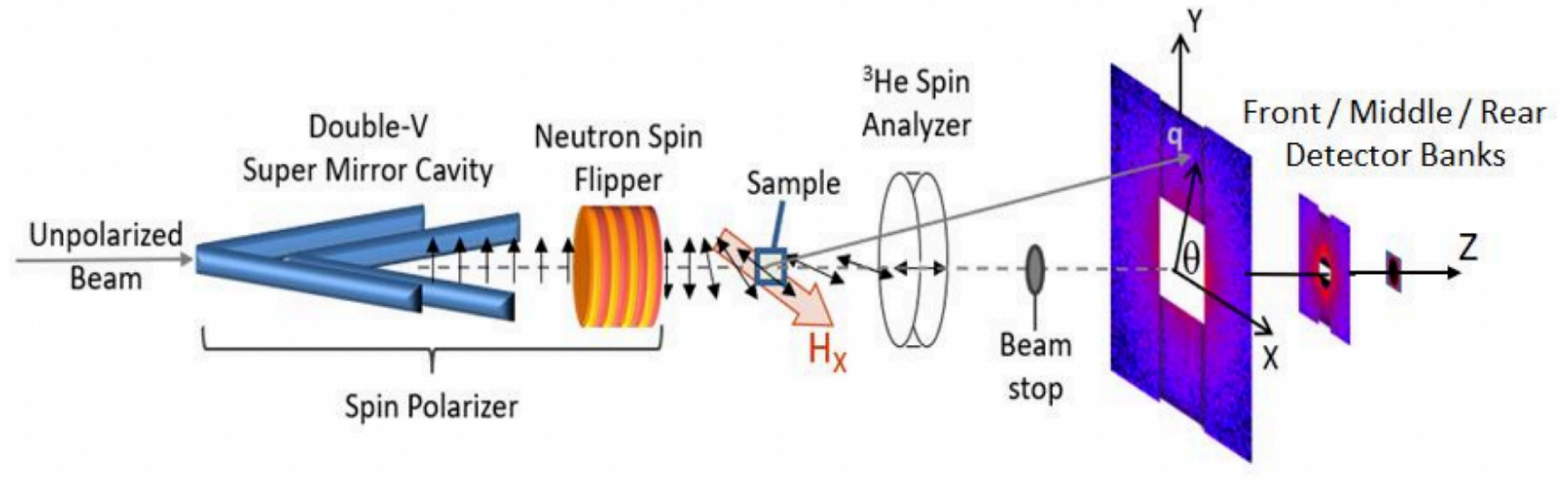
Small-Angle Neutron Scattering

And Polarization Analysis Of Magnetic Materials



NCNR Summer School 2024

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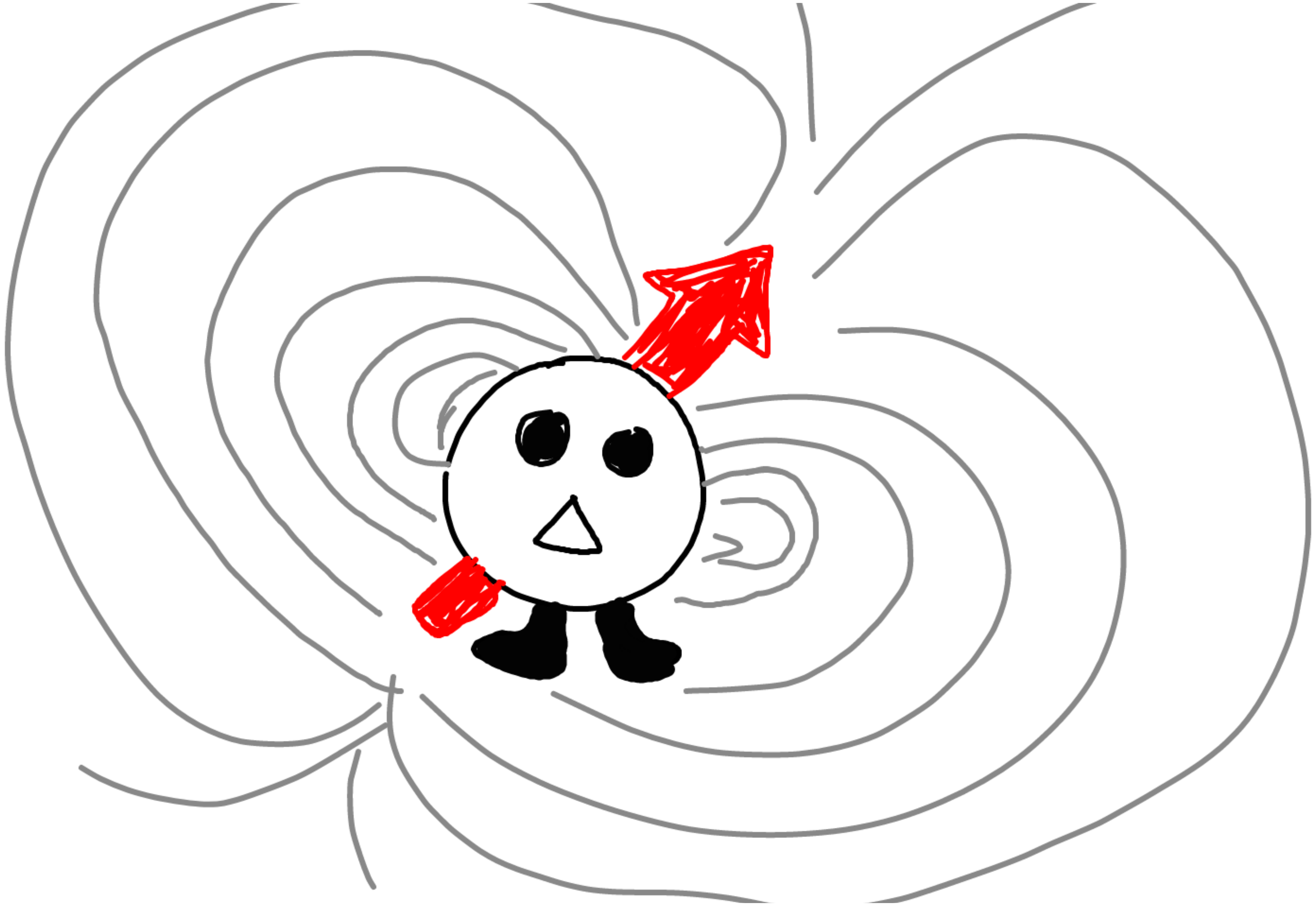
Goal of this talk

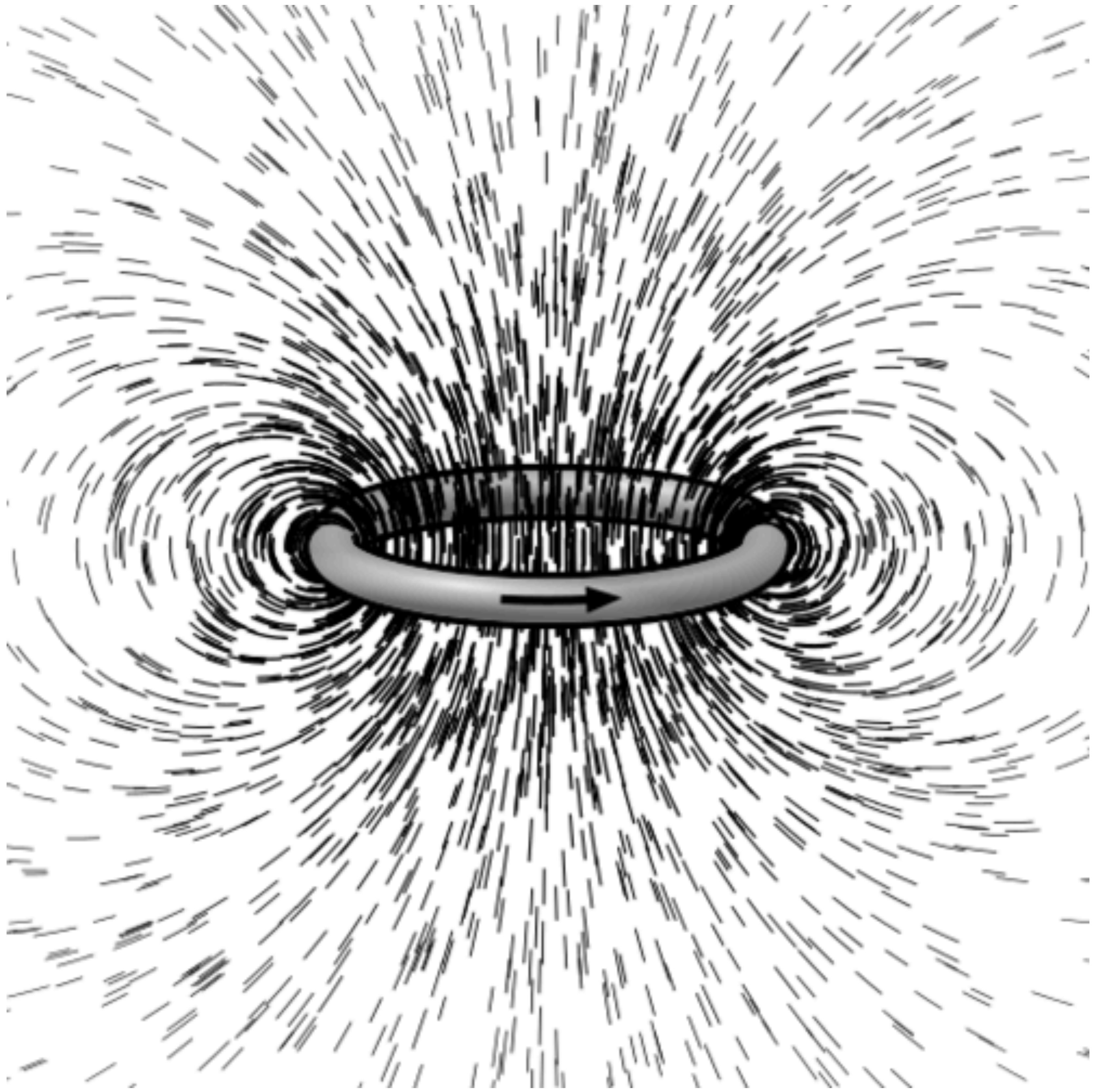
- What is Small-Angle Neutron Scattering (SANS) and how can we use it with polarized neutrons to gain insights into magnetic properties of materials?

The neutron properties are well tuned to study materials



- Lifetime ~ 15 min
- No charge
- Mass = $1.67492 * 10^{-27}$ kg
- Spin = 1/2

As a crude approximation, a spin can be seen as an intrinsic angular momentum (“spinning”) that produces a magnetization



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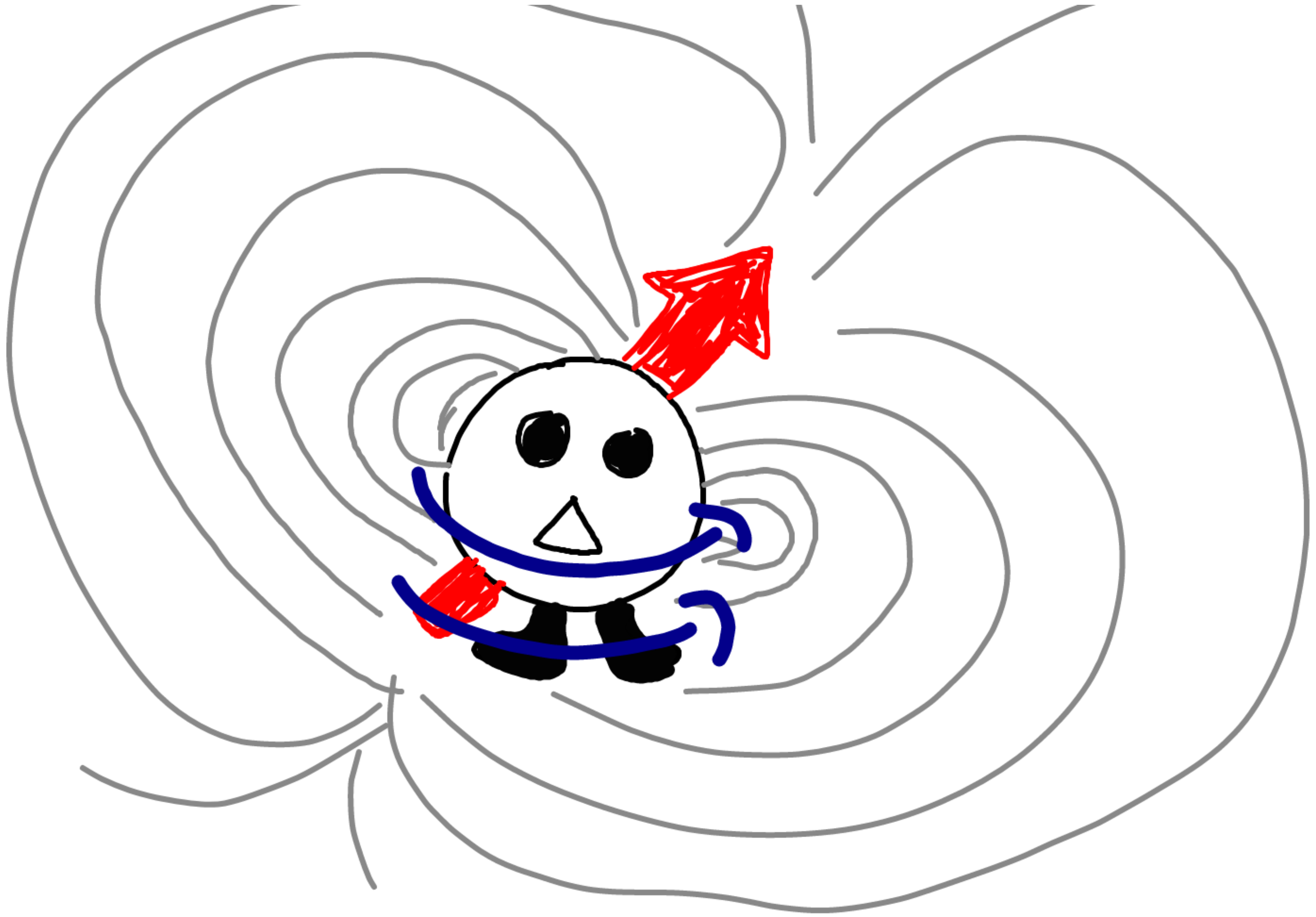
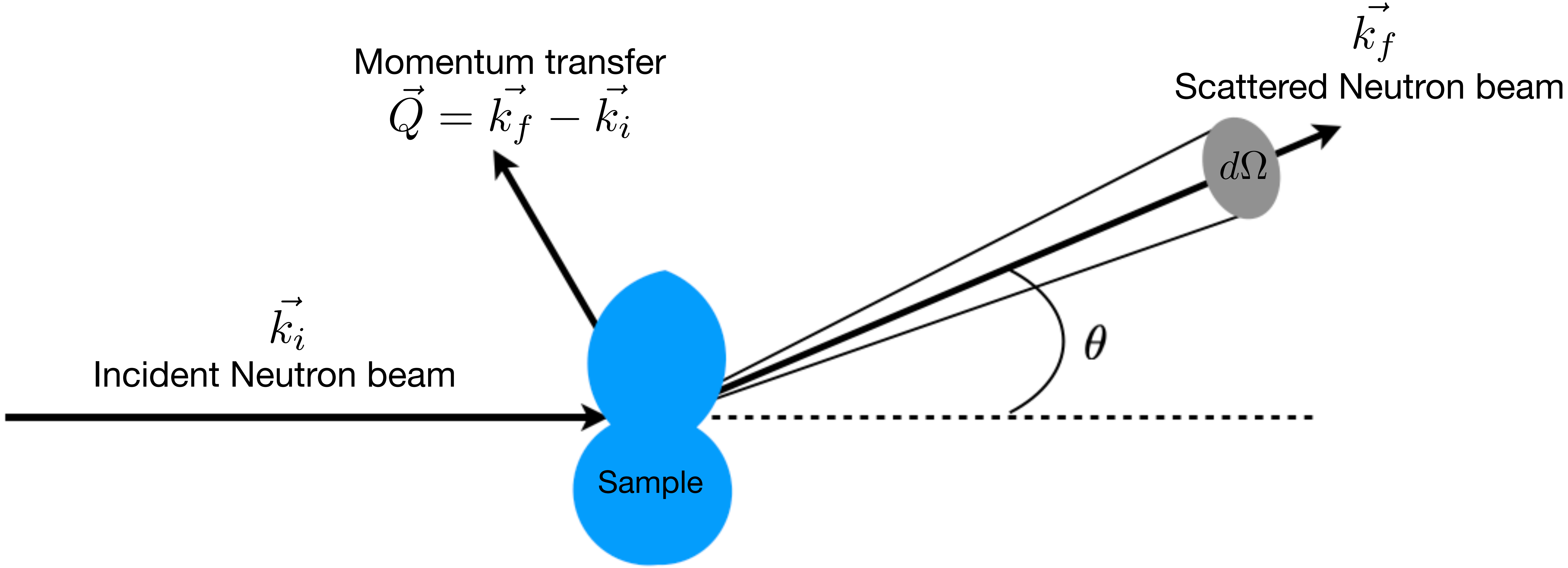


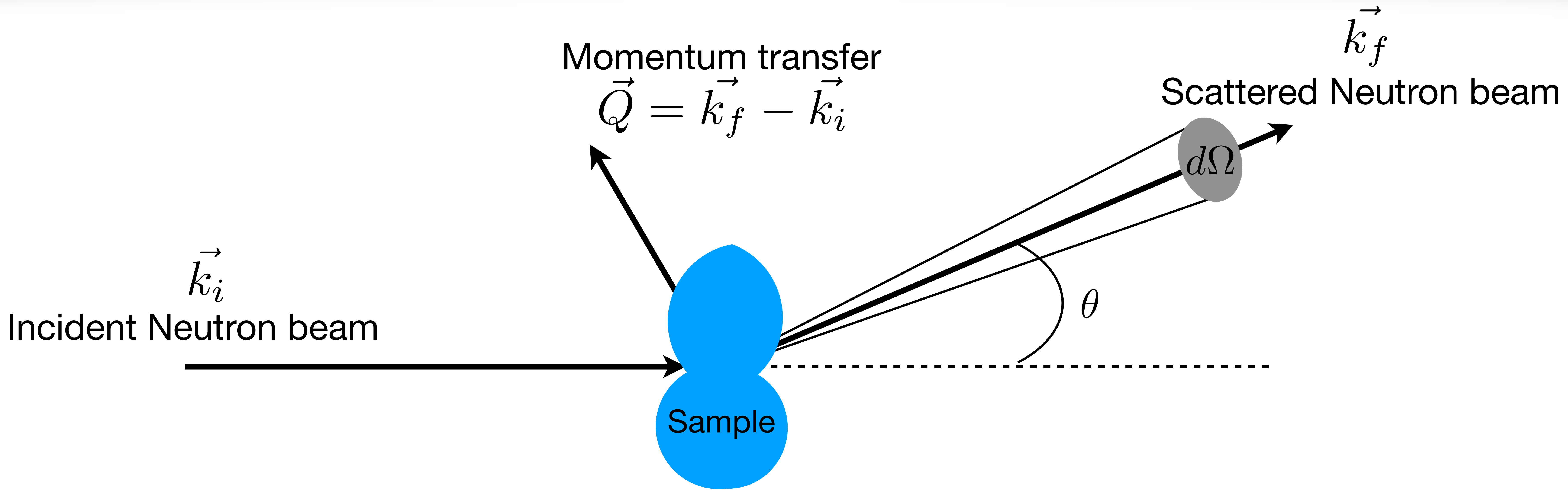
Generally, a neutron scattering experiment consists of counting the number of neutrons scattered by a sample in different directions.

