcal{H}'_2$, $\mathcal{H}'_3$, $\mathcal{H}'_4$ — Refers to *Blume, 1985*

- Terms square in **A** contribute to the first order scattering term
- Terms linear in **A** contribute to the second order scattering term

$$w_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\,\mathcal{H}'_1+\mathcal{H}'_4\,|i\rangle + \sum_g \frac{\langle f|\,\mathcal{H}'_2+\mathcal{H}'_3\,|g\rangle\langle g|\,\mathcal{H}'_2+\mathcal{H}'_3\,|i\rangle}{E_i-E_g}\right|^2\delta(E_a-E_b+\hbar\omega_i-\hbar\omega_f)$$

First and second order terms

$$\langle f|\, H_1' \,|i\rangle = \mathcal{N}^2 \frac{e^2}{m} \langle b| \sum_j e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}} \,|a\rangle\, \boldsymbol{\epsilon}_i \cdot \boldsymbol{\epsilon}_f$$

$$\langle f|\, H_4' \,|i\rangle = -\mathcal{N}^2 \frac{e^2}{m} \frac{i\hbar\omega}{mc^2} \langle b| \frac{1}{2} \sum_j \boldsymbol{\sigma_j} e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}} \,|a\rangle\, \boldsymbol{\epsilon_f^*} \times \boldsymbol{\epsilon_i}$$

$$\sum_g \frac{\langle f|\, \mathcal{H}_2' + \mathcal{H}_3' \,|g\rangle \langle g|\, \mathcal{H}_2' + \mathcal{H}_3' \,|i\rangle}{E_i - E_g} =$$

$$\mathcal{N}^2 \frac{e^2}{m^2} \sum_g \sum_{j,k} \frac{\langle f|\, e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_k}} \left[\boldsymbol{p_k}\cdot\boldsymbol{\epsilon_f^*} - i\frac{\hbar}{2}\boldsymbol{\sigma_k}(\boldsymbol{k_f}\times\boldsymbol{\epsilon_f^*})\right] |g\rangle \langle g|\, e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_j}} \left[\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_i} + i\frac{\hbar}{2}\boldsymbol{\sigma_j}(\boldsymbol{k_i}\times\boldsymbol{\epsilon_i})\right] |a\rangle}{E_a + \hbar\omega_i - E_g + i\Gamma}$$

$$+ \frac{\langle f|\, e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_k}} \left[\boldsymbol{p_k}\cdot\boldsymbol{\epsilon_i} + i\frac{\hbar}{2}\boldsymbol{\sigma_k}(\boldsymbol{k_i}\times\boldsymbol{\epsilon_i})\right] |g\rangle \langle g|\, e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_j}} \left[\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_f^*} - i\frac{\hbar}{2}\boldsymbol{\sigma_j}(\boldsymbol{k_f}\times\boldsymbol{\epsilon_f^*})\right] |a\rangle}{E_a - E_g - \hbar\omega_f}$$

Annihilate photon first

Create photon first

Non-resonant contribution of second-order terms

Using $\hbar\omega_f \sim \hbar\omega_i \gg E_i - E_g \qquad \sum_g |g\rangle\langle g| = 1$

$$\sum_g \frac{\langle f| \mathcal{H}'_2 + \mathcal{H}'_3 |g\rangle \langle g| \mathcal{H}'_2 + \mathcal{H}'_3 |i\rangle}{E_i - E_g}$$

$$\sim \mathcal{N}^2 \frac{e^2}{\hbar\omega m^2} \sum_{j,k} \langle f| \left[e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_k}} \left(\boldsymbol{p_k}\cdot\boldsymbol{\epsilon_f^*} - i\frac{\hbar}{2}\boldsymbol{\sigma_k}(\boldsymbol{k_f}\times\boldsymbol{\epsilon_f^*}) \right), e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_j}} \left(\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_i} + i\frac{\hbar}{2}\boldsymbol{\sigma_j}(\boldsymbol{k_i}\times\boldsymbol{\epsilon_i}) \right) \right] |i\rangle$$

Need to evaluate 4 commutators, with the help of :

$$[\boldsymbol{\sigma_a}, \boldsymbol{\sigma_b}] = 2i\epsilon_{abc}\boldsymbol{\sigma_c}$$

$$[p_a, f(\boldsymbol{r})] = -i\hbar\frac{\partial f}{\partial_a}$$

$$(\boldsymbol{a}\cdot\boldsymbol{c})(\boldsymbol{b}\cdot\boldsymbol{d}) - (\boldsymbol{a}\cdot\boldsymbol{d})(\boldsymbol{b}\cdot\boldsymbol{c}) = (\boldsymbol{a}\times b)(\boldsymbol{c}\times\boldsymbol{d})$$

$$\mathbf{k} = \frac{\omega}{c}\hat{\boldsymbol{k}}$$

$$\left[e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_j}}(\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_f^*}), e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_j}}(\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_i}) \right] = \hbar(\boldsymbol{Q}\times\boldsymbol{p_j})(\boldsymbol{\epsilon_f^*}\times\boldsymbol{\epsilon_i})$$

$$\left[\boldsymbol{\sigma_j}(\boldsymbol{k_f}\times\boldsymbol{\epsilon_f^*}), \boldsymbol{\sigma_j}(\boldsymbol{k_i}\times\boldsymbol{\epsilon_i}) \right] = 2i\frac{\omega^2}{c^2}\boldsymbol{\sigma_j}(\hat{\boldsymbol{k_f}}\times\boldsymbol{\epsilon_f^*})\times(\hat{\boldsymbol{k_i}}\times\boldsymbol{\epsilon_i})$$

$$\left[e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_j}}\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_f^*}, \boldsymbol{\sigma_j}\cdot(\boldsymbol{k_i}\times\boldsymbol{\epsilon_i})e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_j}} \right] = \hbar\frac{\omega^2}{c^2}\boldsymbol{\sigma_j}e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}}(\hat{\boldsymbol{k_i}}\cdot\boldsymbol{\epsilon_f^*})(\hat{\boldsymbol{k_i}}\times\boldsymbol{\epsilon_i})$$

$$\left[e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_j}}\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_i}, \boldsymbol{\sigma_j}\cdot(\boldsymbol{k_f}\times\boldsymbol{\epsilon_f^*})e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_j}} \right] = -\hbar\frac{\omega^2}{c^2}\boldsymbol{\sigma_j}e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}}(\hat{\boldsymbol{k_f}}\cdot\boldsymbol{\epsilon_i})(\hat{\boldsymbol{k_f}}\times\boldsymbol{\epsilon_f^*})$$

Magnetic contribution

$$\langle f|\, H_4' \,|i\rangle + \sum_g \frac{\langle f|\, \mathcal{H}_2' + \mathcal{H}_3' \,|g\rangle \langle g|\, \mathcal{H}_2' + \mathcal{H}_3' \,|i\rangle}{E_i - E_g}$$

$$\sim -\mathcal{N}^2 \frac{e^2}{m}\frac{i\hbar\omega}{mc^2}\left[\langle 0|\sum_j \frac{i\boldsymbol{Q}\times\boldsymbol{p_j}}{\hbar k^2} e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}}\,|0\rangle\cdot\boldsymbol{A} + \langle 0|\,\frac{1}{2}\sum_j \boldsymbol{\sigma_j} e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}}\,|0\rangle\cdot\boldsymbol{B}\right]$$

$$= -\mathcal{N}^2 \frac{e^2}{m}\frac{i\hbar\omega}{mc^2}\left[4sin^2(\theta)\left(\frac{1}{2}\hat{\boldsymbol{q}}\times\sum_j \boldsymbol{l_j} e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}}\times\hat{\boldsymbol{q}}\right)\cdot\boldsymbol{A} + \left(\sum_j \boldsymbol{s_j} e^{i\hat{\boldsymbol{Q}}\cdot\boldsymbol{r_j}}\right).\boldsymbol{B}\right]$$