For this talk, we assume elastic scattering only

$$\Delta E = 0$$



Neutron cross-sections are helpful to characterize the strength of interaction between the sample and the neutron



Total Cross-section

$$\sigma_{tot} = \frac{\text{Number of neutrons scattered in all directions per second}}{\text{Incident flux } (I_0)}$$

Units of area in barns (1 barn = 10^{-28} m^2)

Differential Cross-section

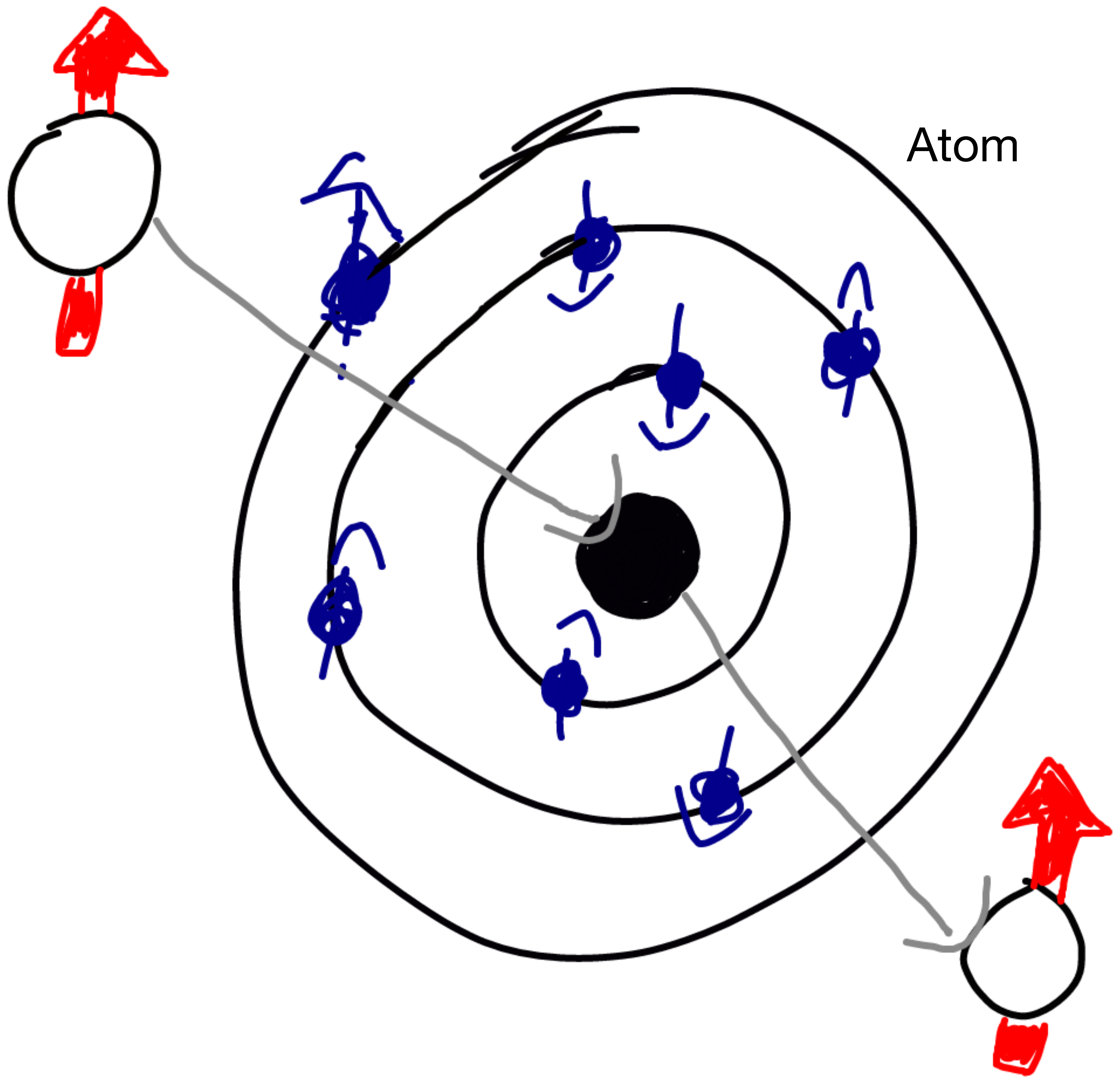
$$\frac{d\sigma}{d\Omega} = \frac{\text{Number of neutrons scattered per sec. into a solid angle } d\Omega}{\text{Incident flux } (I_0)}$$

Units are barns/steradian

** A macroscopic diff. cross-section is often used, which divides the diff. cross-section by the volume of the sample.

A neutron interacts with the atoms within a material via 2 different ways

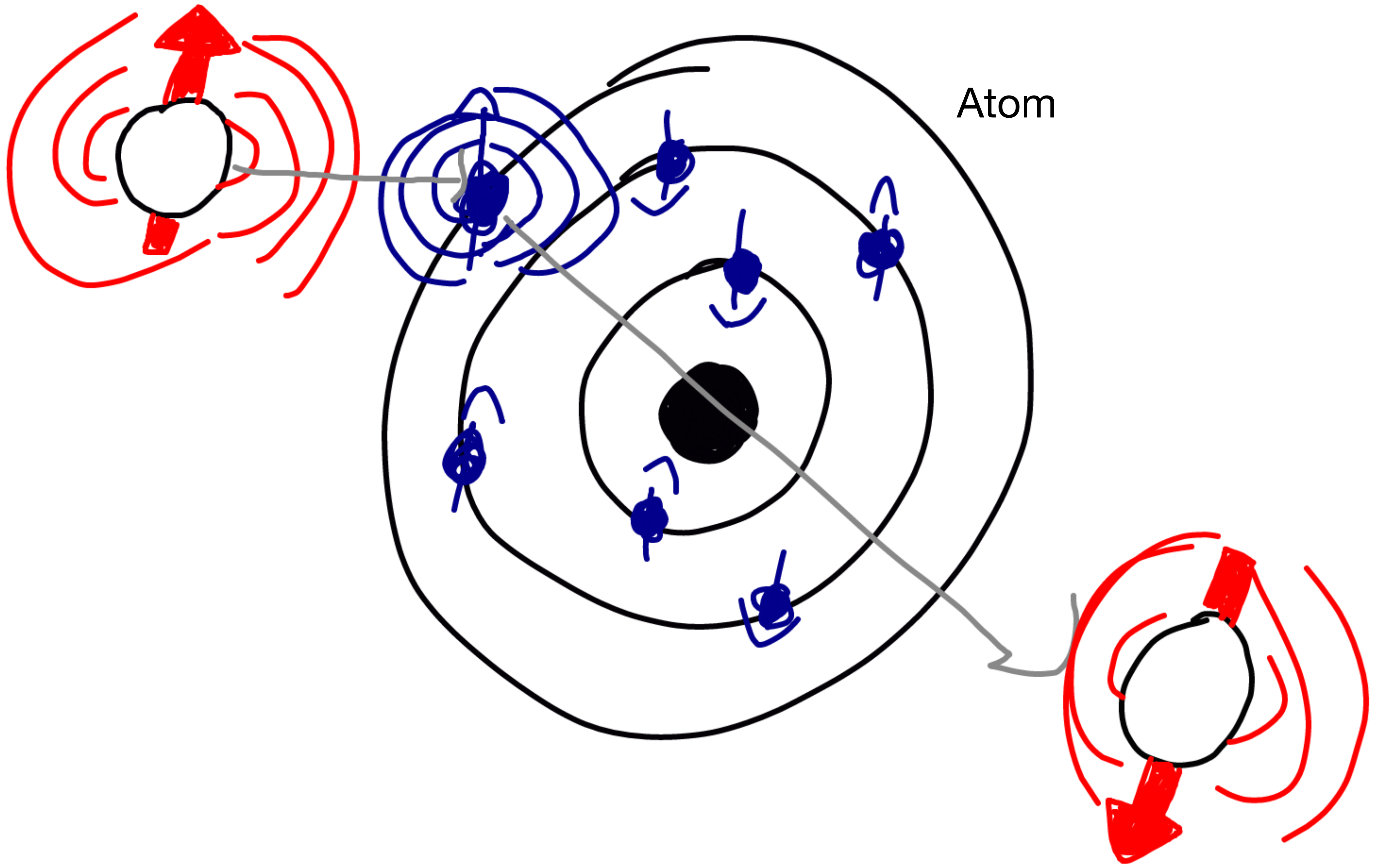
Nuclear Interaction



$$\hat{V}_N(\boldsymbol{r}_n, \boldsymbol{R}_N) = -\frac{2\pi\hbar^2}{m_n} b\,\delta(\boldsymbol{r}_n - \boldsymbol{R}_N)$$

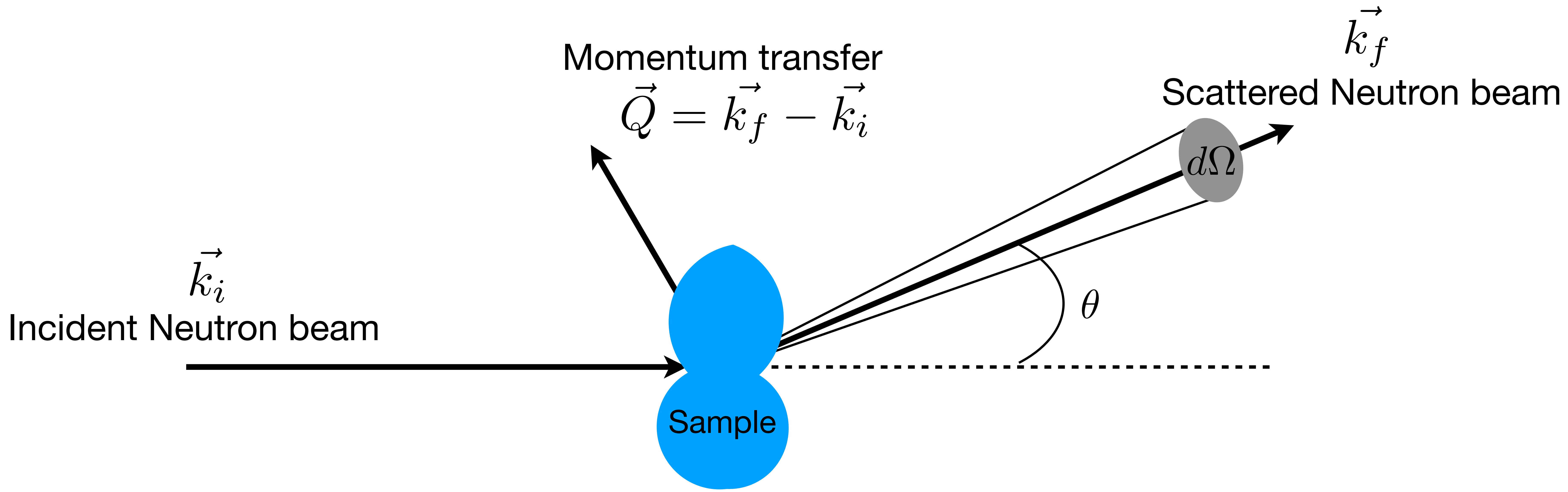
b: Neutron Scattering length (~ 1fm = 1e-15 m)

Magnetic Dipole-Dipole Interaction

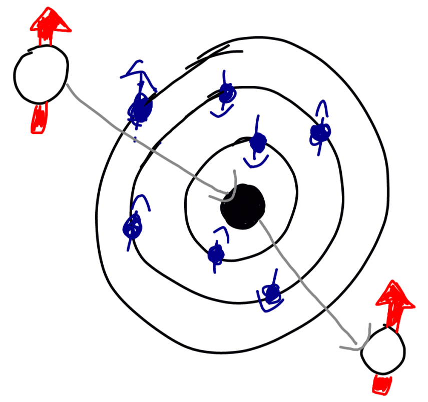


$$\hat{V}_M(\vec{r_n}, \vec{r_e}) = -\vec{S_n} \cdot \vec{B}(\vec{r_n} - \vec{r_e})$$

The neutron differential cross-section probes the Fourier transformation of the density (ρ) and magnetization (M) of a material



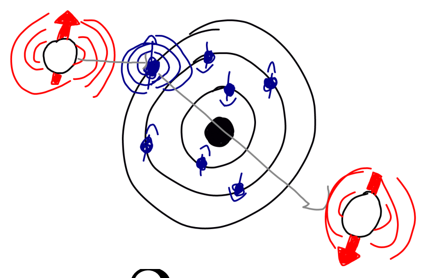
Nuclear Neutron diff. Cross-section



$$\frac{d\sigma}{d\Omega}(\vec{Q}) \propto \left| \int_V \rho(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r} \right|^2$$

Nuclear Scattering Density

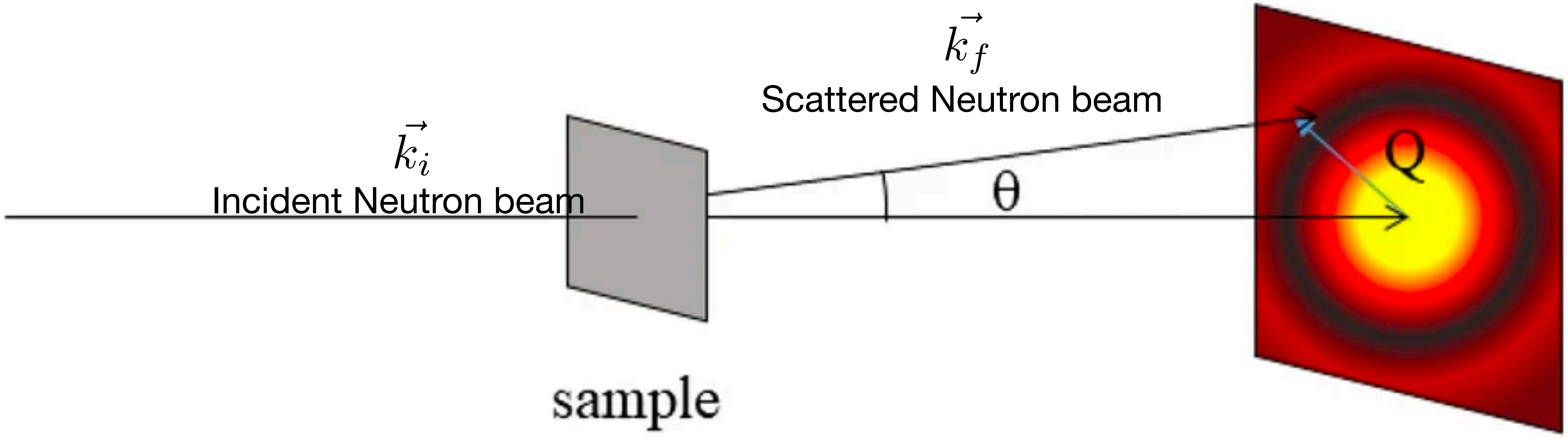
Magnetic Neutron diff. Cross-section



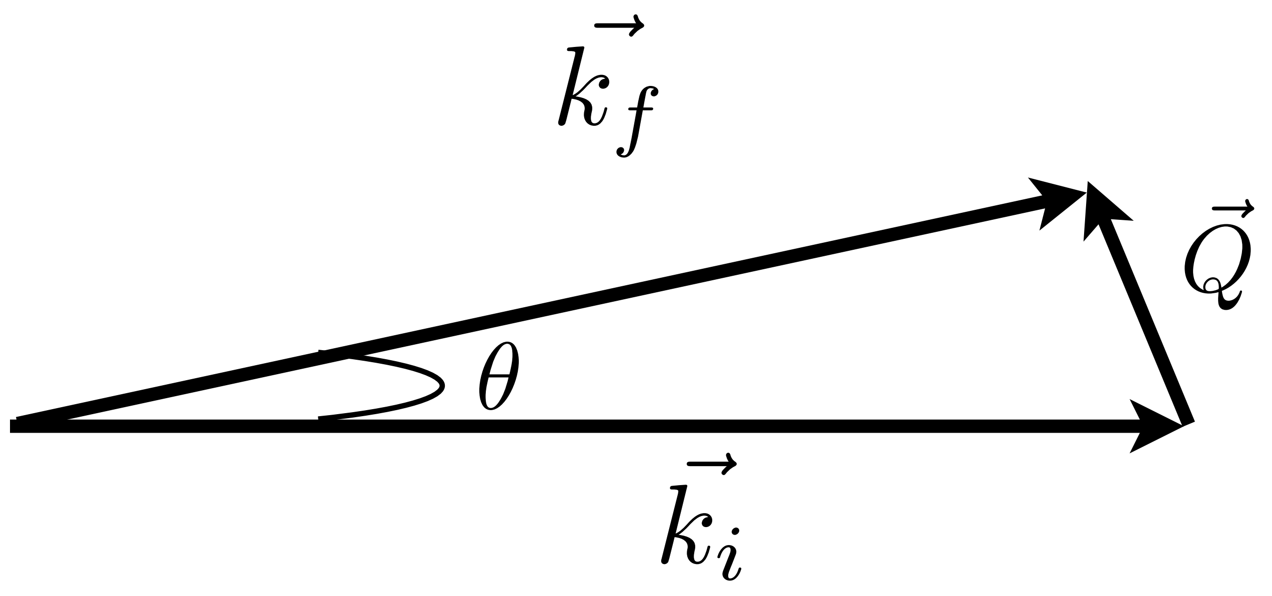
$$\frac{d\sigma}{d\Omega}(\vec{Q}) \propto \left| \int_V M_{\perp Q}(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r} \right|^2$$

Magnetization Density

SANS: Small-Angle (low Q) neutron scattering is a technique designed to probe “long” length scale structures.



$$Q = 2ksin(\frac{\theta}{2}) \sim k\theta$$



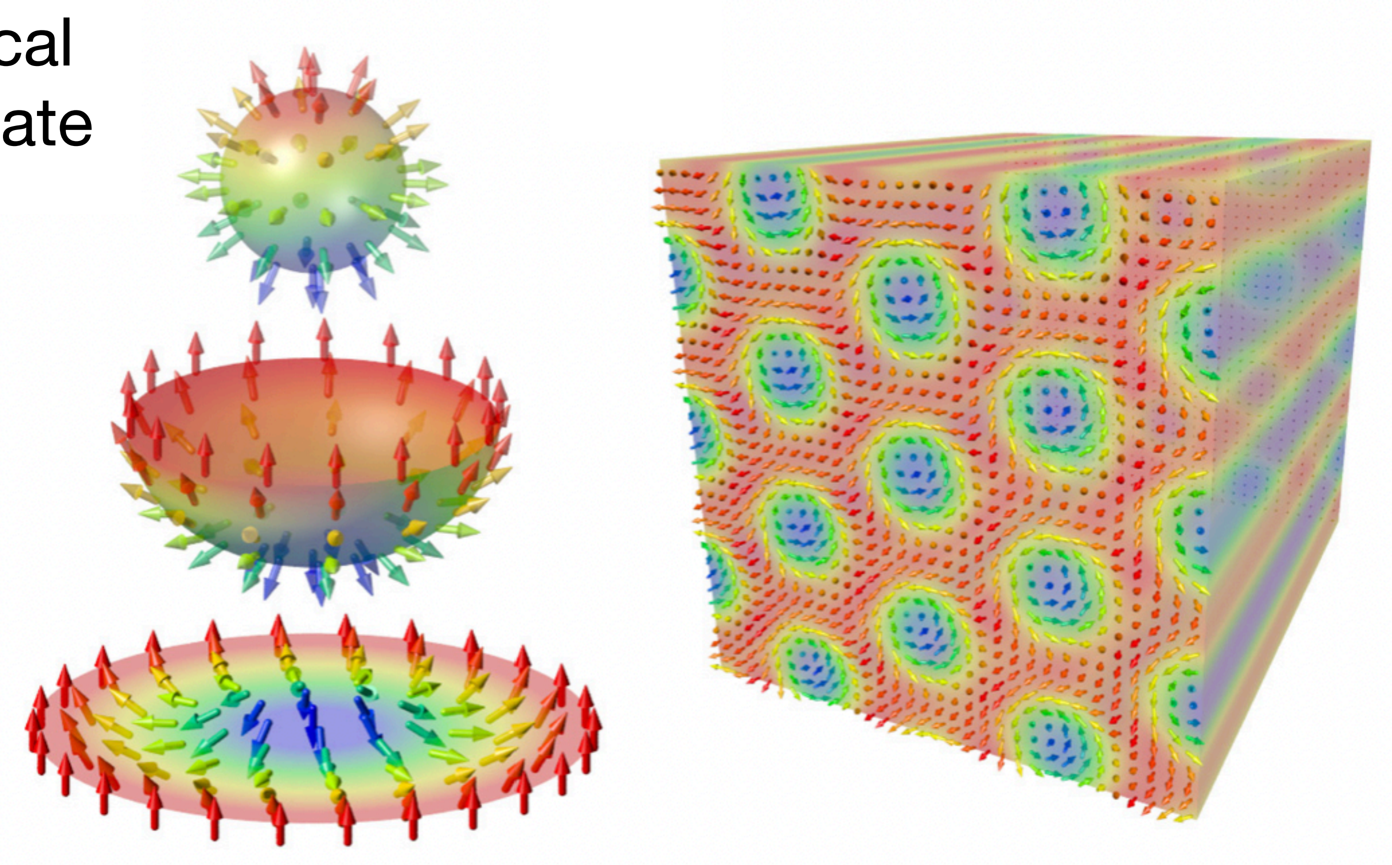
$$D = \frac{2\pi}{|\vec{Q}|}$$

D (length scale) ~ 1 to 10 000 nm

Liu, Dong et al. "Current progresses of small-angle neutron scattering on soft-matters investigation." *Nuclear Analysis* (2022): 100011.

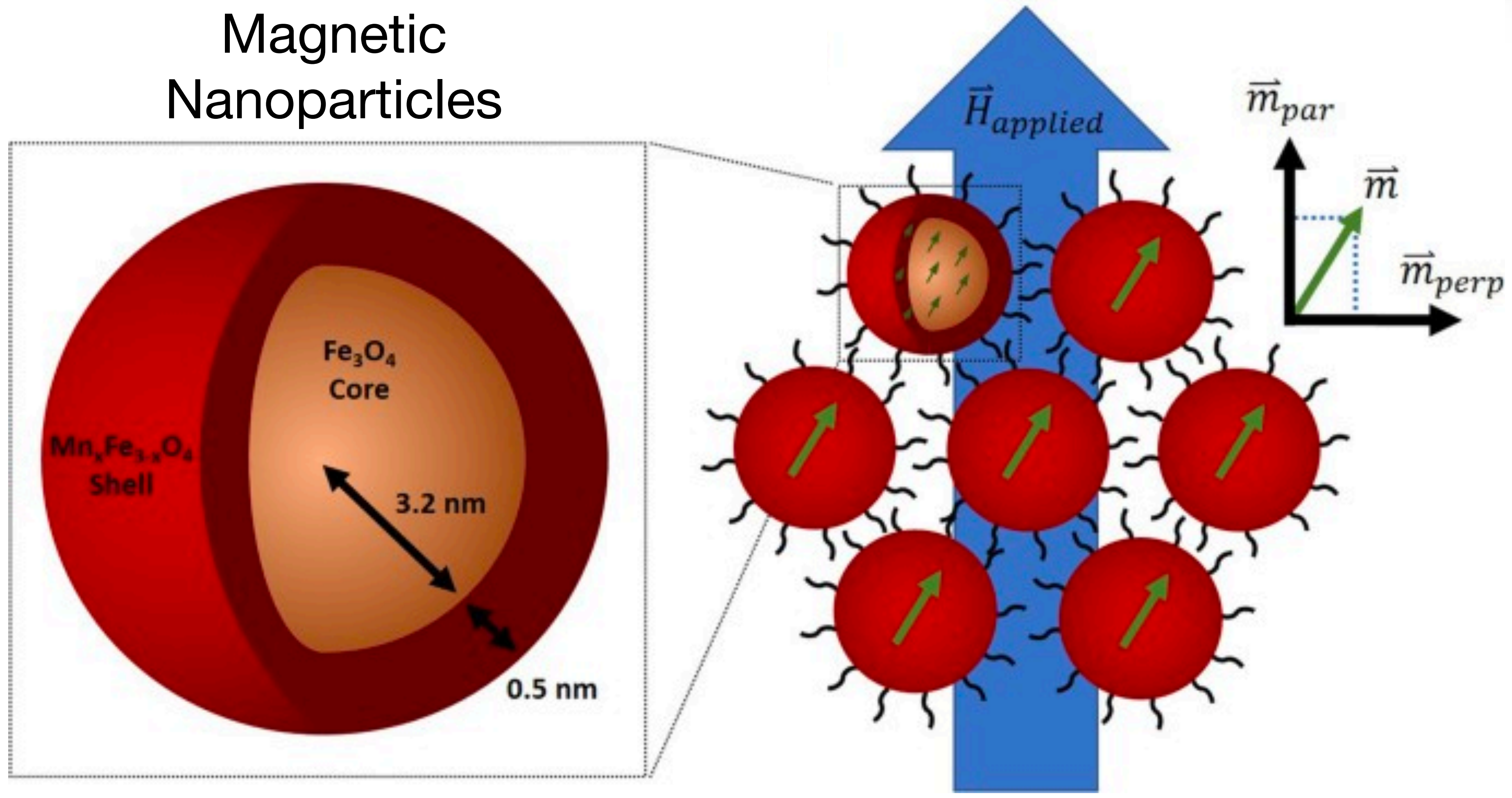
SANS is useful for various hard condensed matter systems

Topological Multi-**q** state



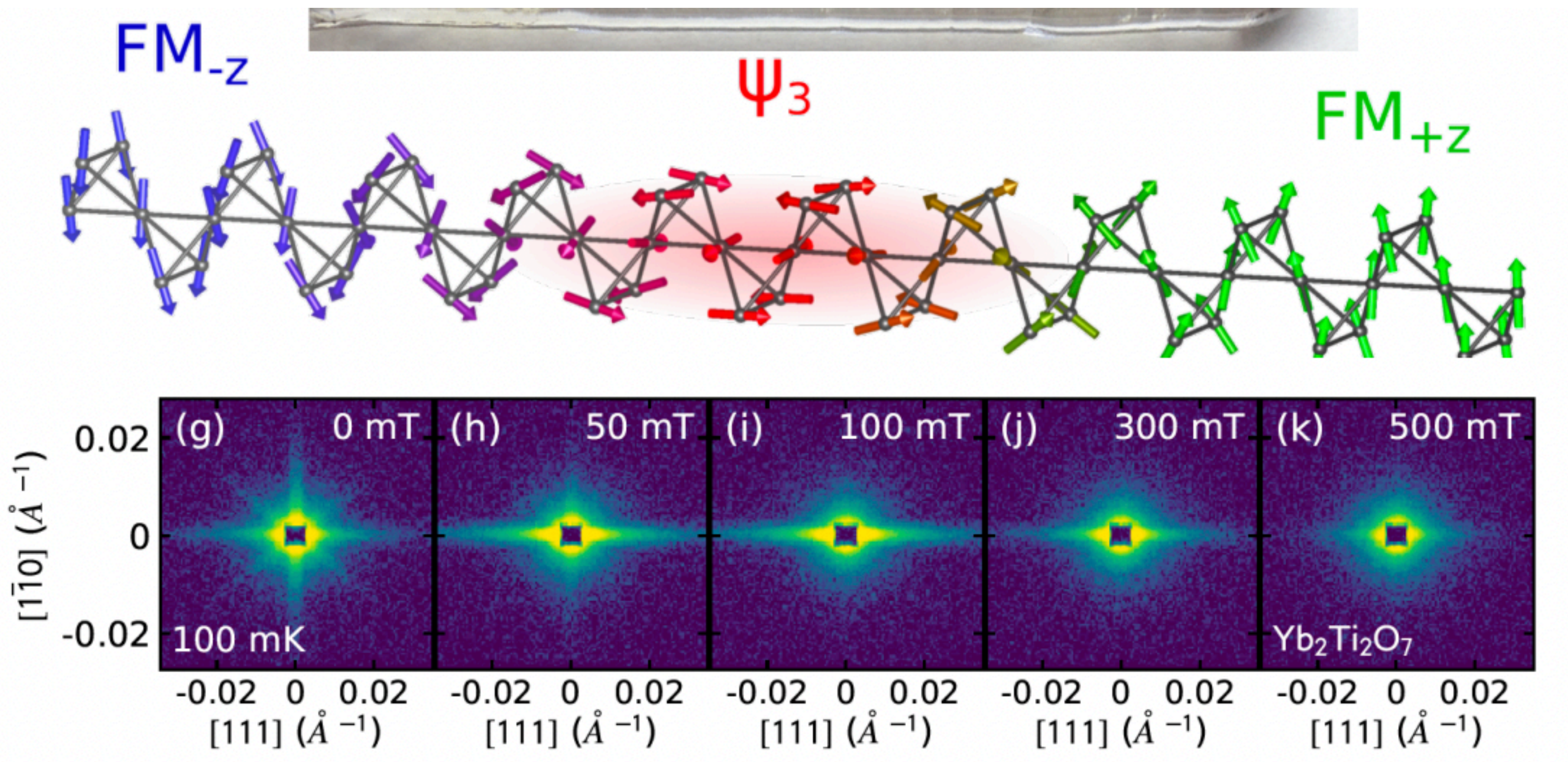
K. Everschor-Sitte et al., J. Appl. Phys. 115, 172602(2014)

Magnetic Nanoparticles



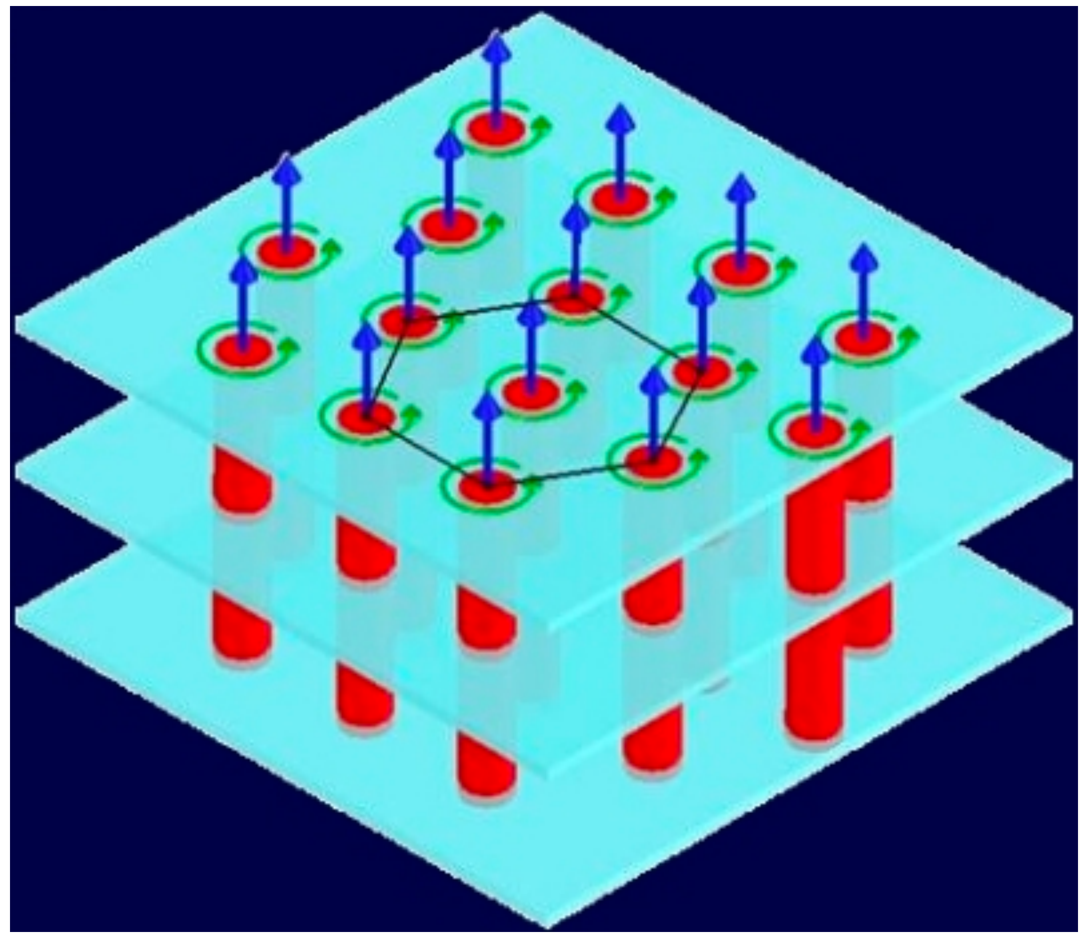
S. Oberdick et al., Sci. Reports 8, 3425 (2018)