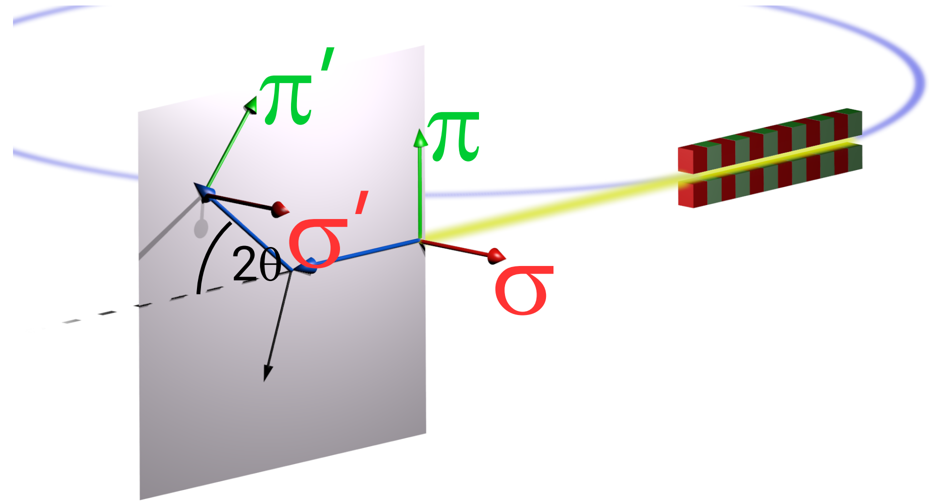
Here, l_j and s_j are given in units of $\hbar$

$$\boldsymbol{A} = \boldsymbol{\epsilon_f^*}\times\boldsymbol{\epsilon_i}$$

$$\boldsymbol{B} = \boldsymbol{\epsilon_f^*}\times\boldsymbol{\epsilon_i} - (\hat{\boldsymbol{k_f}}\times\boldsymbol{\epsilon_f^*})\times(\hat{\boldsymbol{k_i}}\times\boldsymbol{\epsilon_i}) - (\hat{\boldsymbol{k_i}}\times\boldsymbol{\epsilon_i})(\hat{\boldsymbol{k_i}}\cdot\boldsymbol{\epsilon_f^*}) + (\hat{\boldsymbol{k_f}}\times\boldsymbol{\epsilon_f^*})(\hat{\boldsymbol{k_f}}\cdot\boldsymbol{\epsilon_i})$$

Separation of L and S

$$< M >= \frac{1}{2}\mathbf{L}(\mathbf{Q})\cdot\mathbf{A}+\mathbf{S}(\mathbf{Q})\cdot\mathbf{B}$$



$$\begin{array}{ccccc} & & \sigma & \pi & \\ B = & \Bigg(& \hat{\mathbf{k}}_{\mathbf{i}}\times\hat{\mathbf{k}}_{\mathbf{f}} & -\hat{\mathbf{k}}_{\mathbf{f}}(1-\hat{\mathbf{k}}_{\mathbf{i}}\cdot\hat{\mathbf{k}}_{\mathbf{f}}) & \Bigg) \; \sigma \\ & & -\hat{\mathbf{k}}_{\mathbf{i}}(1-\hat{\mathbf{k}}_{\mathbf{i}}\cdot\hat{\mathbf{k}}_{\mathbf{f}}) & \hat{\mathbf{k}}_{\mathbf{i}}\times\hat{\mathbf{k}}_{\mathbf{f}} & \;\;\;\; \pi \end{array}$$

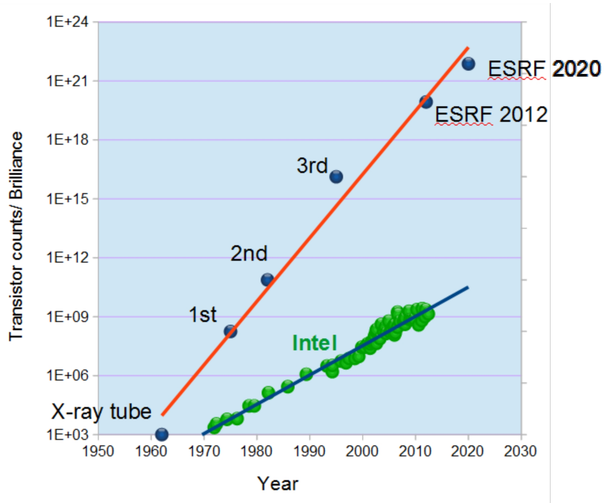
$$A = \frac{Q^2}{2k^2}\begin{pmatrix} 0 & -(\hat{\mathbf{k}}_{\mathbf{i}}+\hat{\mathbf{k}}_{\mathbf{f}}) \\ (\hat{\mathbf{k}}_{\mathbf{i}}+\hat{\mathbf{k}}_{\mathbf{f}}) & 2\hat{\mathbf{k}}_{\mathbf{i}}\times\hat{\mathbf{k}}_{\mathbf{f}} \end{pmatrix}$$

Summary non-resonant magnetic X-ray scattering

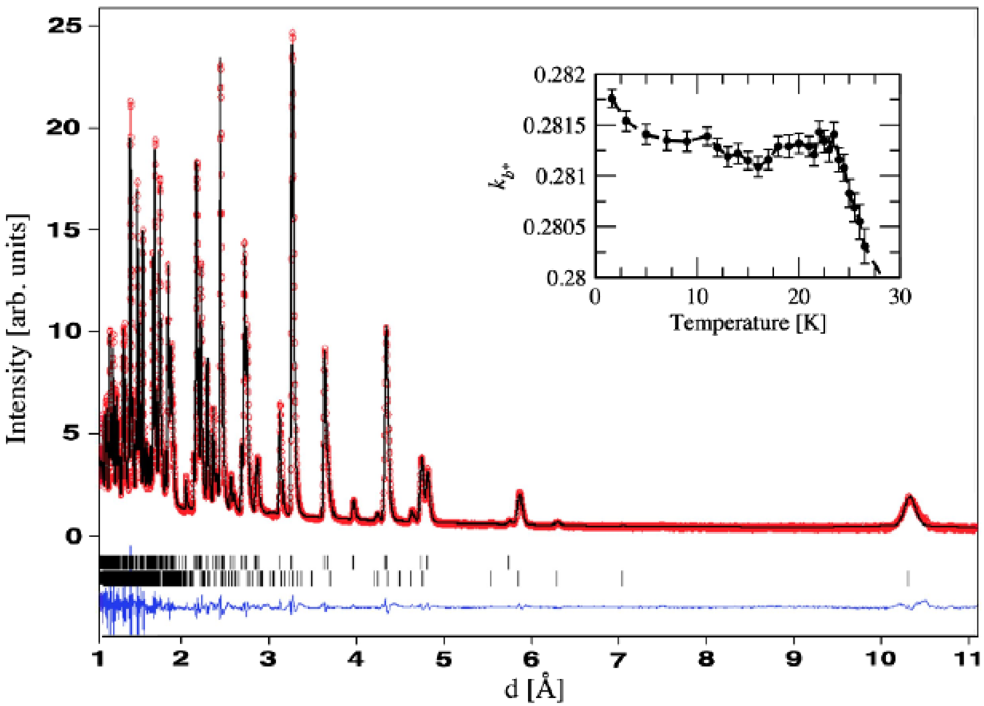
$$\langle f|\, H_1' \,|i\rangle = \mathcal{N}^2 \frac{e^2}{m} \langle b| \sum_j e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}} |a\rangle\, \boldsymbol{\epsilon}_i \cdot \boldsymbol{\epsilon}_f$$

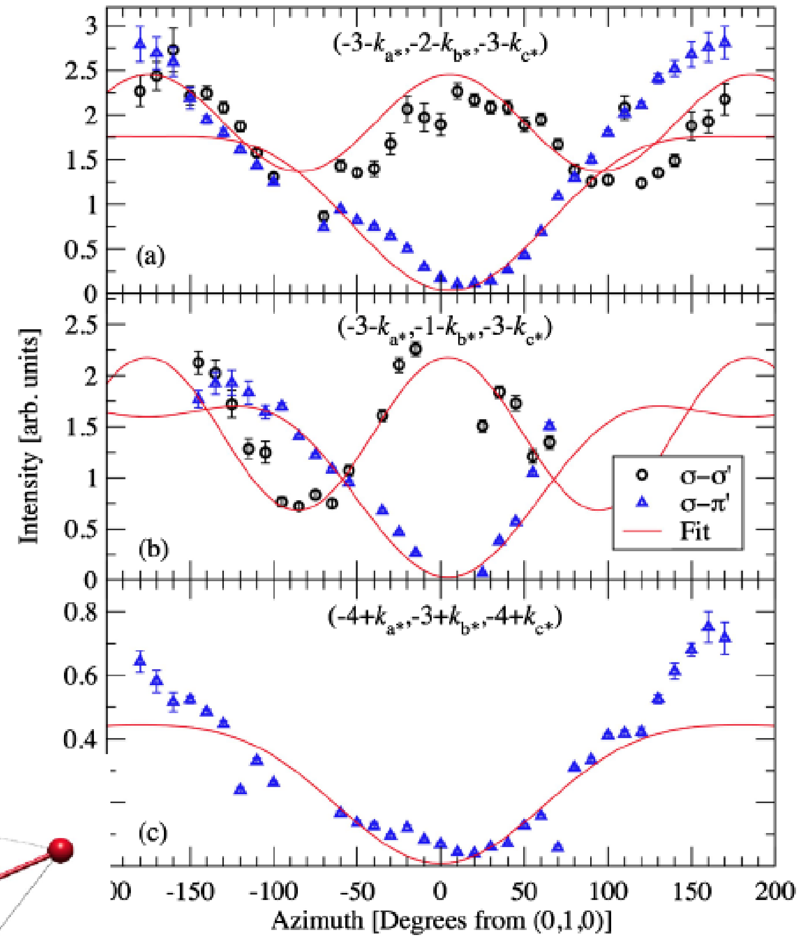
$$-\mathcal{N}^2 \frac{e^2}{m} \frac{i\hbar\omega}{mc^2} \left[4sin^2(\theta) \left(\frac{1}{2}\hat{\boldsymbol{q}} \times \sum_j \boldsymbol{l_j} e^{i\boldsymbol{Q}\cdot\boldsymbol{r_j}} \times \hat{\boldsymbol{q}} \right) \cdot \boldsymbol{A} + \left(\sum_j \boldsymbol{s_j} e^{i\hat{\boldsymbol{Q}}\cdot\boldsymbol{r_j}} \right) .\boldsymbol{B} \right]$$