Magnetic domain Walls



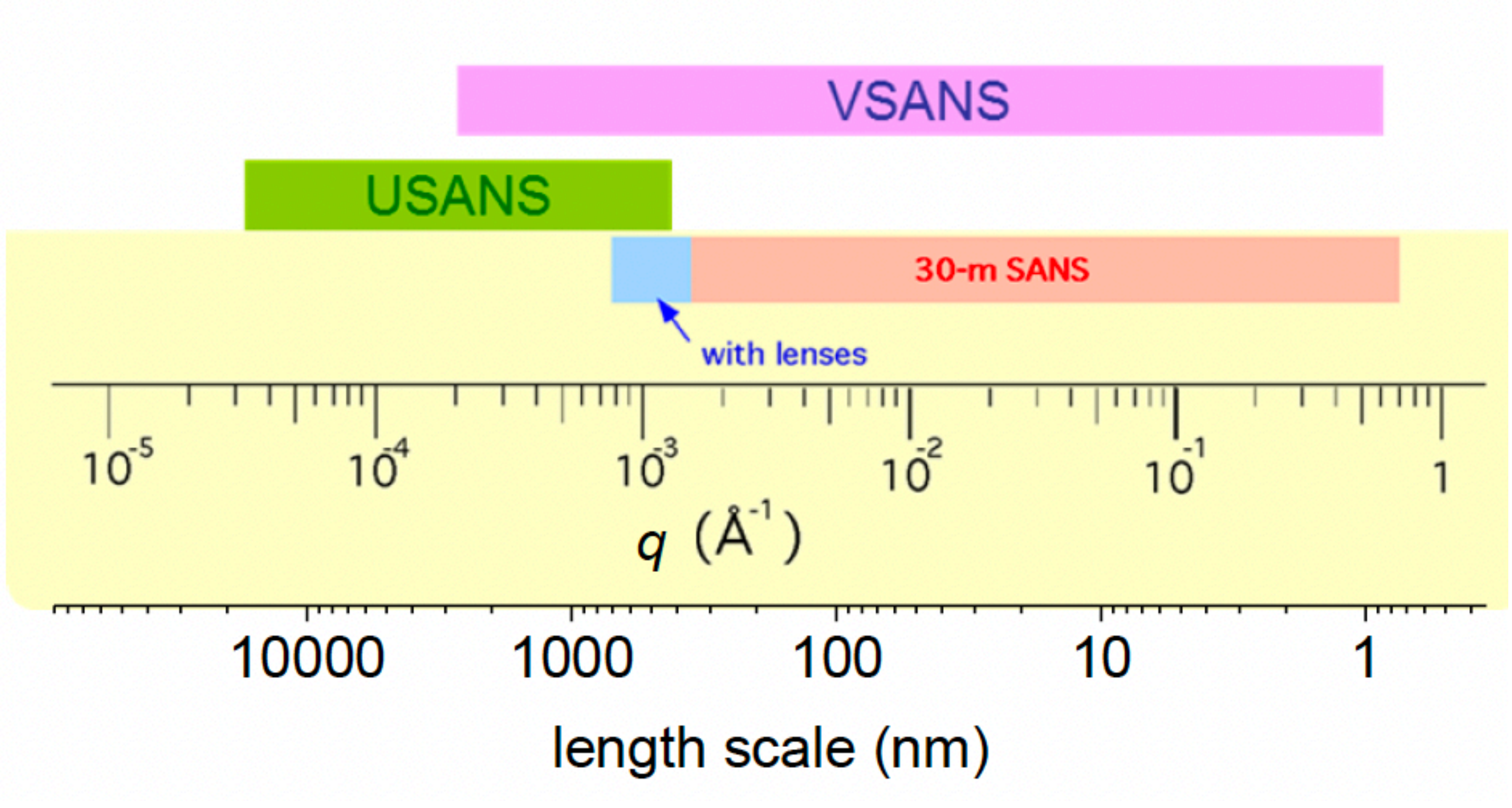
A. Scheie et al., PNAS 117 (44) 2020

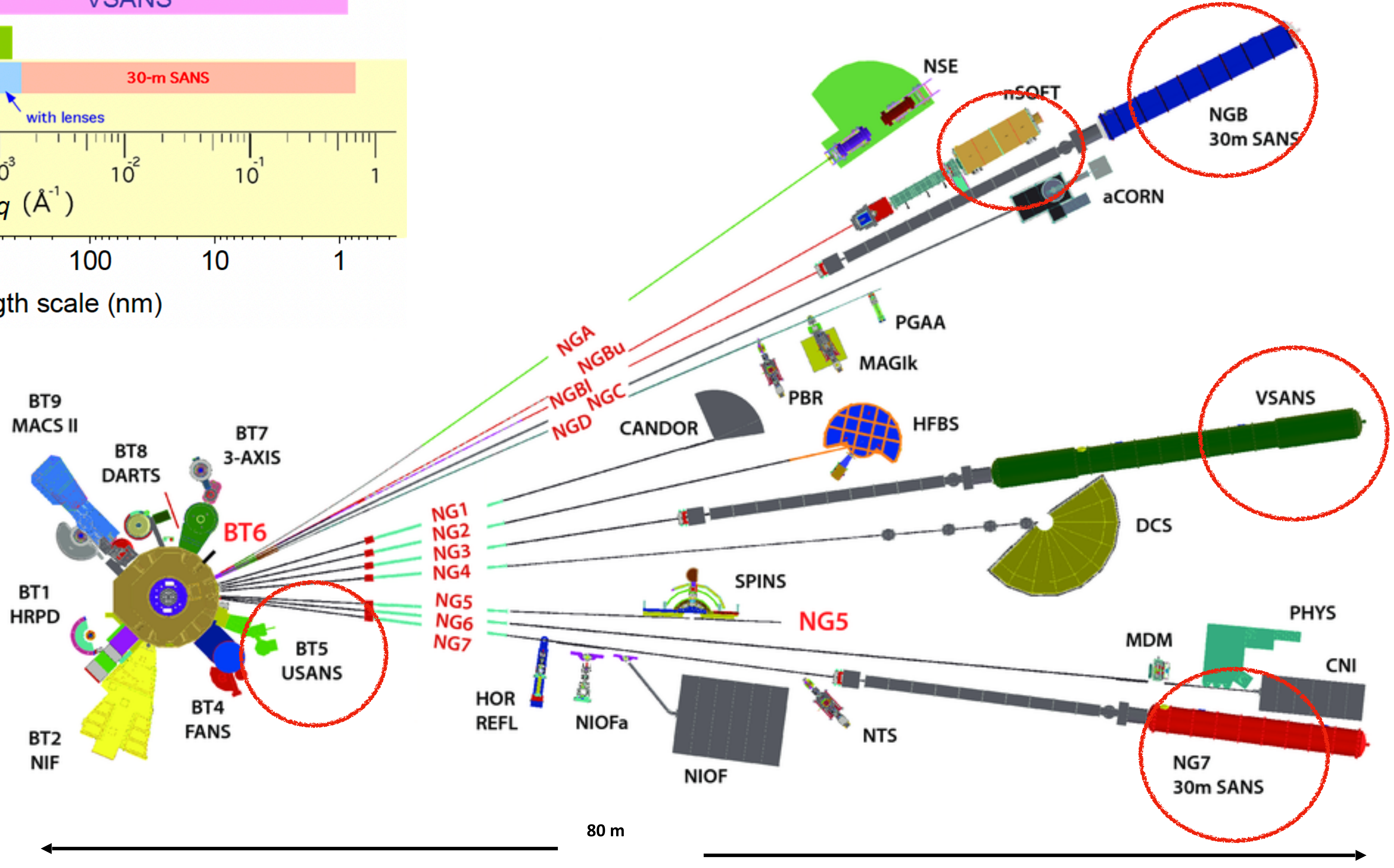
Flux lattice
In superconductors



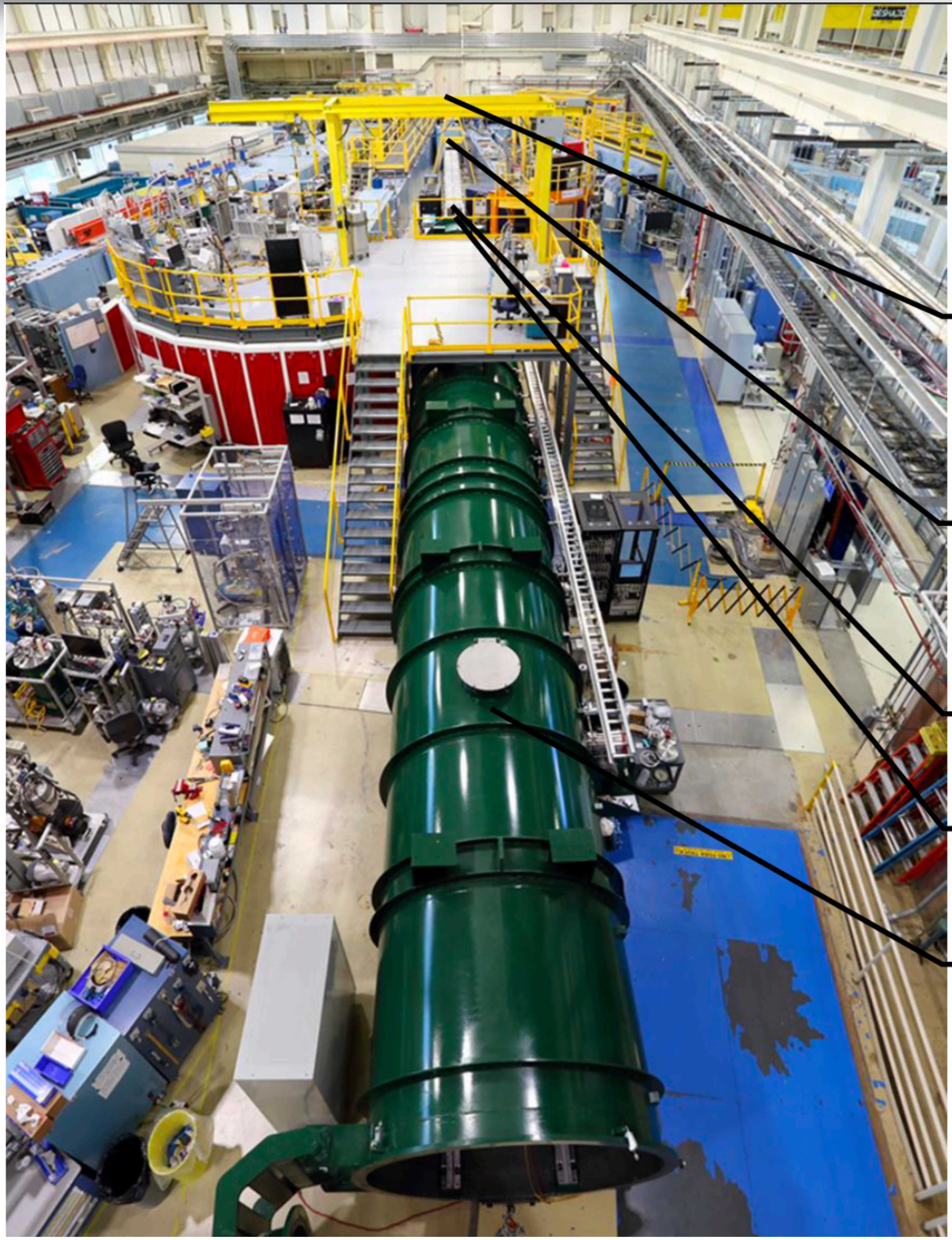
J. Hoffman STM Lab

NCNR is the host of 5 different SANS instruments





V-SANS is an extremely versatile neutron instrument



Various ways to select a specific distribution of incident neutrons wavelength

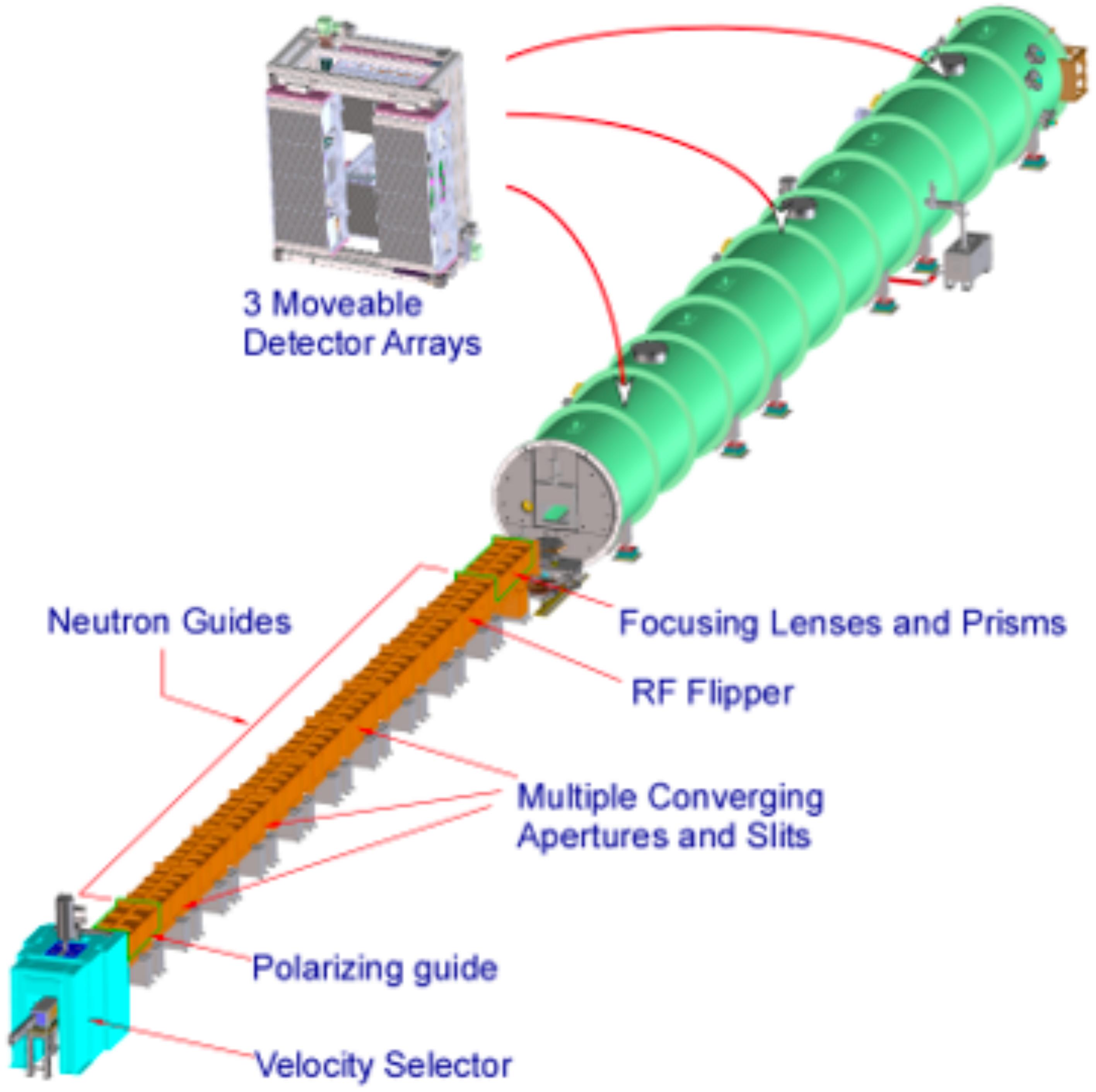
Multiple beam collimation options

Polarization capability

Large sample area

Three movable detectors

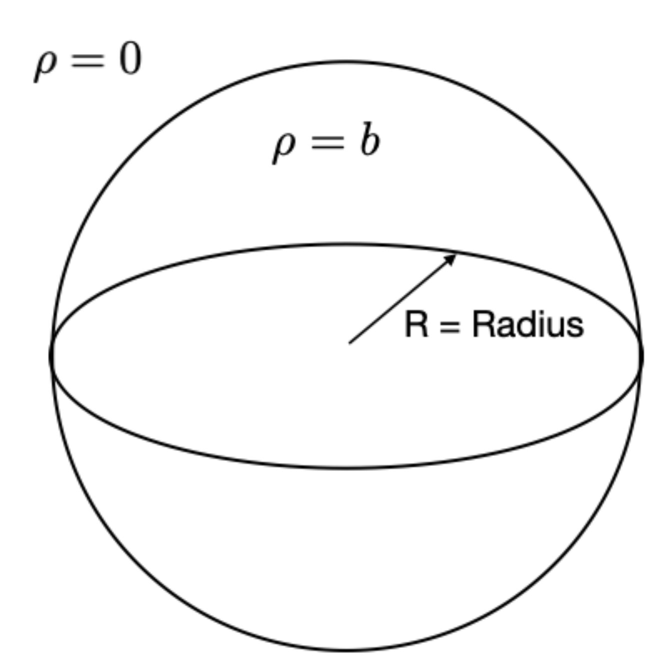
Barker J, et al. *J Appl. Cryst.* **55**(2) 271 (2022)



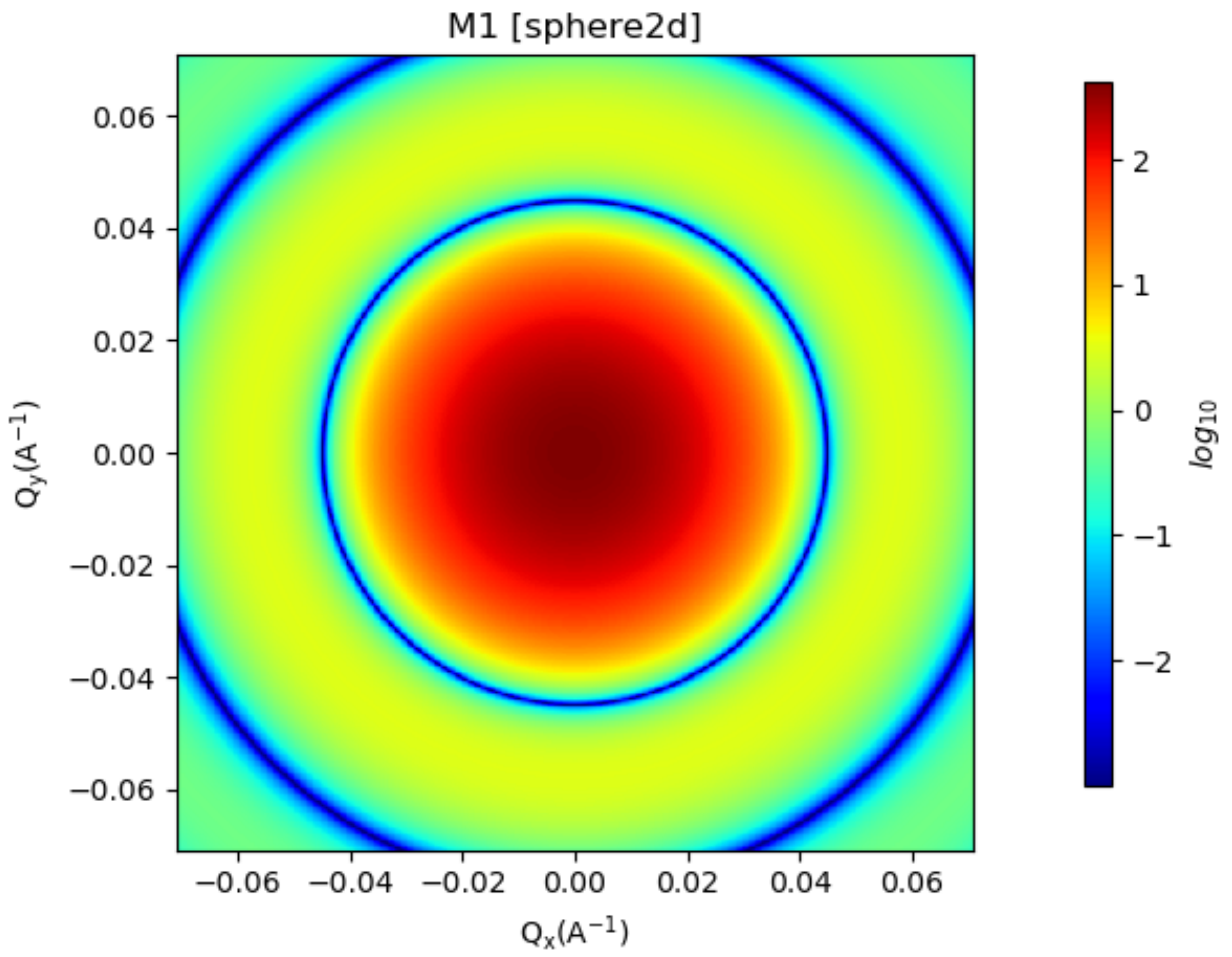
Q ~ 2e-4 to 0.7 $Å^{-1}$

D ~ 0.8 nm to 3 microns

SANS from Nuclear Scattering: Scattering from uncorrelated (diluted) spheres

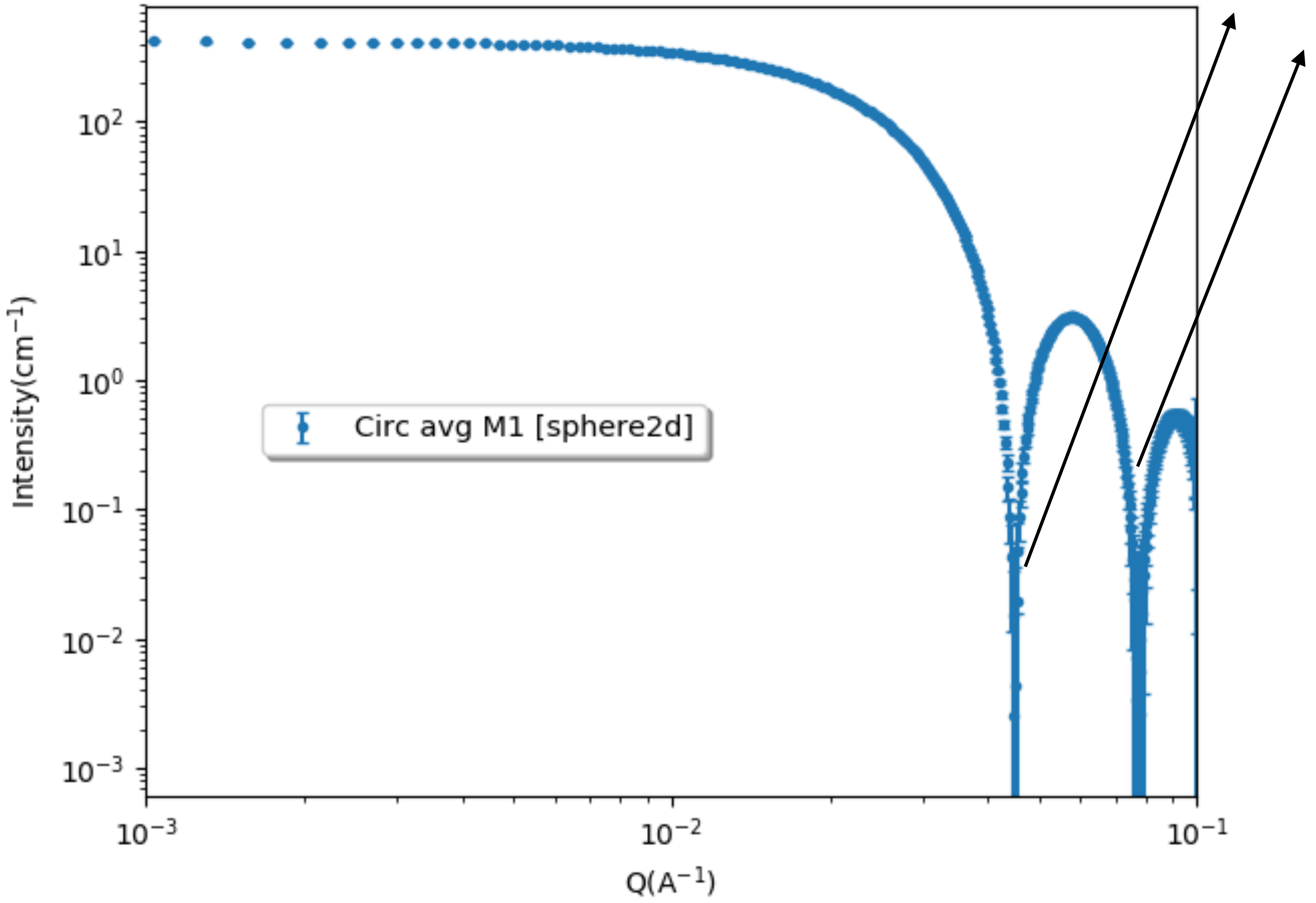


$$\frac{d\sigma}{d\Omega}(\vec{Q}) \propto |\int_V \rho(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r}\,|^2 = 9b\left(\frac{sin(QR) - QRcos(QR)}{(QR)^3}\right)^2$$

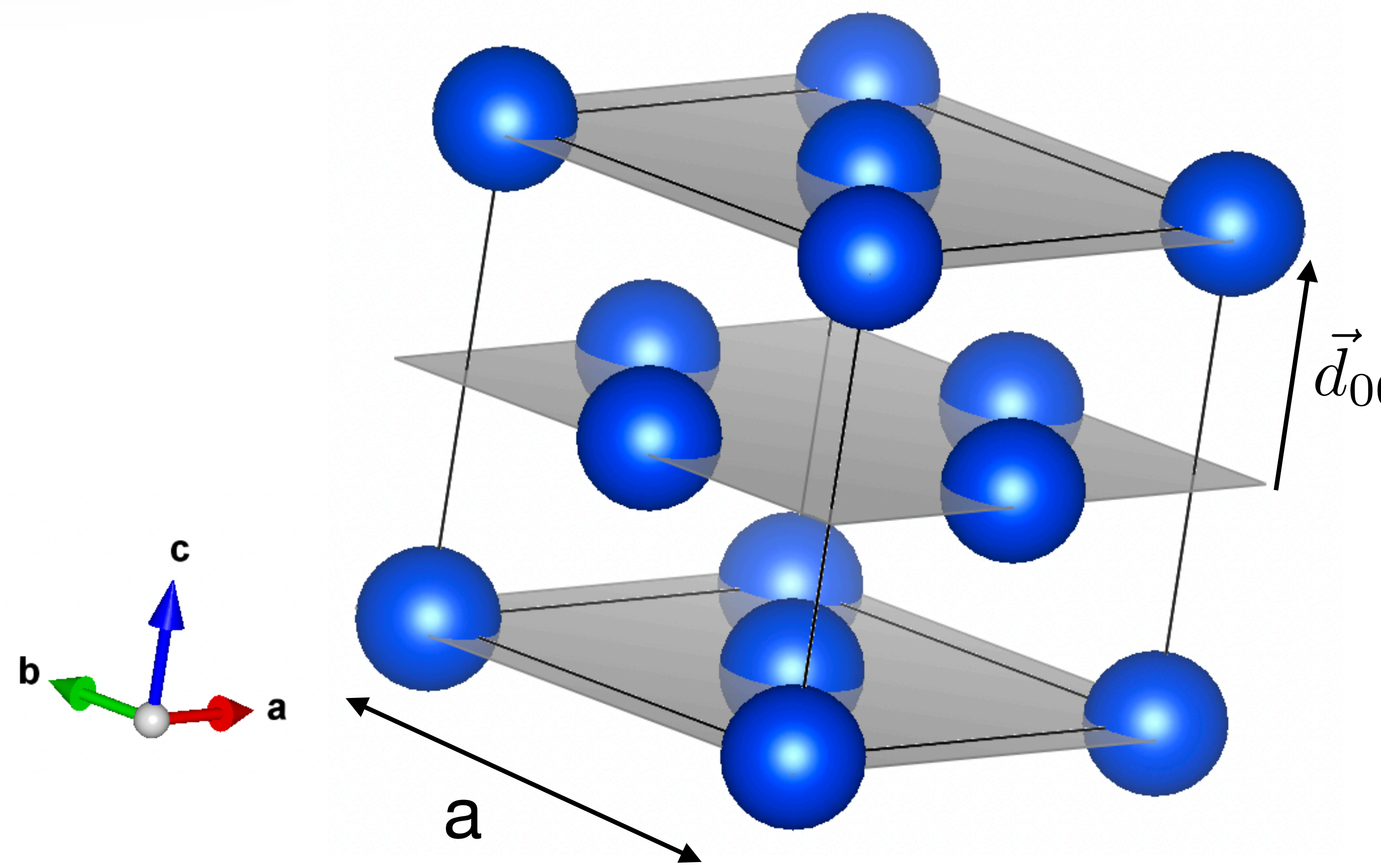


Zeros of the function are located at:

$$QR \sim \pi(n + 1/2)$$



SANS from Nuclear Scattering:
Scattering from a face-centered cubic (fcc) crystal lattice



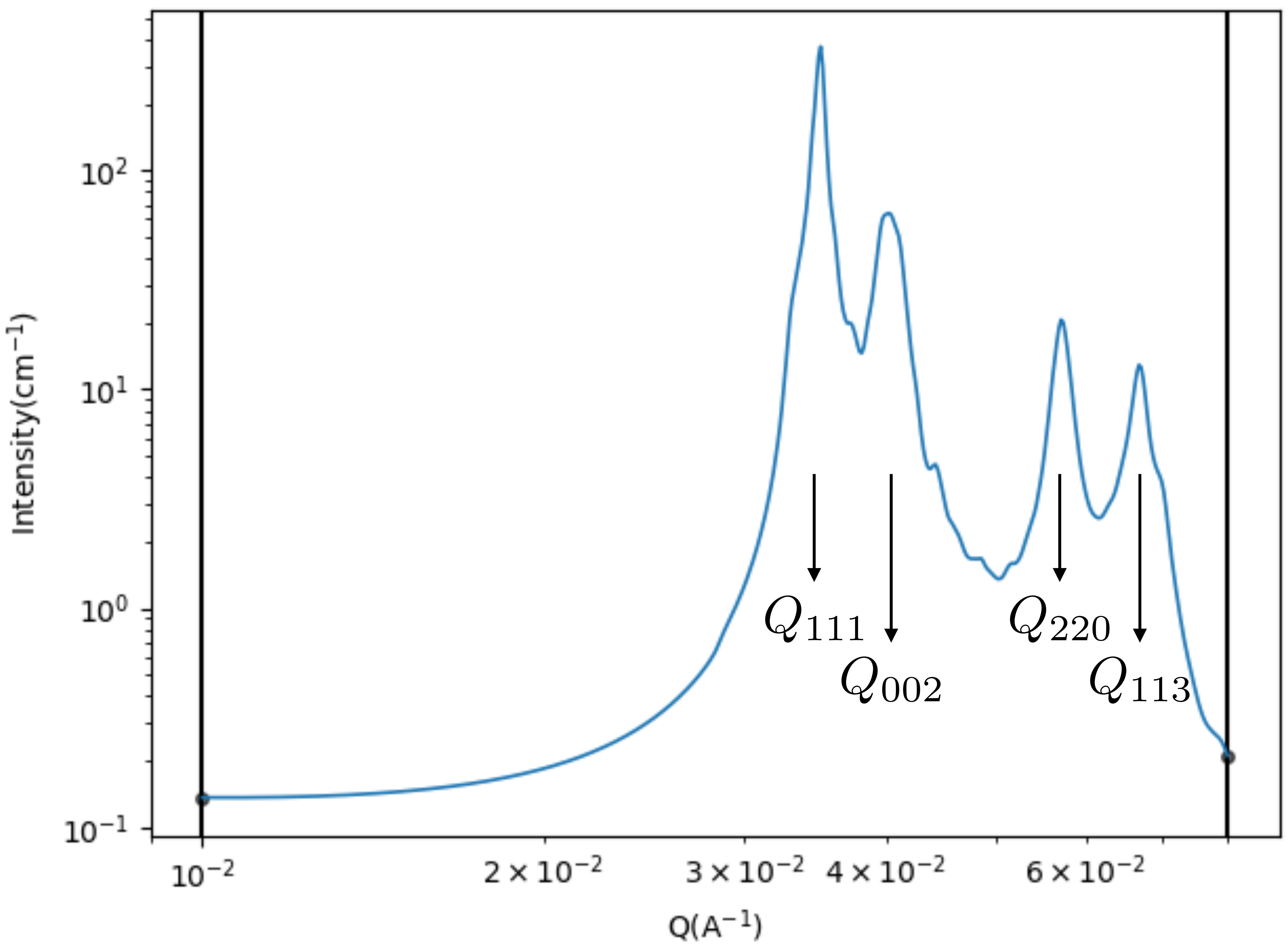
$$\vec{d}_{002} = \frac{2\pi}{\vec{Q}_{002}}$$

$$\frac{d\sigma}{d\Omega}(\vec{Q}) \propto \left| \int_V \rho(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r} \right|^2$$

Produce scattering peaks (Bragg reflections) indexed by

↓

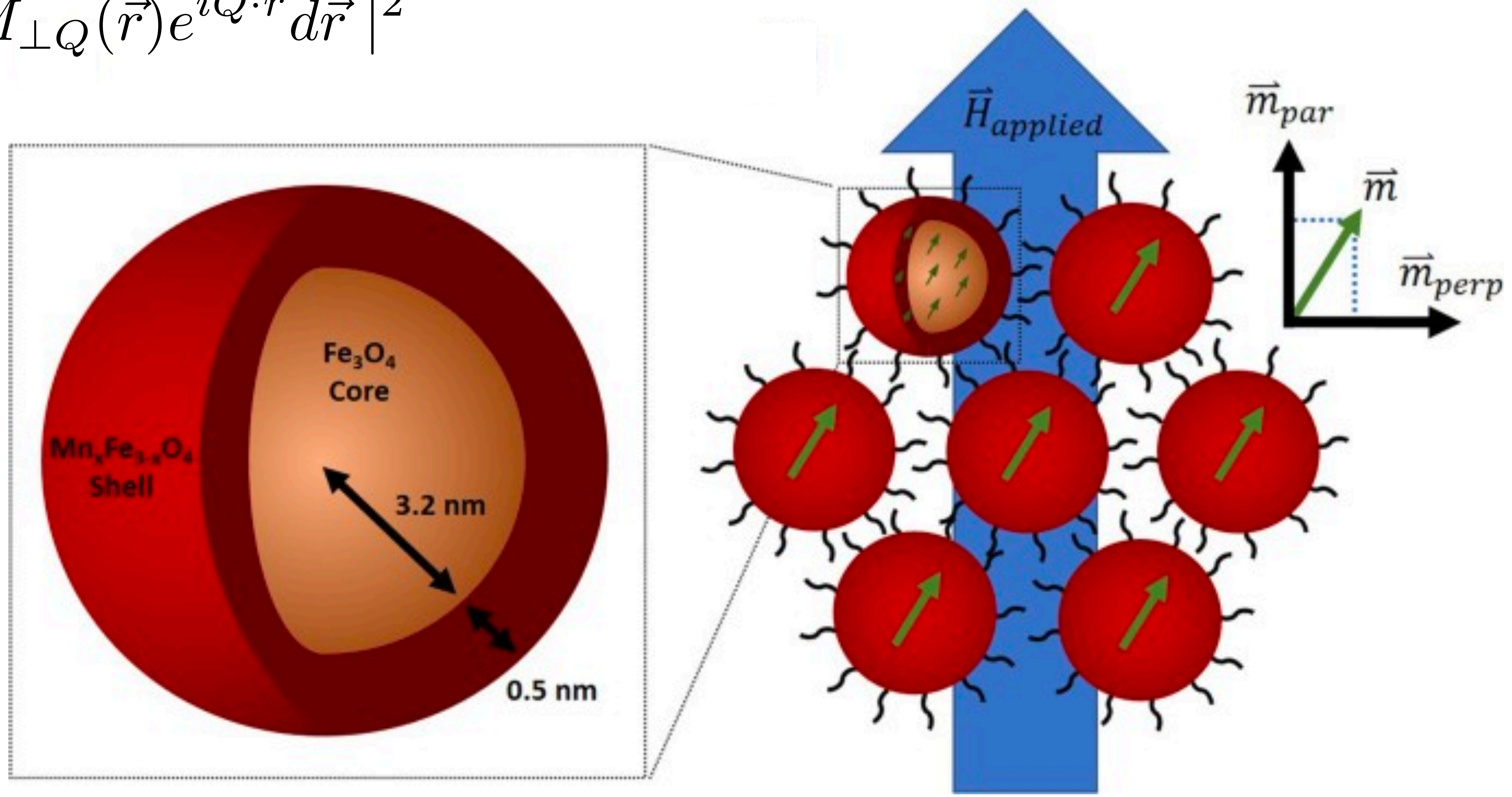
$$|Q_{Bragg}| = \frac{2\pi}{a}\sqrt{H^2 + K^2 + L^2}$$



For the fcc lattice, the peaks have finite intensity if the integers H,K, and L are all odd or all even.