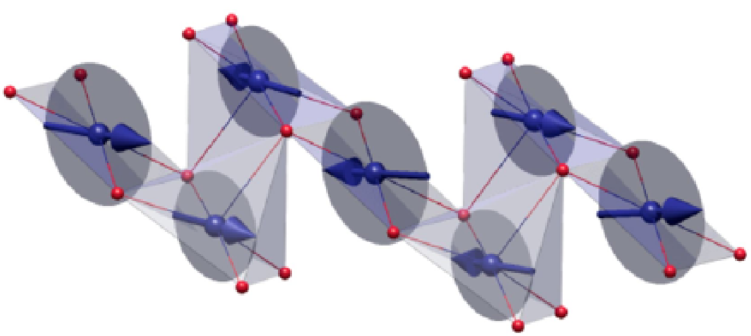
- Rest mass of the electron =511 keV
- At 1 keV, scattering cross section 3.8 10^{-6} smaller than Thomson scattering.
- Only a few unpaired electrons contribute to the magnetic scattering vs. all electrons in the Thomson scattering.
- However, the flux available largely compensate for the weak scattering cross section.

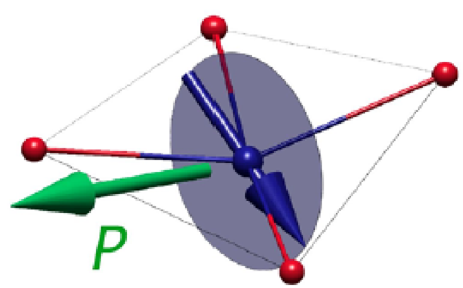


Non-resonant magnetic scattering $Cu_3Nb_2O_8$