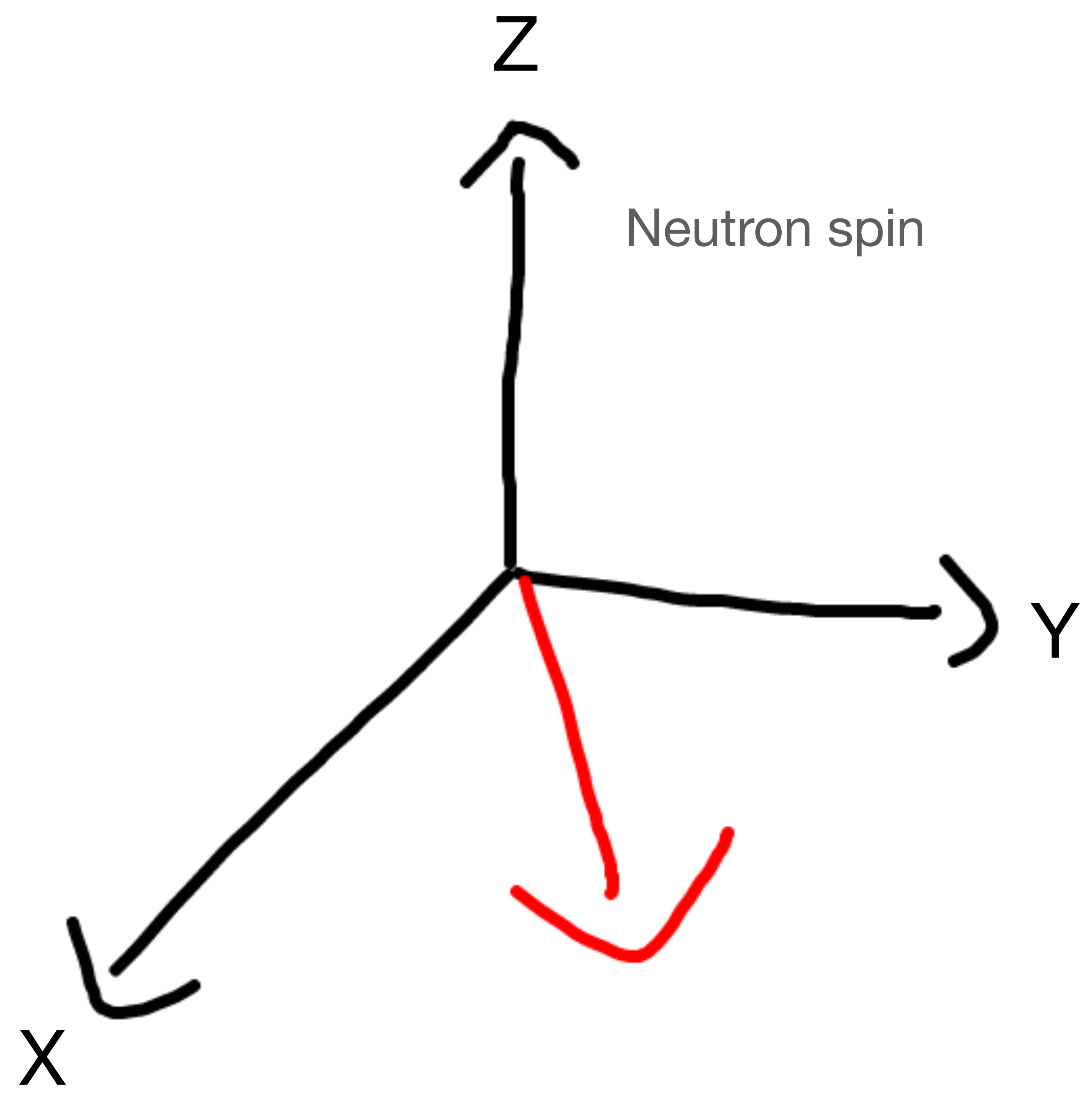
SANS from Magnetic Scattering

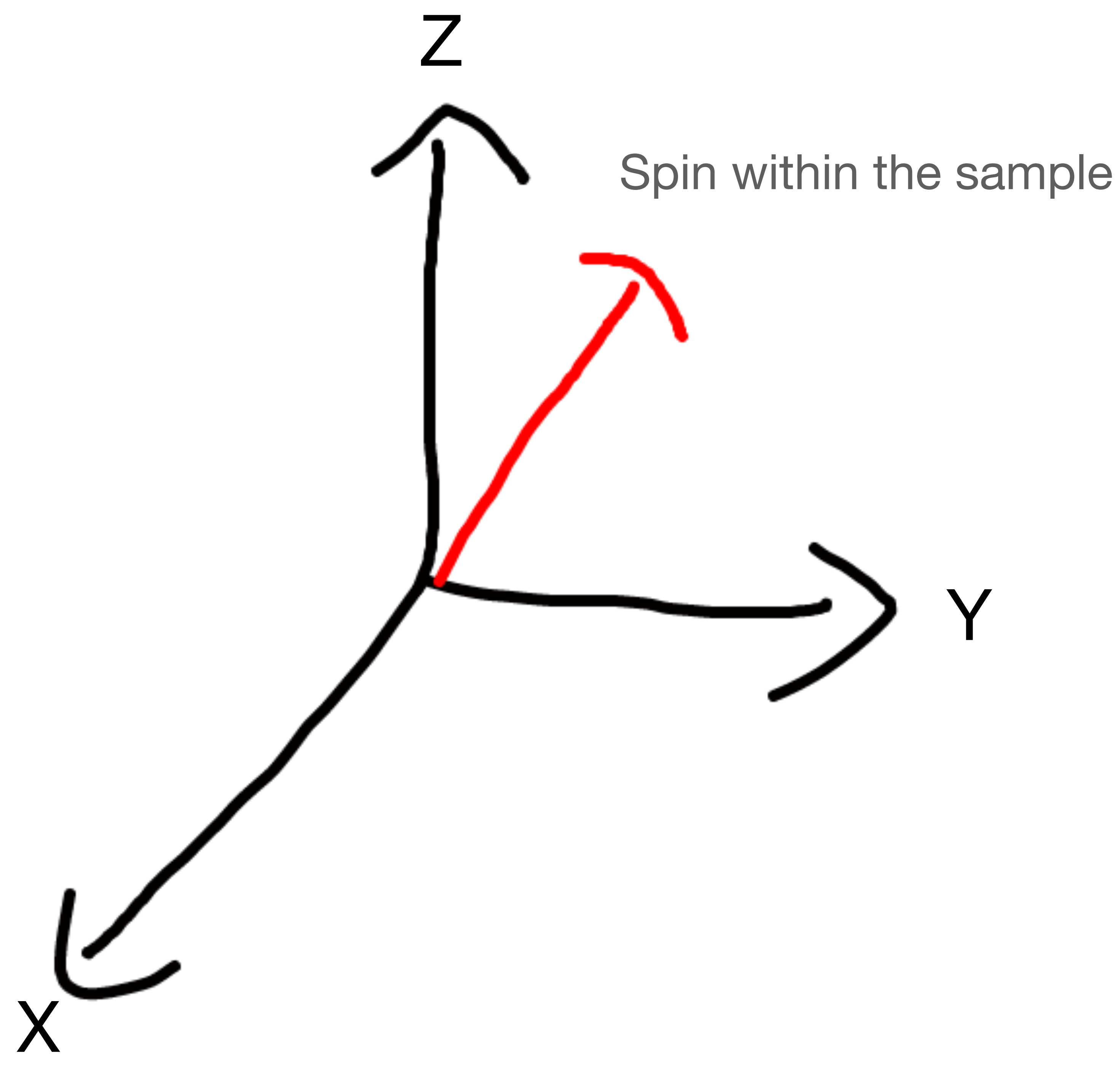
$$\frac{d\sigma}{d\Omega}(\vec{Q}) \propto |\int_V M_{\perp Q}(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r}\,|^2$$

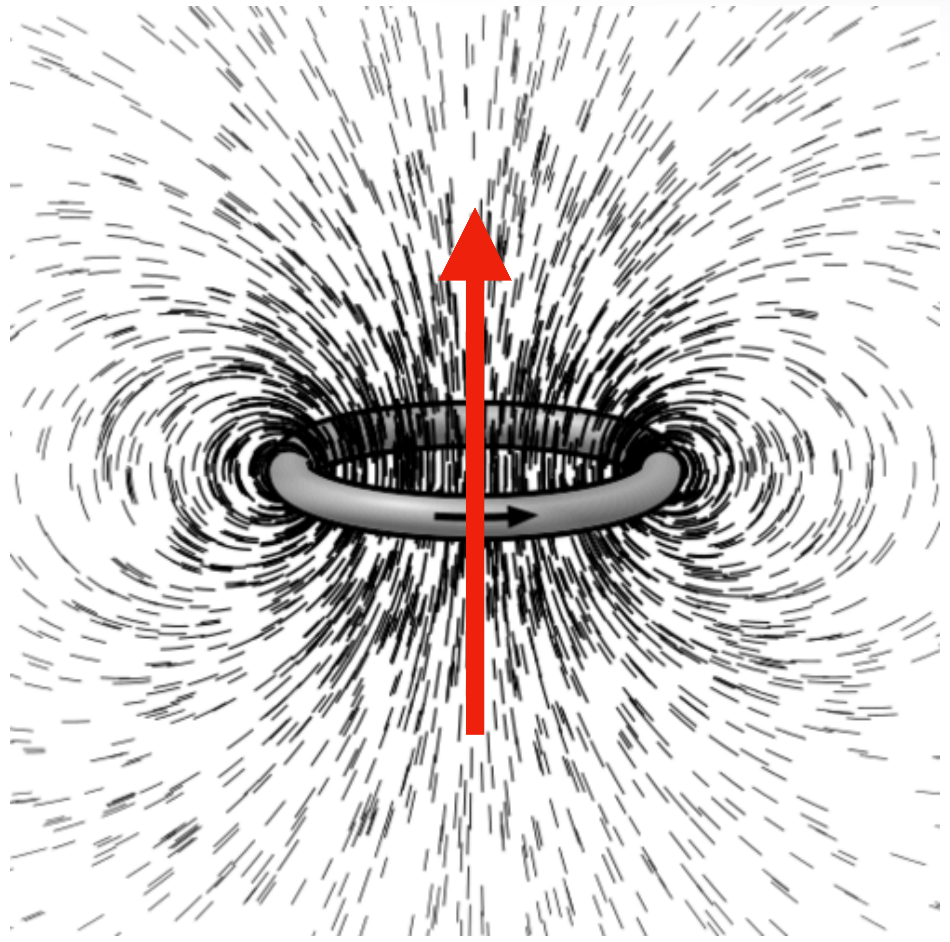


S. Oberdick et al., Sci. Reports 8, 3425 (2018)

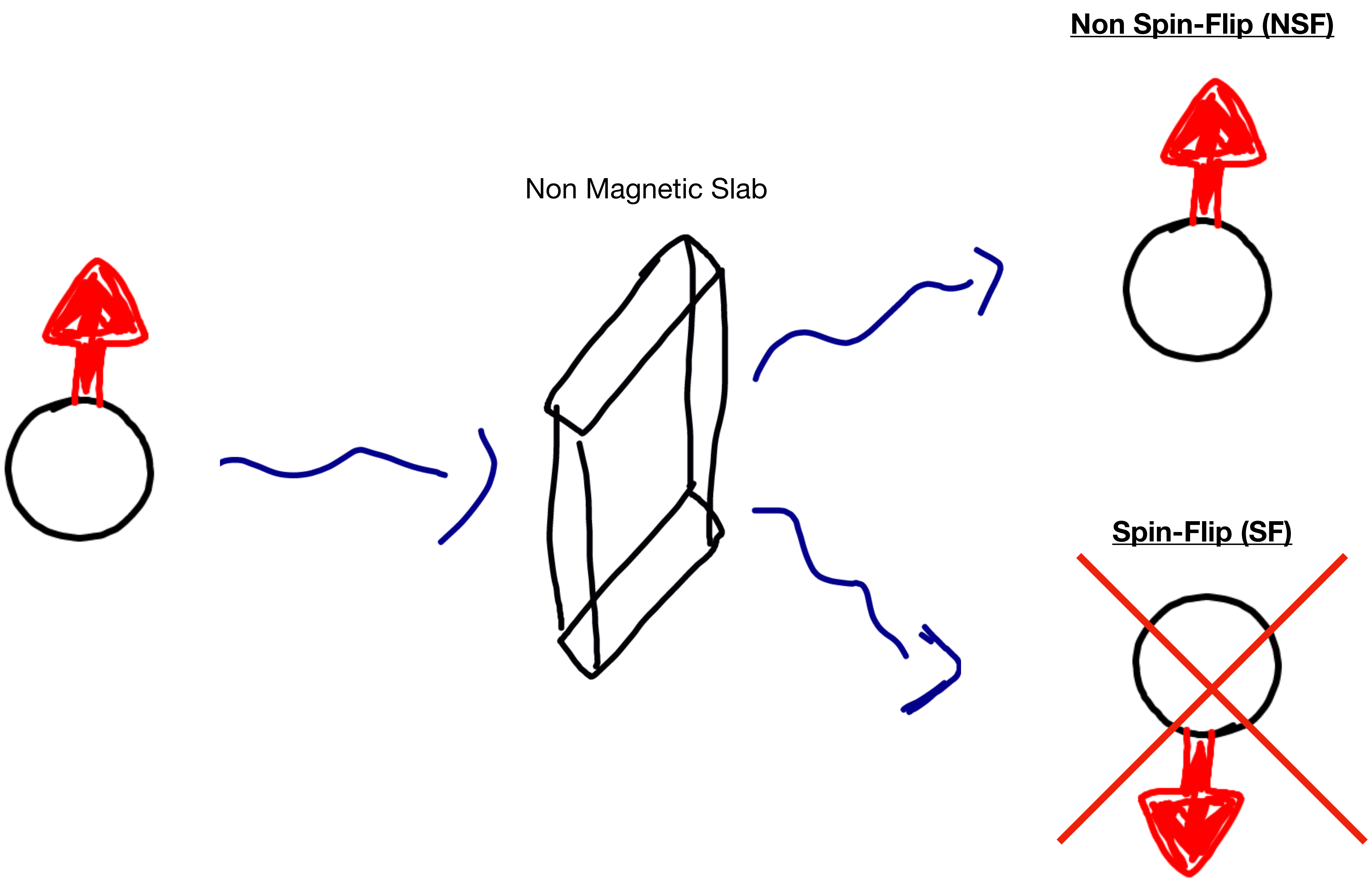
The magnetic interaction depends on the relative orientation of the spins within the probed sample



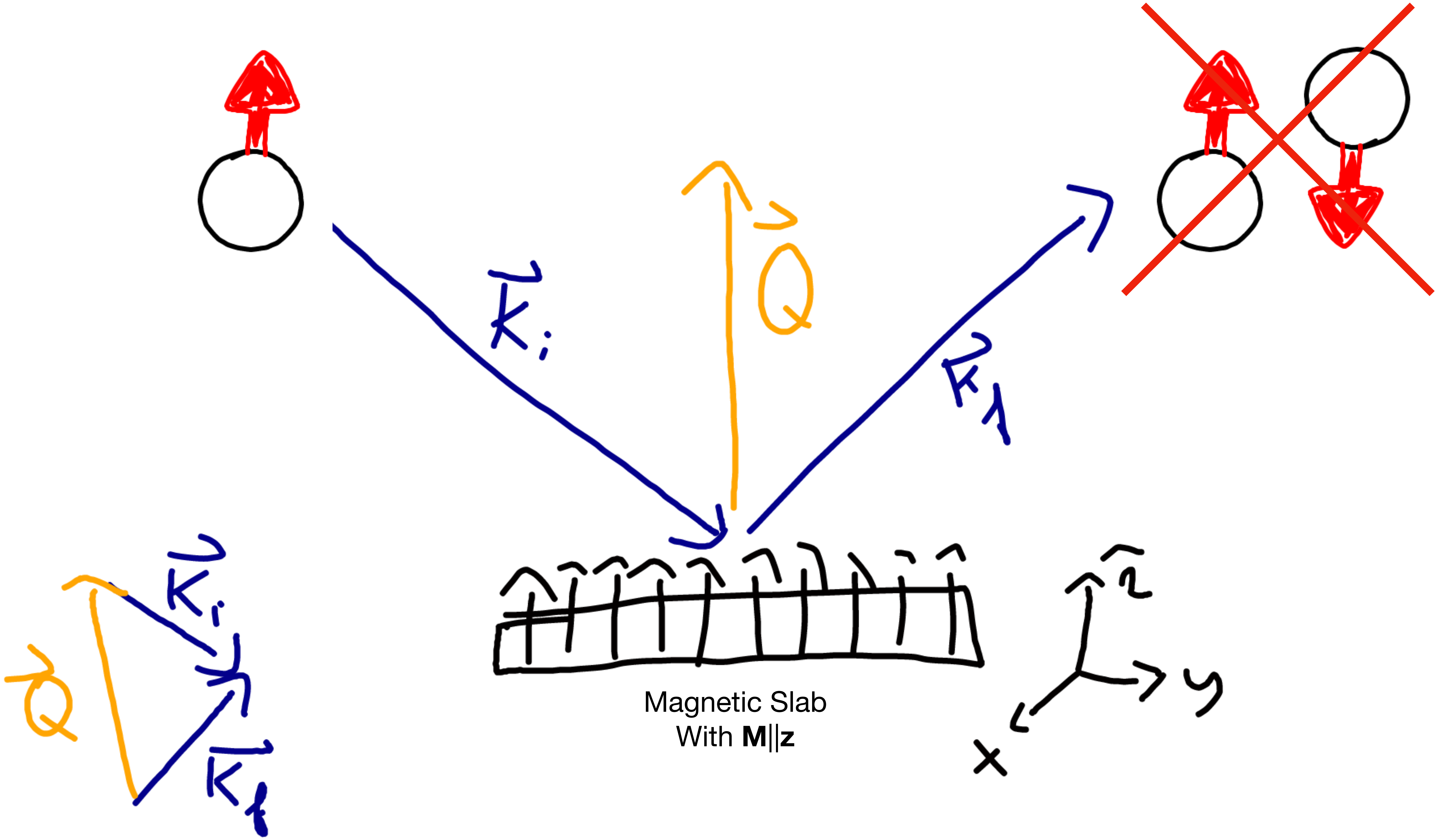




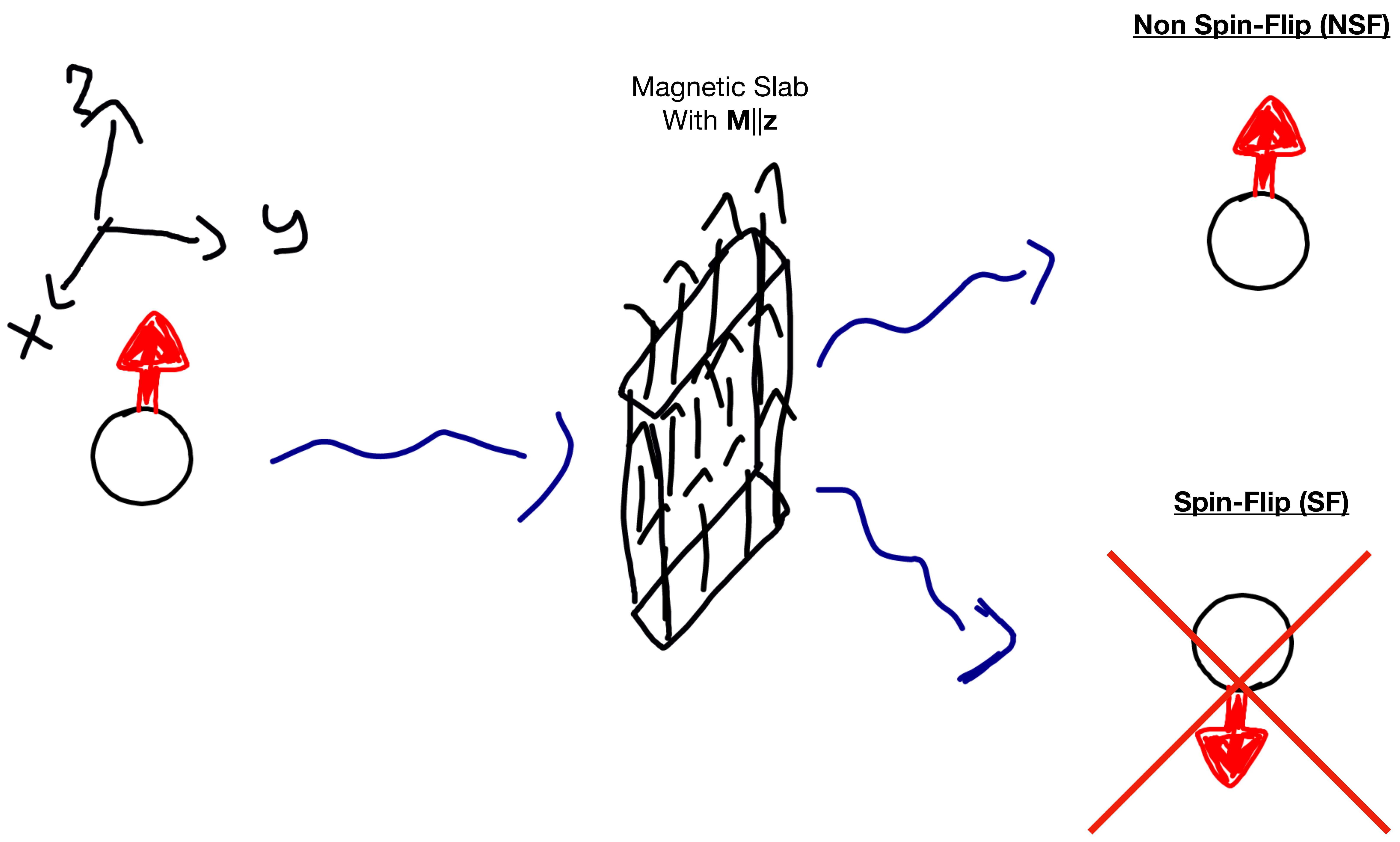
Rule 1: Nuclear scattering does not flip the neutron spin



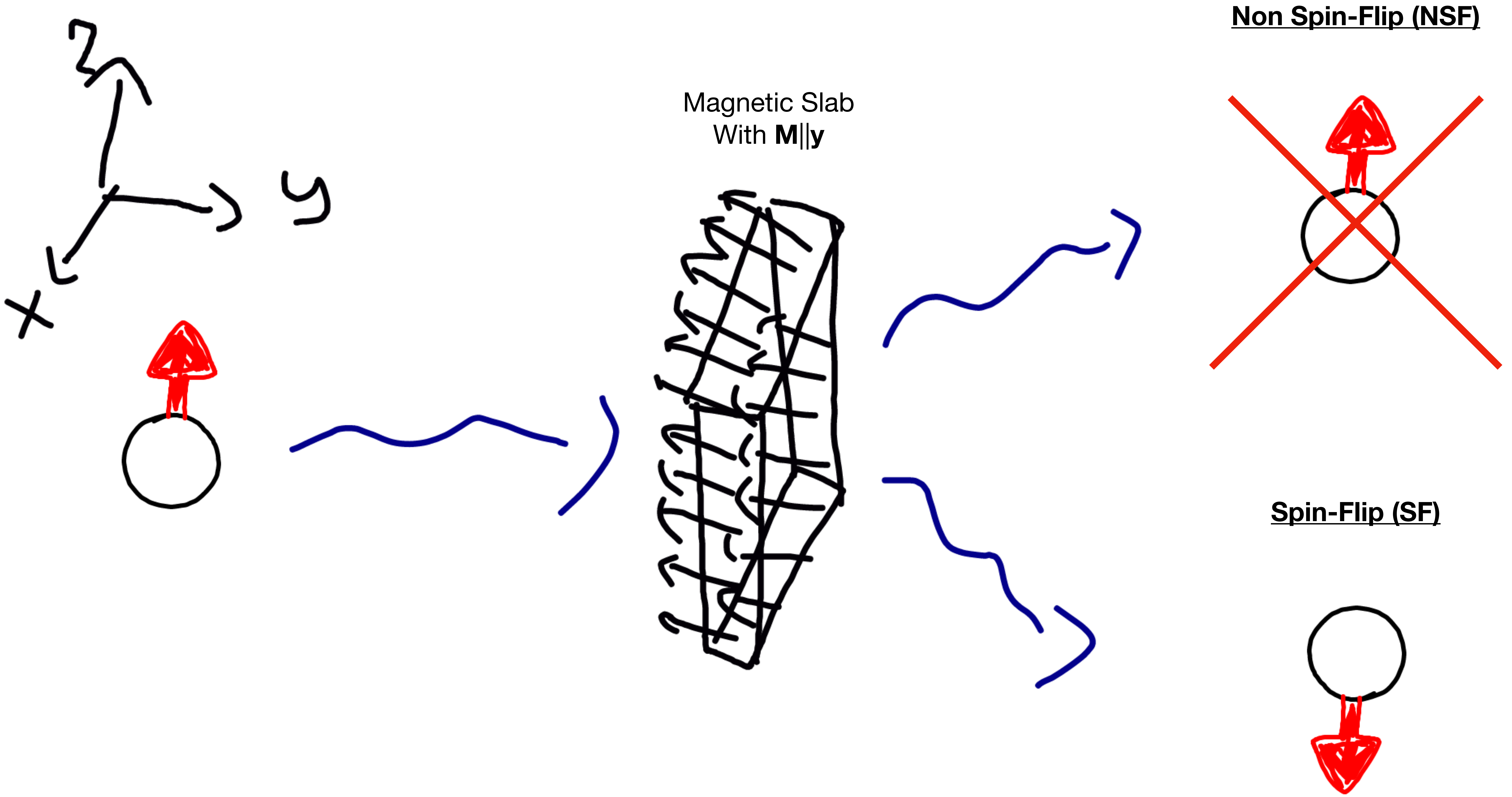
Rule 2: Magnetic scattering is only sensitive to magnetization perpendicular to the momentum transfer Q



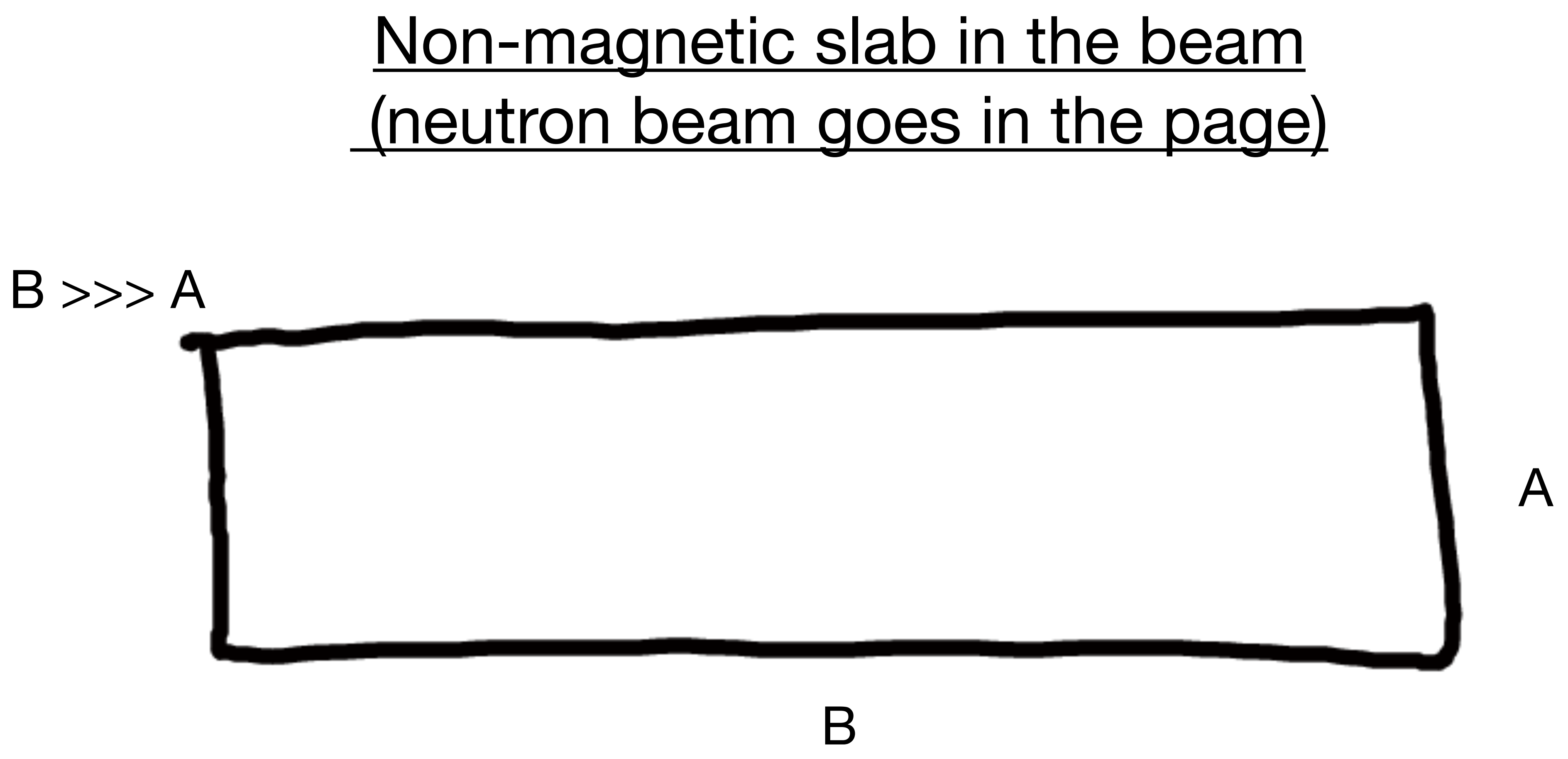
Rule 3: The non spin-flip scattering is only sensitive to magnetization parallel to the neutron spin

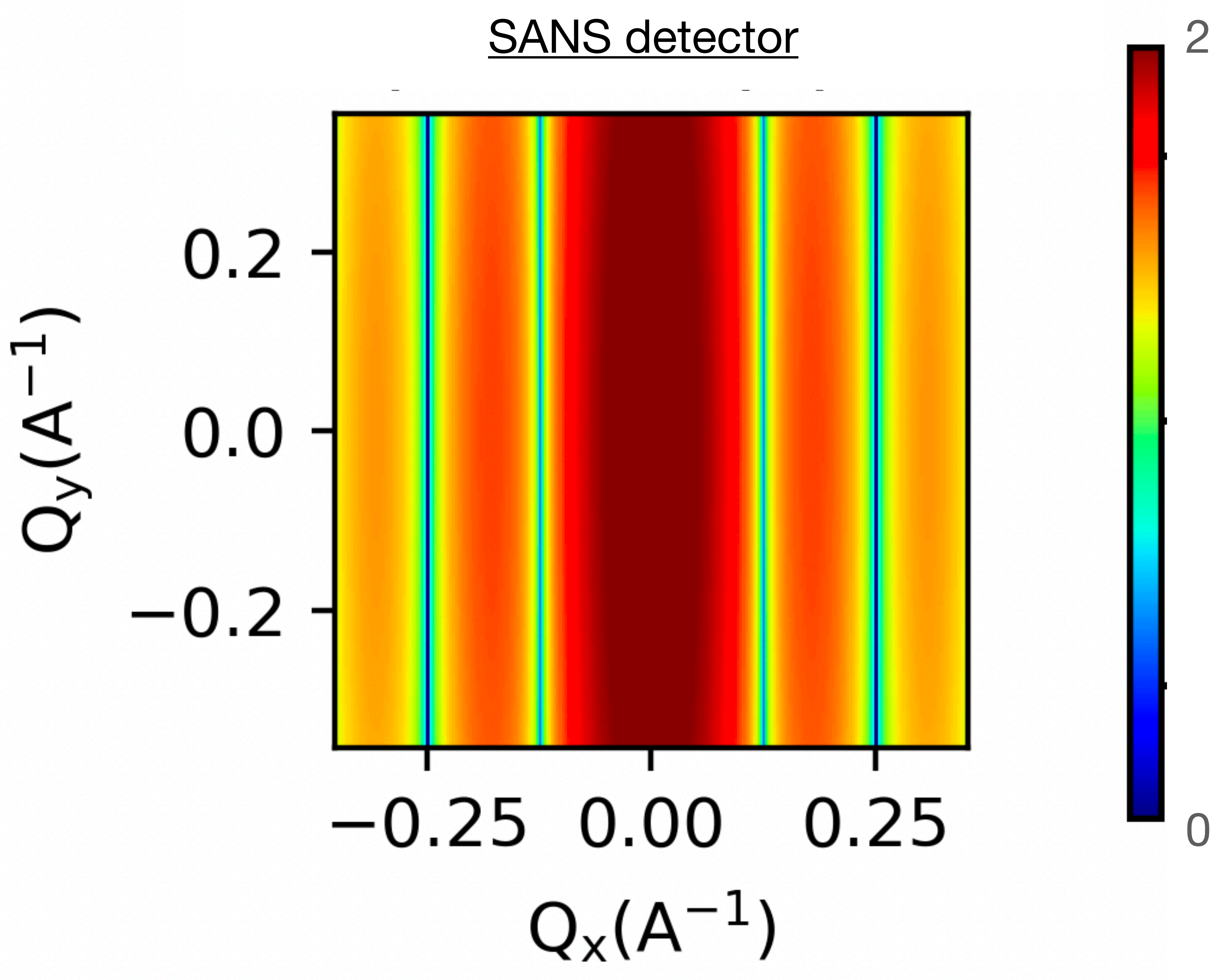


Rule 4: Magnetization perpendicular to the neutron spin only contributes to spin-flip scattering