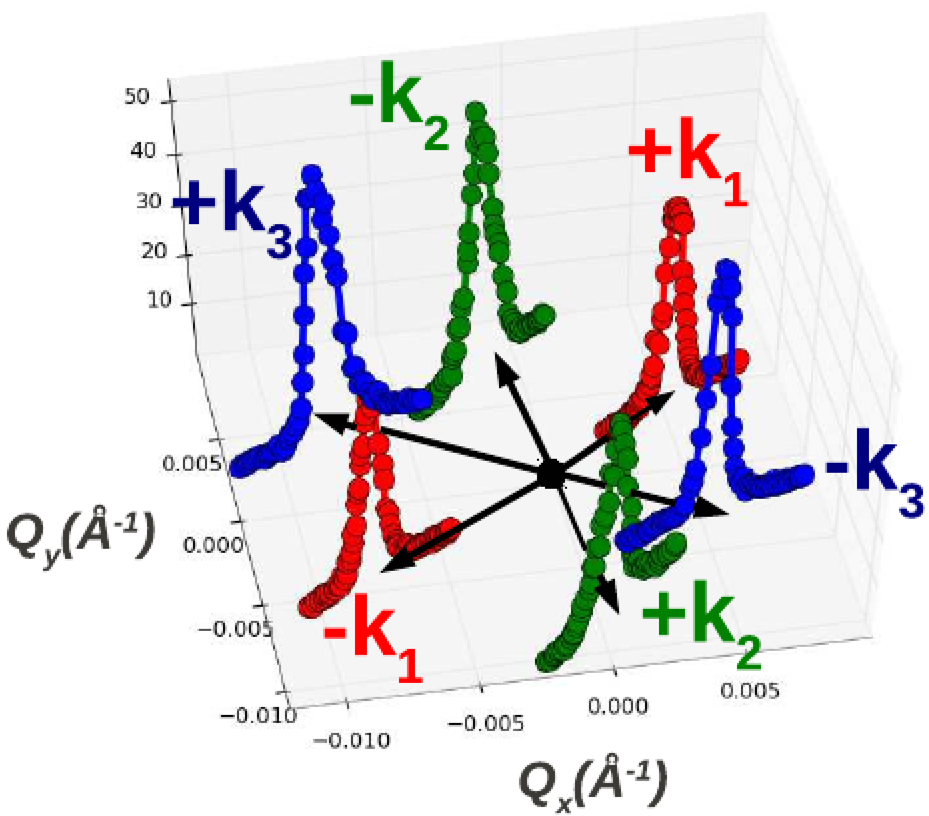


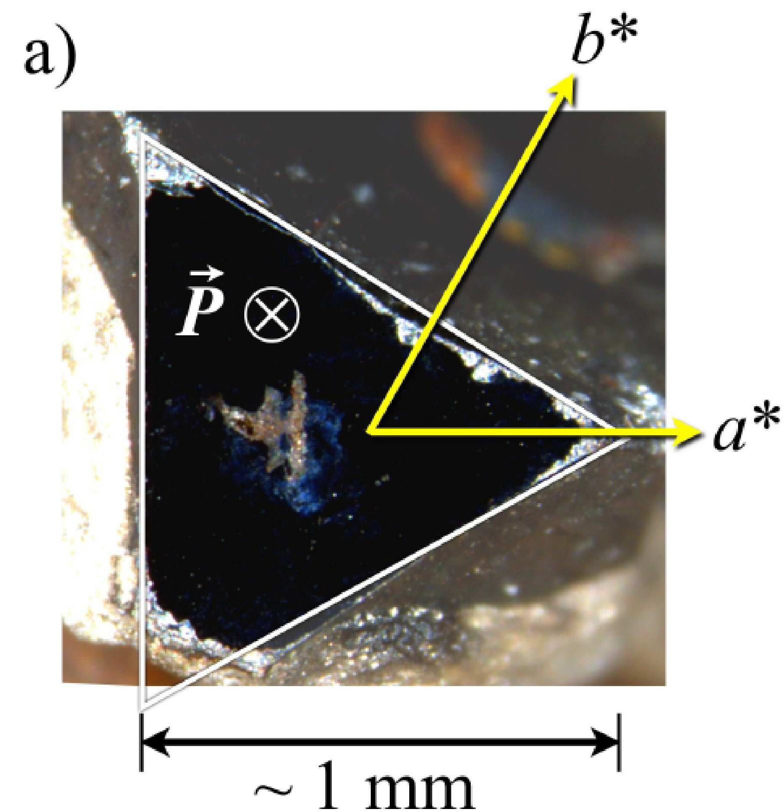


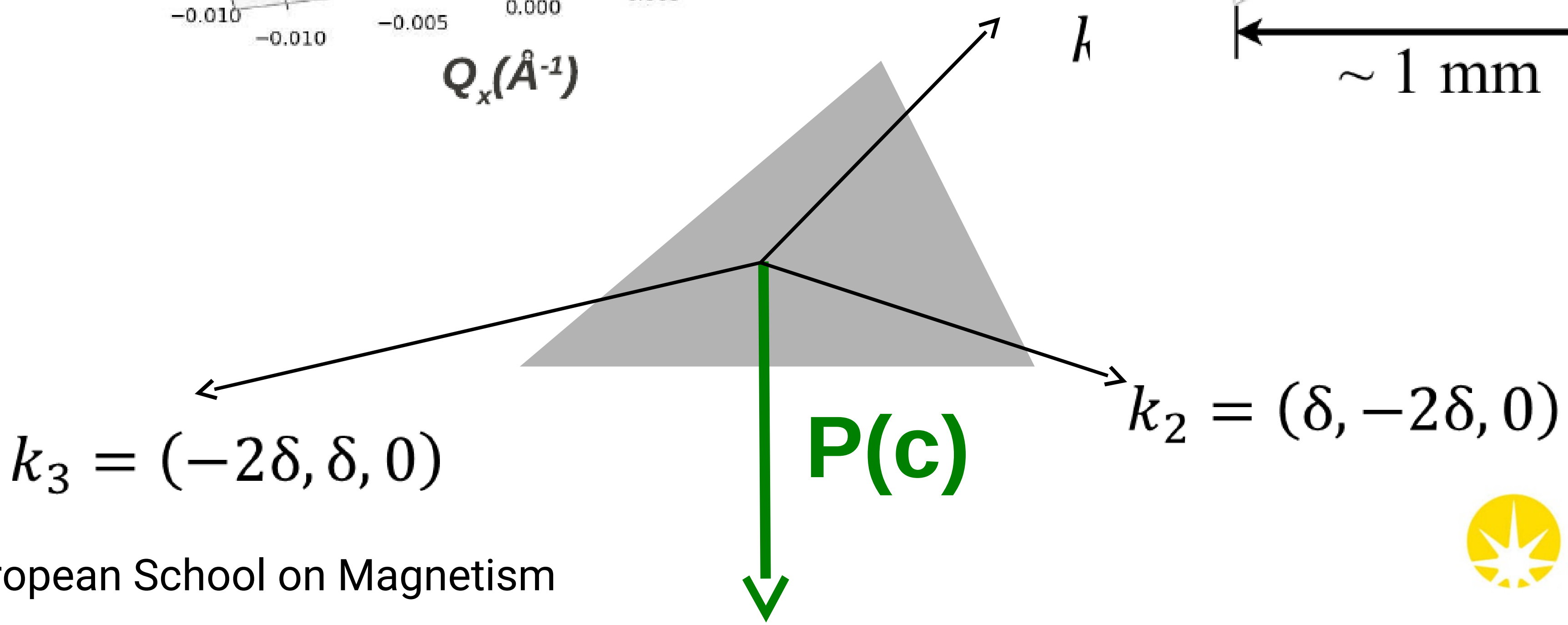


R. Johnson , Phys. Rev. Lett. (2011)

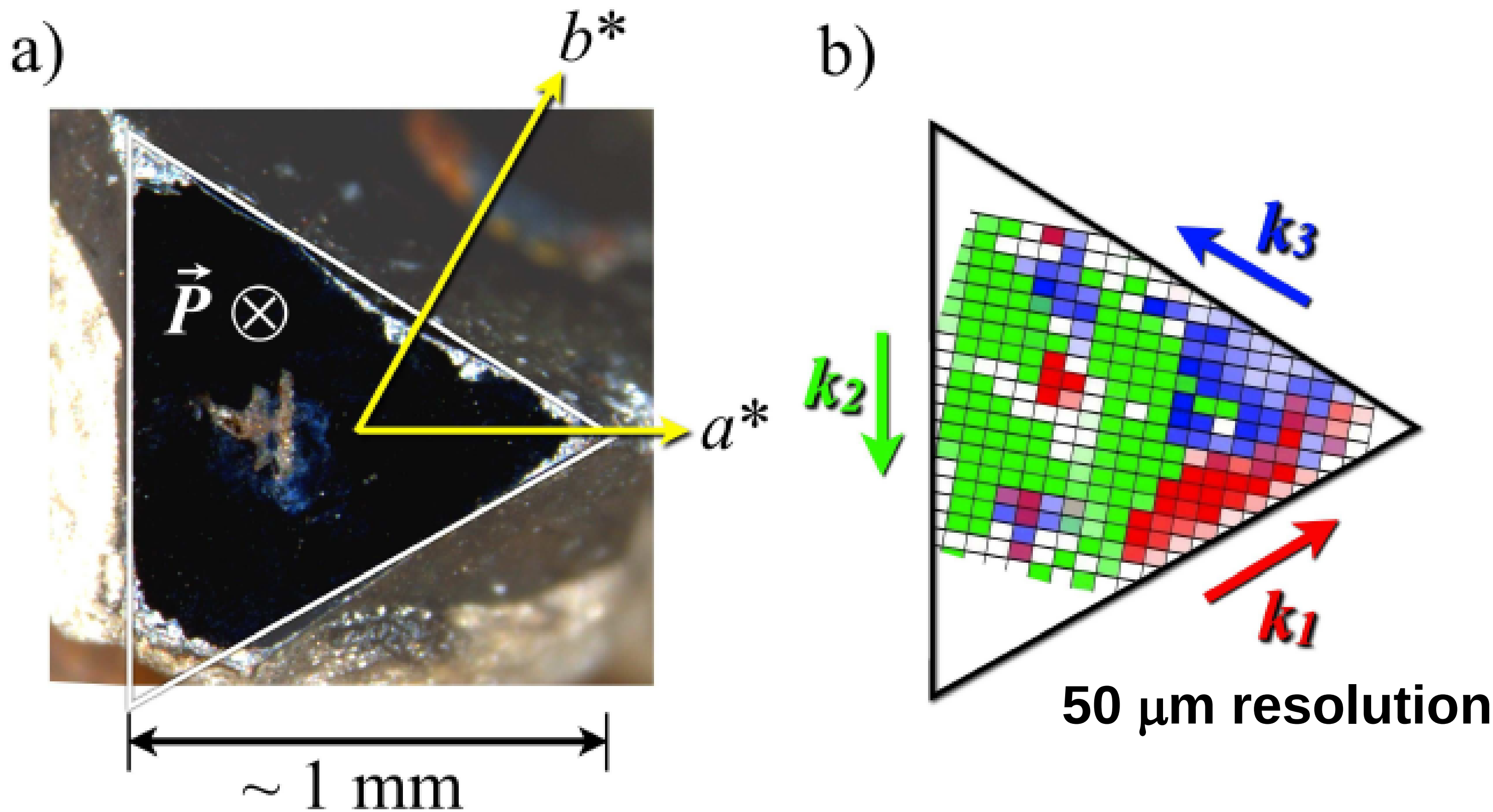
$BiFeO_3$: Non resonant micro-focused magnetic diffraction

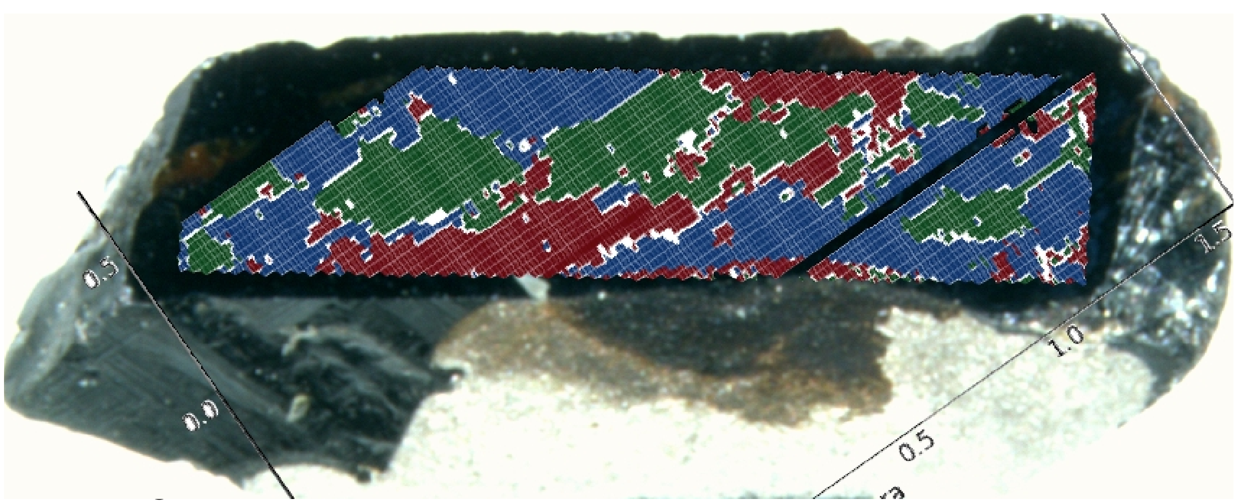






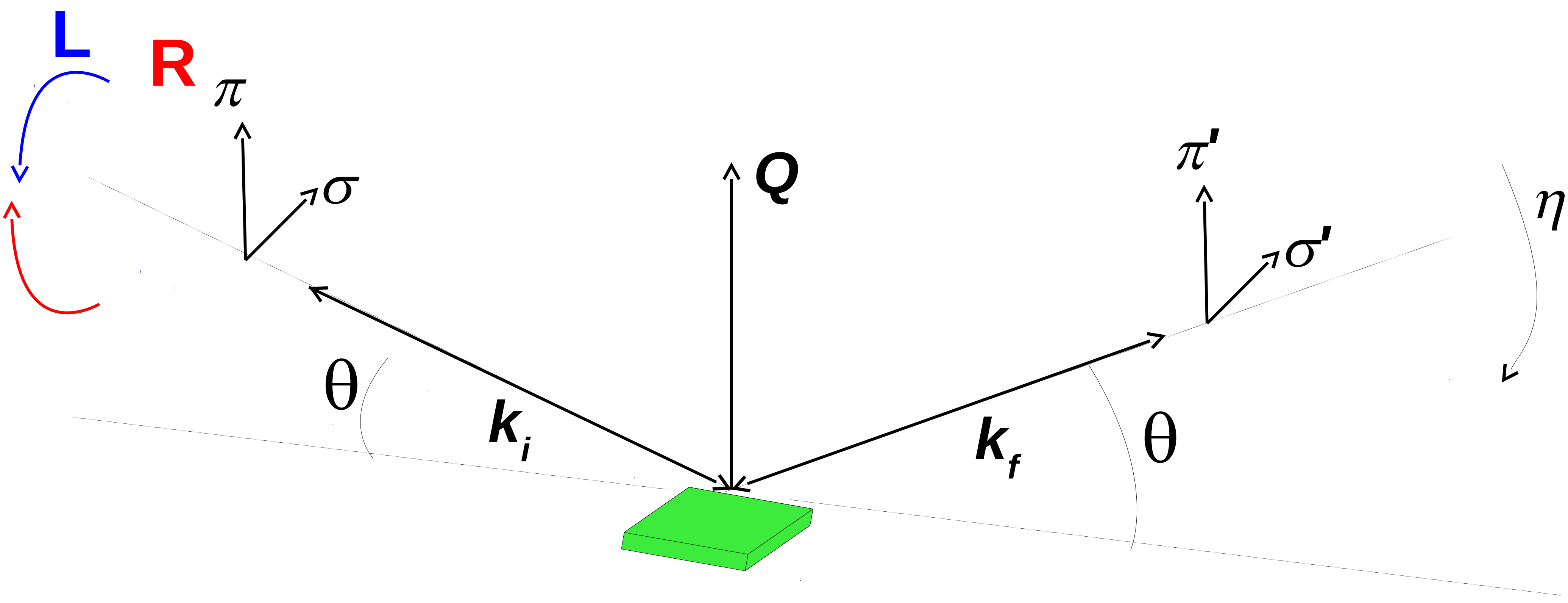
$BiFeO_3$: Non resonant micro-focused magnetic diffraction





diamond

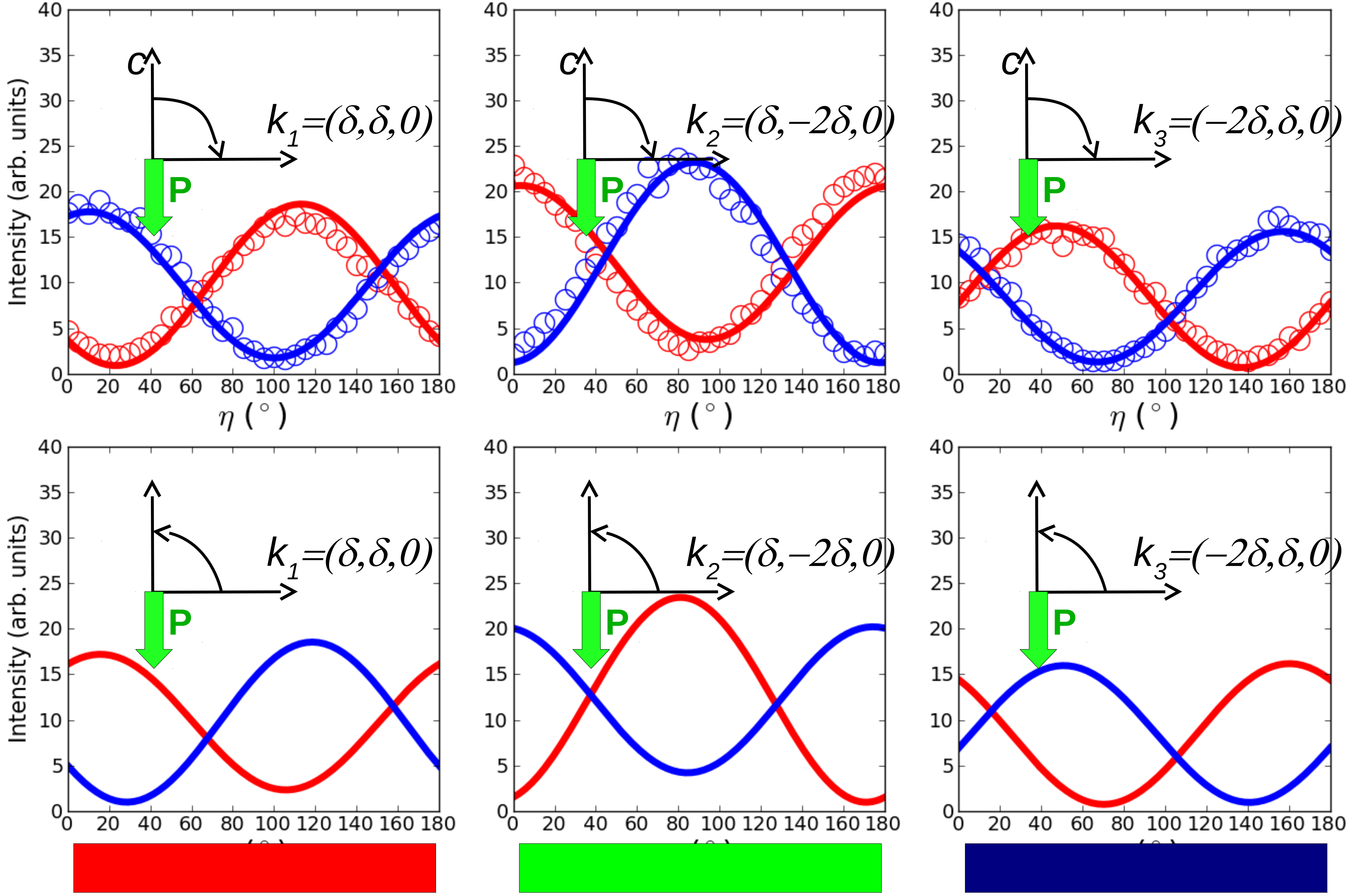
$BiFeO_3$: Non resonant micro-focused magnetic diffraction



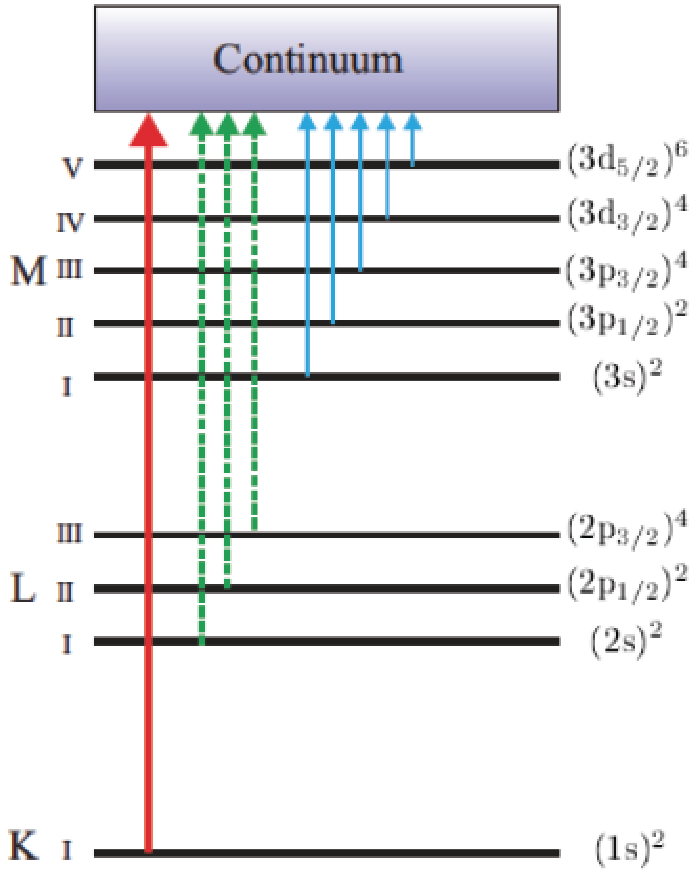
Experiment off resonance, 5.8 KeV

R. D. Johnson,et al., Phys. Rev. Lett. 110, 217206 (2013)

$BiFeO_3$: “Homochiral” domains



Resonant X-ray magnetic scattering



$j = l \pm ½$ $(nl_j)^{2j+1}$

- Tune the energy of the X-ray beam to an absorption edge
- Photon is absorbed and the system re-emit a photon with the same energy
- Element specific information
- Combine the element specific information from spectroscopy techniques with Bragg scattering
- Polarization dependence effects
- Possibility to probe magnetic order but also other E/M-multipoles

diamond

Resonant X-ray magnetic scattering

$$f_{Resonant} \sim \frac{\langle f| e^{-i\boldsymbol{k_f}\cdot\boldsymbol{r_k}} \left[\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_f^*} - i\frac{\hbar}{2}\boldsymbol{\sigma_j}(\boldsymbol{k_f}\times\boldsymbol{\epsilon_f^*})\right] |g\rangle \langle g| e^{i\boldsymbol{k_i}\cdot\boldsymbol{r_j}} \left[\boldsymbol{p_j}\cdot\boldsymbol{\epsilon_i} + i\frac{\hbar}{2}\boldsymbol{\sigma_j}(\boldsymbol{k_i}\times\boldsymbol{\epsilon_i})\right] |a\rangle}{E_a + \hbar\omega_i - E_g + i\Gamma}$$

We need to evaluate the matrix elements:

$$\mathrm{O}_2 = \langle g| \mathcal{H}_2' |i\rangle = \langle g| \boldsymbol{p}\cdot\boldsymbol{\epsilon}(1 + i\boldsymbol{k}\cdot\boldsymbol{r} - \frac{1}{2}(\boldsymbol{k}\cdot\boldsymbol{r})^2 + \ldots) |i\rangle$$

E_1 E_2 E_3

$$\mathrm{O}_3 = \langle g| \mathcal{H}_2' |i\rangle = \langle g| \boldsymbol{\sigma}\cdot(\boldsymbol{k}\times\boldsymbol{\epsilon})(1 + i\boldsymbol{k}\cdot\boldsymbol{r} - \frac{1}{2}(\boldsymbol{k}\cdot\boldsymbol{r})^2 + \ldots) |i\rangle$$

M_1 M_2 M_3

The power expansion is justified by the fact that the spatial extend of the core electron is relatively small (~0.1 A)

We also use the following commutator, to switch to position representation

$$\left[\frac{p^2}{2m}, r\right] = \frac{\hbar}{im}p$$

Resonant X-ray magnetic scattering : E1-E1

$$f_{nE1}^{\mathrm{XRES}} = [(\hat{\boldsymbol{\varepsilon}}' \cdot \hat{\boldsymbol{\varepsilon}})F^{(0)} - i(\hat{\boldsymbol{\varepsilon}}' \times \hat{\boldsymbol{\varepsilon}}) \cdot \hat{\mathbf{z}}_n F^{(1)} + (\hat{\boldsymbol{\varepsilon}}' \cdot \hat{\mathbf{z}}_n)(\hat{\boldsymbol{\varepsilon}} \cdot \hat{\mathbf{z}}_n)F^{(2)}]$$

$$\begin{pmatrix} 0 & \boldsymbol{k}_i \\ -\boldsymbol{k}_f & \boldsymbol{k}_i \times \boldsymbol{k}_f \end{pmatrix}$$

$$F^{(0)} = (3/4k)[F_{11} + F_{1-1}]$$

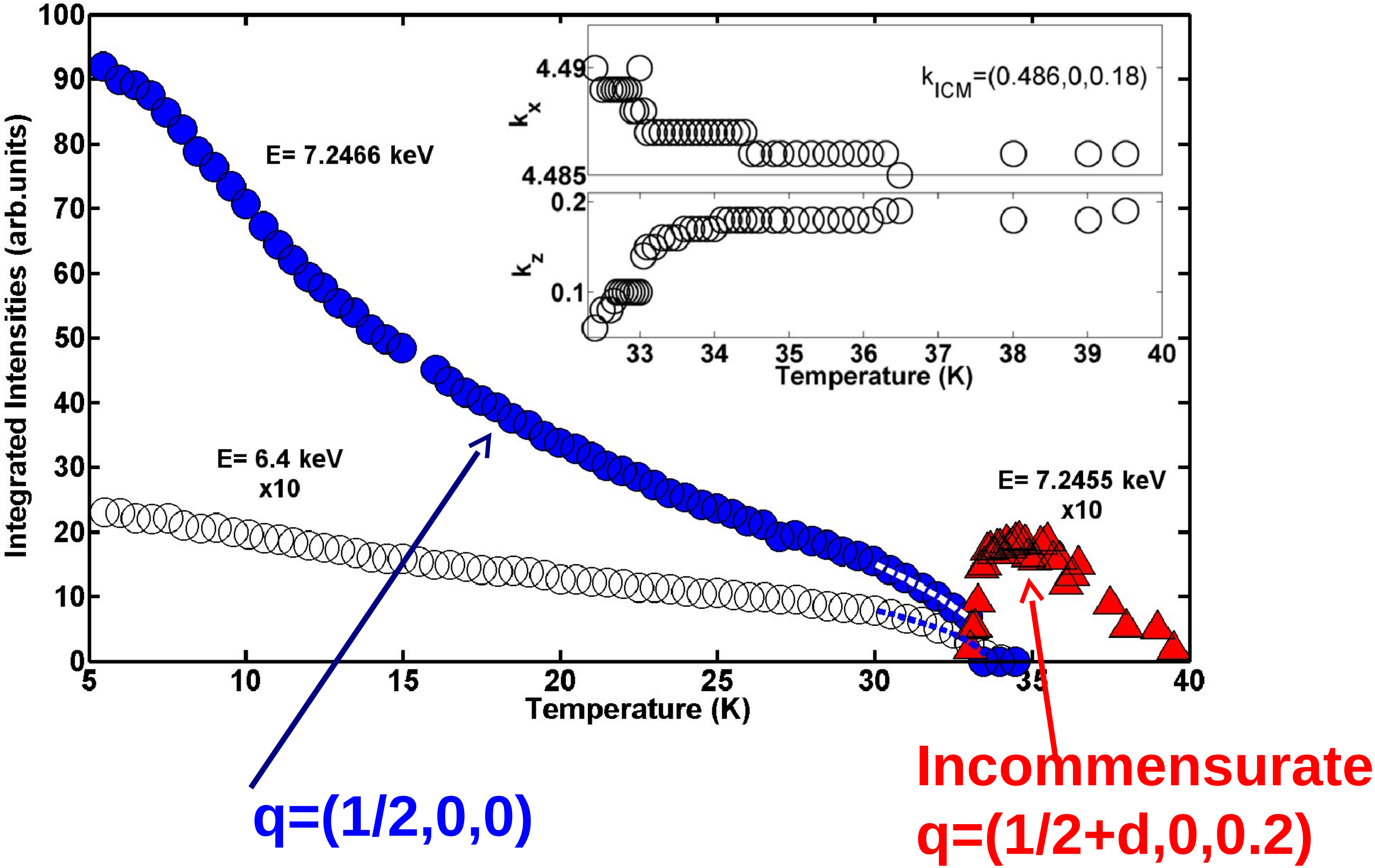
$$F^{(1)} = (3/4k)[F_{11} - F_{1-1}]$$

$$F^{(2)} = (3/4k)[2F_{10} - F_{11} - F_{1-1}].$$

$$F_{LM}^{(e)}(\omega) = \sum_{\alpha,\eta}[P_\alpha P_\alpha(\eta)\Gamma_x(\alpha M\eta;\mathrm{EL})/\Gamma(\eta)]/[x(\alpha,\eta) - i].$$

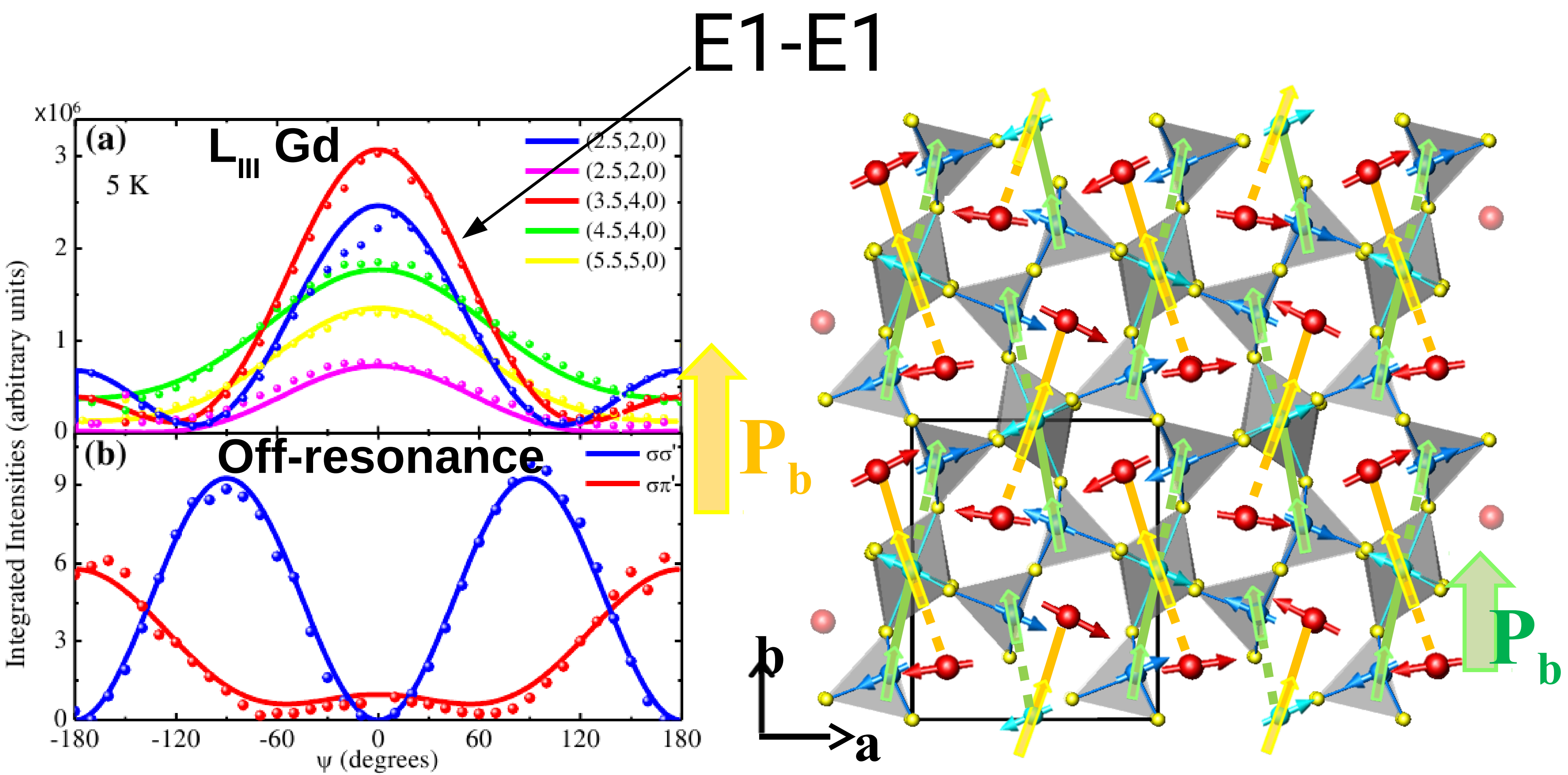
[1] J. P. Hill and D. F. McMorrow, "X-ray resonant exchange scattering: polarization dependence and correlation functions," Acta Crystallogr., vol. A52, pp. 236−244, 1996.

Resonant X-ray magnetic scattering $GdMn_2O_5$



N. Lee, Phys. Rev. Lett. 110, 137203 (2013)

Resonant X-ray magnetic scattering $GdMn_2O_5$



European School on Magnetism

N. Lee, Phys. Rev. Lett. 110, 137203 (2013)

Probing different multipolar orders

$$A = \sum_{\alpha,\beta} \epsilon_\alpha^{o*}\epsilon_\beta^i D_{\alpha\beta} + \frac{i}{2}\sum_{\alpha,\beta,\gamma} \epsilon_\alpha^{o*}\epsilon_\beta^i \left(k_\gamma^i I_{\alpha\beta\gamma} - k_\gamma^o I_{\alpha\beta\gamma}^*\right)$$
$$+\frac{1}{4}\sum_{\alpha,\beta,\gamma,\delta} \epsilon_\alpha^{o*}\epsilon_\beta^i k_\gamma^o k_\delta^i Q_{\alpha\beta\gamma\delta} + \frac{1}{2m\omega_{ng}}$$
$$\times \sum_{\alpha,\beta} \left(\epsilon_\alpha^{o*}(\vec{\epsilon}^i \times \vec{k}^i)_\beta R_{\alpha\beta} + (\vec{\epsilon}^{o*} \times \vec{k}^o)_\beta \epsilon_\alpha^i R_{\alpha\beta}^*\right)$$
$$+\frac{i}{2m\omega_{ng}}\sum_{\alpha,\beta,\gamma} (\epsilon_\alpha^{o*}(\vec{\epsilon}^i \times \vec{k}^i)_\beta k_\gamma^i P_{\alpha\beta\gamma}$$
$$-(\vec{\epsilon}^{o*} \times \vec{k}^o)_\beta k_\gamma^o \epsilon_\alpha^i P_{\alpha\beta\gamma}^*).$$

ℓ	E1–E1	E1–E2	E2–E2
0	Electric charge (++)	*****************	Electric charge (++)
1	Magnetic dipole (+−)	Electric dipole (−+)	Magnetic dipole (+−)
		Polar toroidal dipole (−−)	
2	Electric quadr. (++)	Axial toroidal quadr. (−+)	Electric quadr. (++)
		Magnetic quadrupole (−−)	
3	*****************	Electric octupole (−+)	Magnetic octupole (+−)
		Polar toroidal octup. (−−)	
4	*****************	*****************	Electr. hexadecap. (++)

ℓ	E1–M1	E1–M2
0	Axial toroidal monopole (−+)	Electric charge (++)
	'Magnetic monopole' (−−)	Polar toroidal monopole (+−)
1	Electric dipole (−+)	Axial toroidal dipole (++)
	Polar toroidal dipole (−−)	Magnetic dipole (+−)
2	Axial toroidal quadrupole (−+)	Electric quadrupole (++)
	Magnetic quadrupole (−−)	Polar toroidal quadrupole (+−)
3	*****************	Axial toroidal octupole (++)
		Magnetic octupole (+−)

[1] S. Di Matteo, "Resonant x-ray diffraction: multipole interpretation," J. Phys. D. Appl. Phys., vol. 45, no. 16, p. 163001, 2012.

Note on link between cross section and absorption spectroscopy

Optical theorem

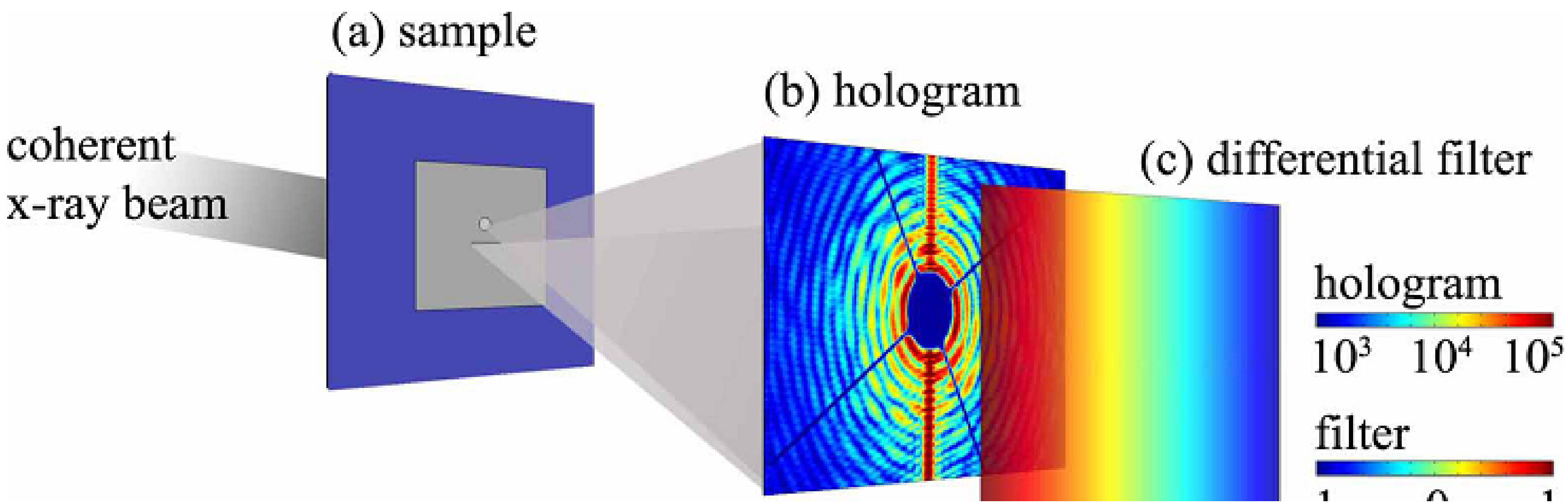
$$\sigma = \frac{4\pi}{k}\,\mathrm{Im}\{f(Q=0)\}$$

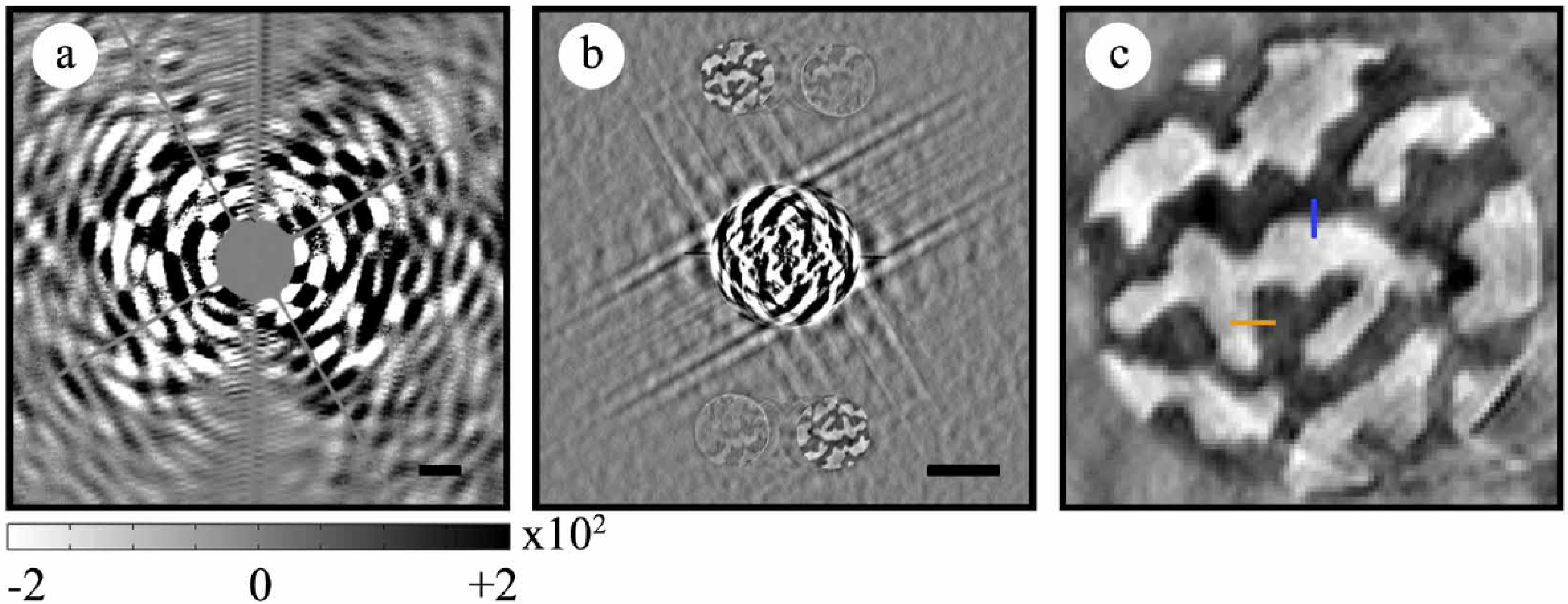
$$f_{nE1}^{\mathrm{XRES}} = [(\hat{\boldsymbol{\varepsilon}}' \cdot \hat{\boldsymbol{\varepsilon}})F^{(0)} - i(\hat{\boldsymbol{\varepsilon}}' \times \hat{\boldsymbol{\varepsilon}}) \cdot \hat{\mathbf{z}}_n F^{(1)} + (\hat{\boldsymbol{\varepsilon}}' \cdot \hat{\mathbf{z}}_n)(\hat{\boldsymbol{\varepsilon}} \cdot \hat{\mathbf{z}}_n)F^{(2)}]$$

XMCD

XMLD

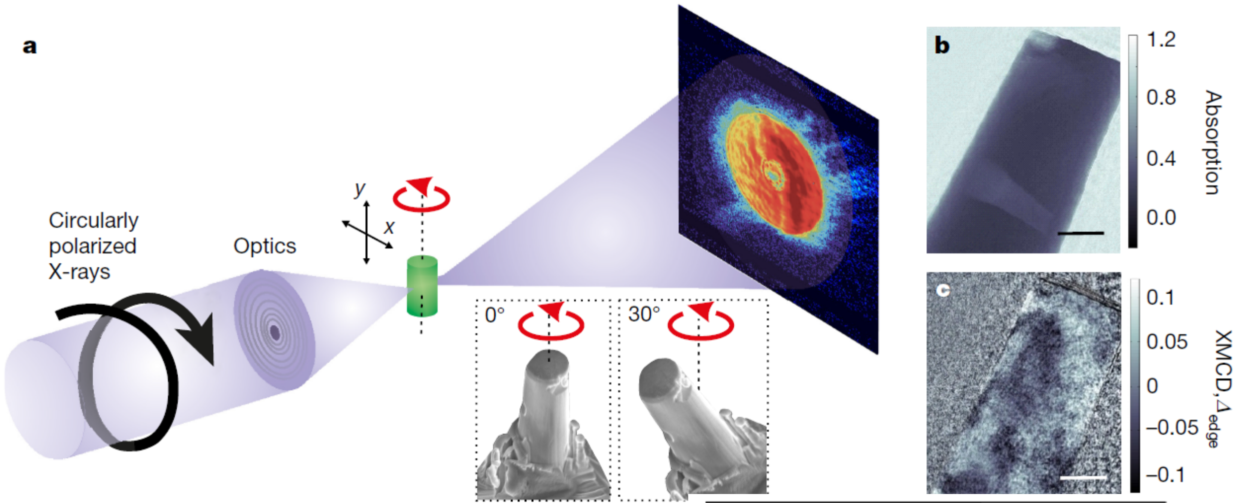
Magnetic X-ray holography

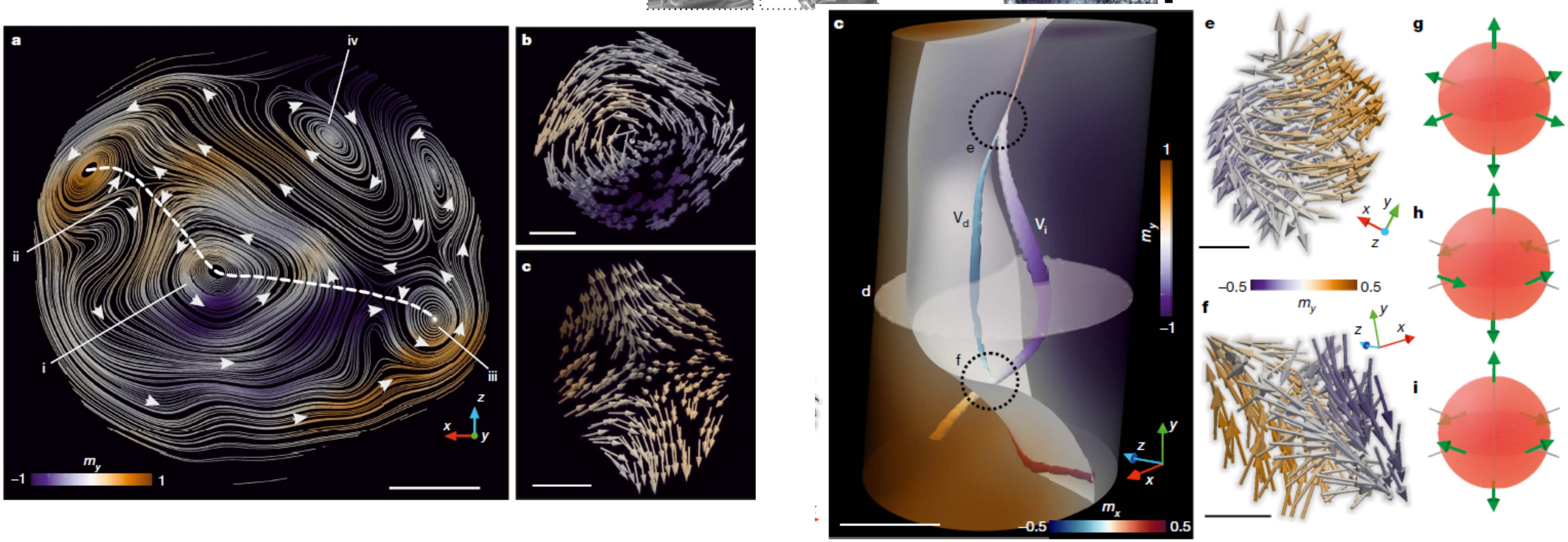




Thomas A. Duckworth, Feodor Ogrin, Sarnjeet S. Dhesi,
Sean Langridge, Amy Whiteside, Thomas Moore, Guillaume Beutier, and Gerrit van der Laan,
"Magnetic imaging by x-ray holography using extended references," Opt. Express 19, 16223-16228 (2011)

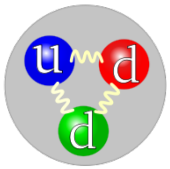
Ptychography





[1] C. Donnelly et al., “Three-dimensional magnetization structures revealed with X-ray vector nanotomography,” Nature, vol. 547, no. 7663, pp. 328–331, 2017.

Neutrons and X-ray for magnetic scattering



Neutron

- Born approximation valid
- Magnetic ~ nuclear scattering amplitude
- Very little beam heating → low T

- Large penetration depth, bulky sample environments (magnets, dilution….)

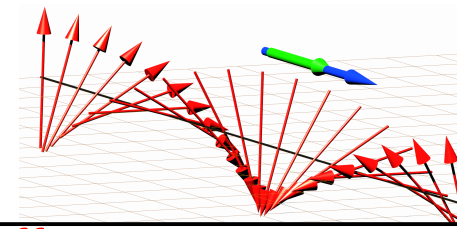
- Manipulate polarization and analysis but costly (flux)

- Large divergence, relatively poor Q-resolution

- Lack of spatial resolution

- Flux typically up to 10^{10} $n.cm^{-2}.s^{-1}$ (scattering volume)

- No direct L/S separation (only by fitting form factor)



X-ray

- Off resonance can get quantitative M but scaling to charge scattering not always easy (use of attenuators for charge scattering...)
- Magnetic Xs much smaller but compensated by flux.
- Beam heating can be a problem not straightforward to go to dilution T
- Not easy to do k=0 work

- Manipulate polarization and analysis

- Highly collimated, excellent Q-resolution

- Spatial resolution down to 20nm

- High brilliance and flux
- Direct L/S separation
- Resonant → element specific
- Resonant → probe tensor beyond magnetic dipole

diamond