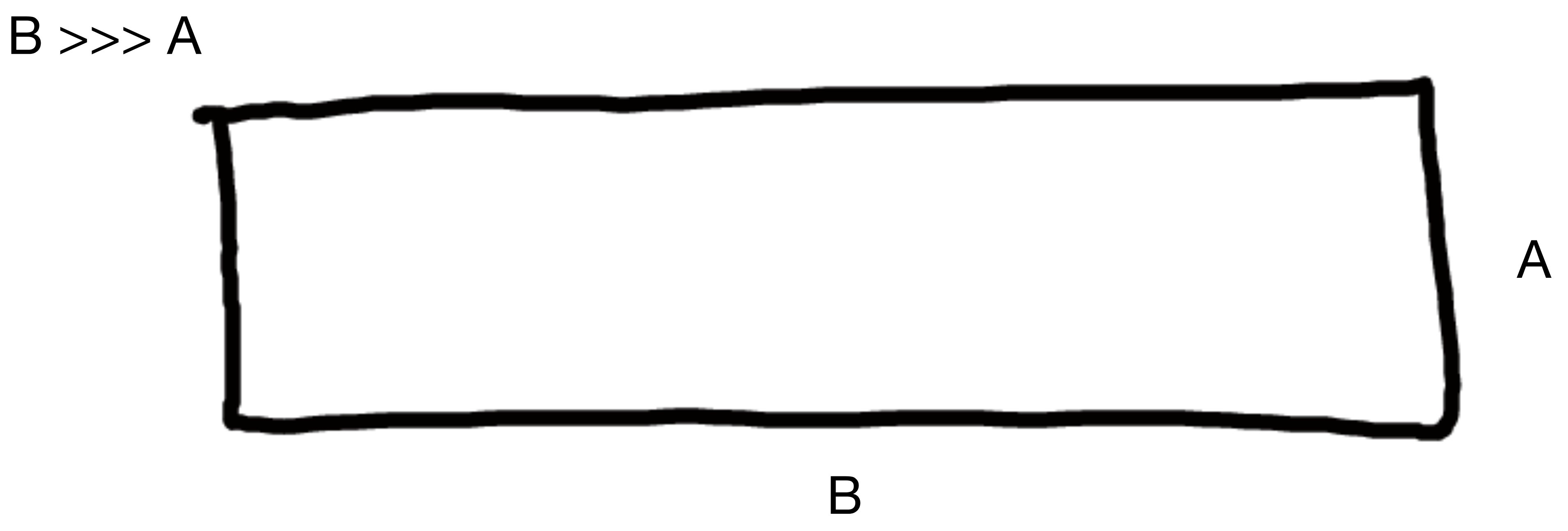
Example: Unpolarized SANS of a non-magnetic slab



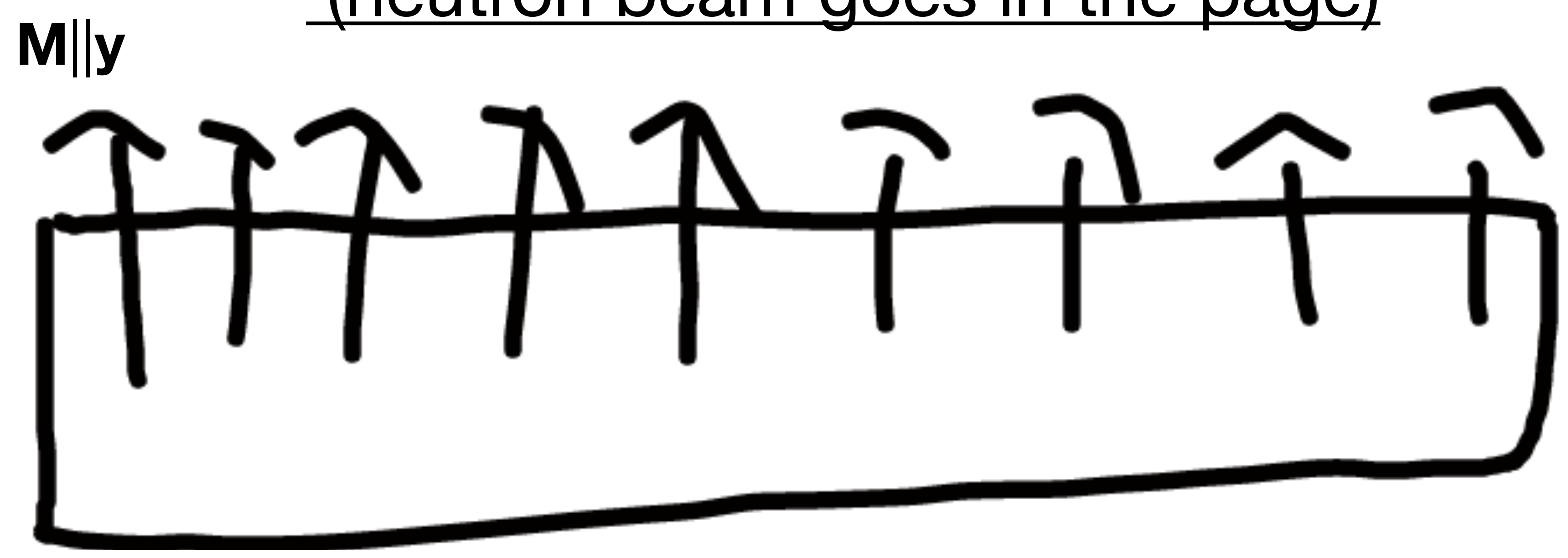


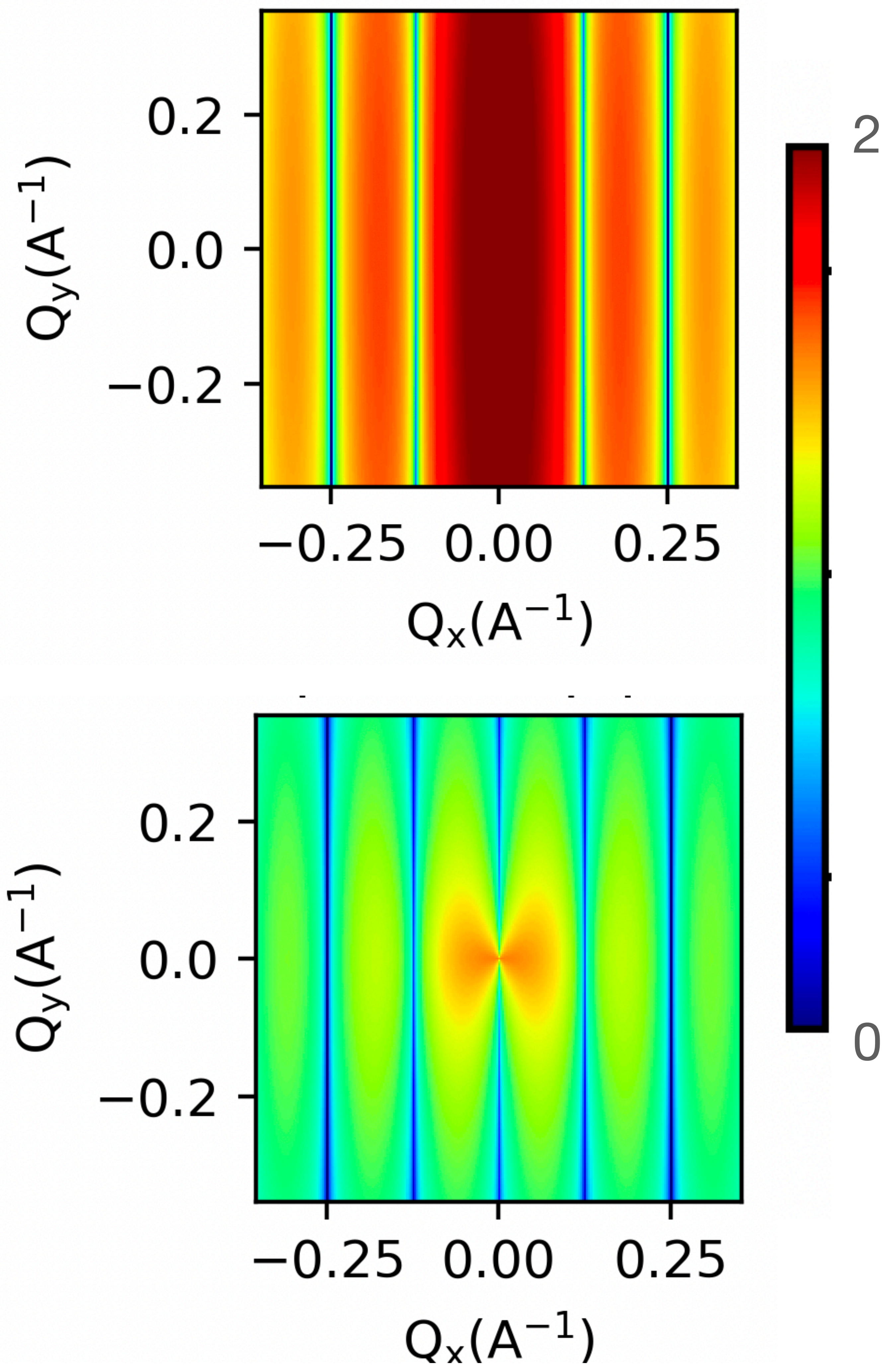
Example:Unpolarized SANS of a magnetic slab

Non-magnetic slab in the beam
(neutron beam goes in the page)



Magnetic slab in the beam
(neutron beam goes in the page)





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Non-magnetic slab in the beam
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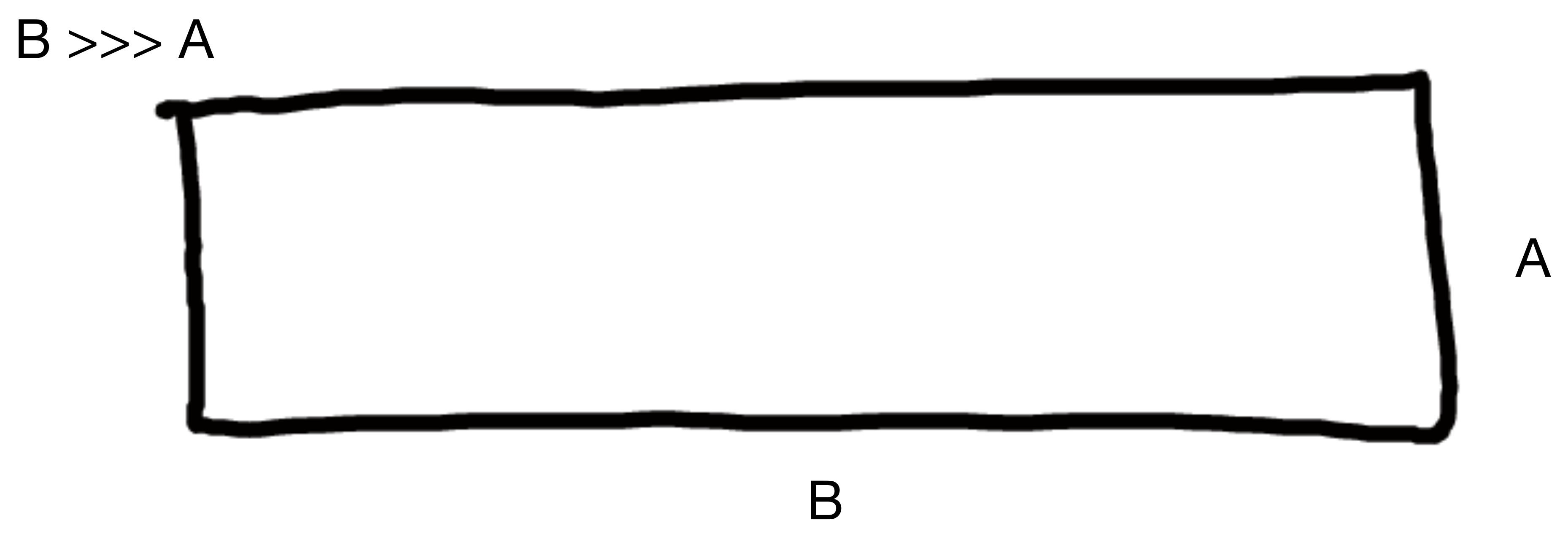
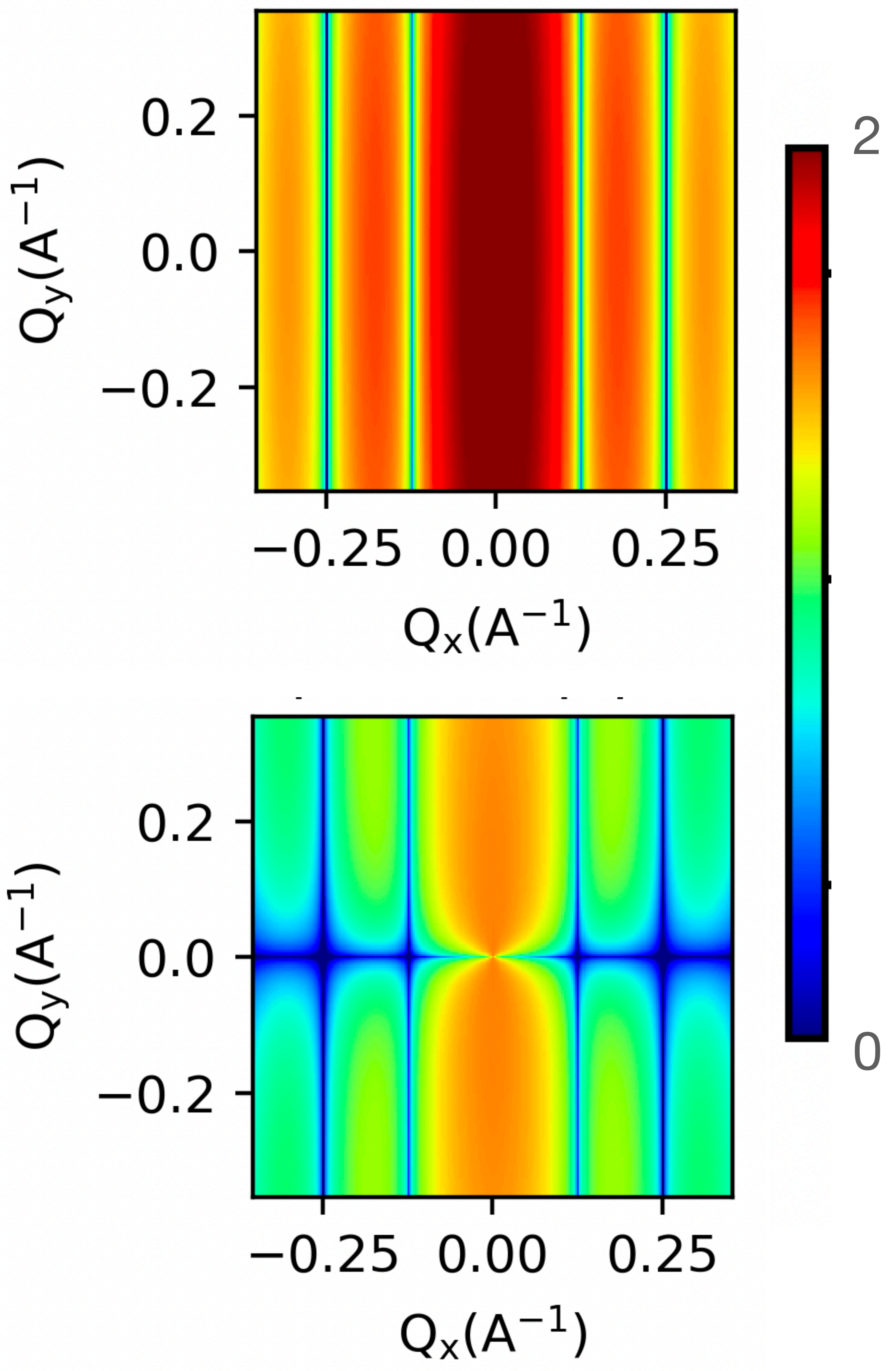
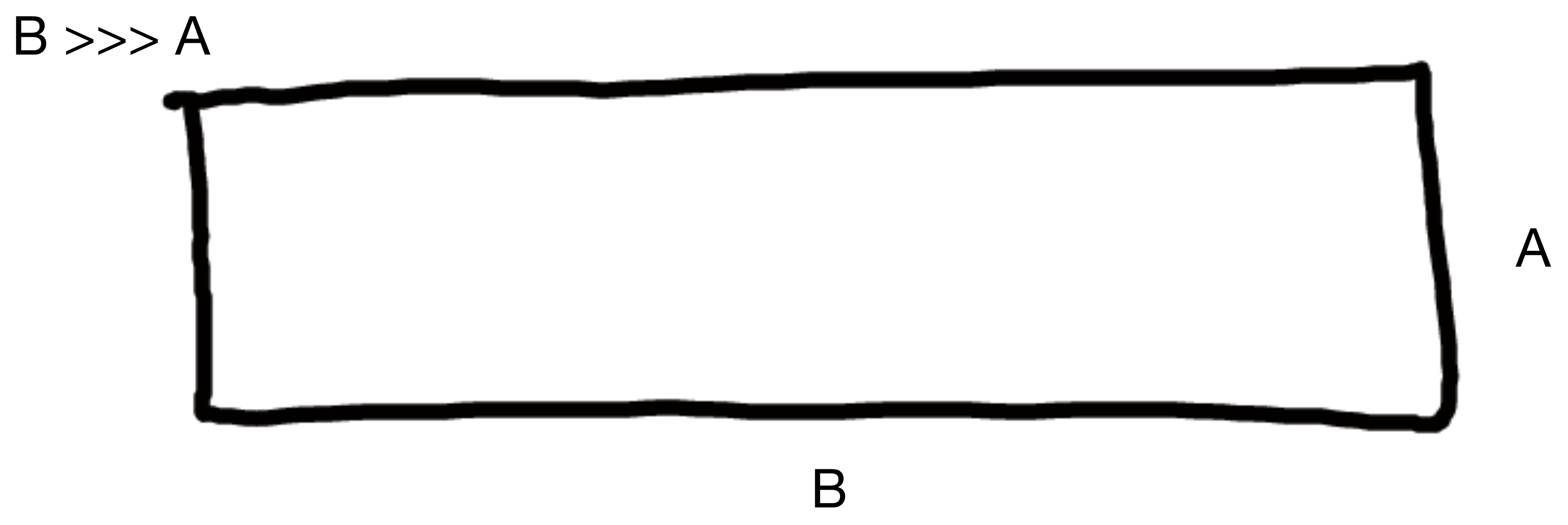


Magnetic slab in the beam
(neutron beam goes in the page)

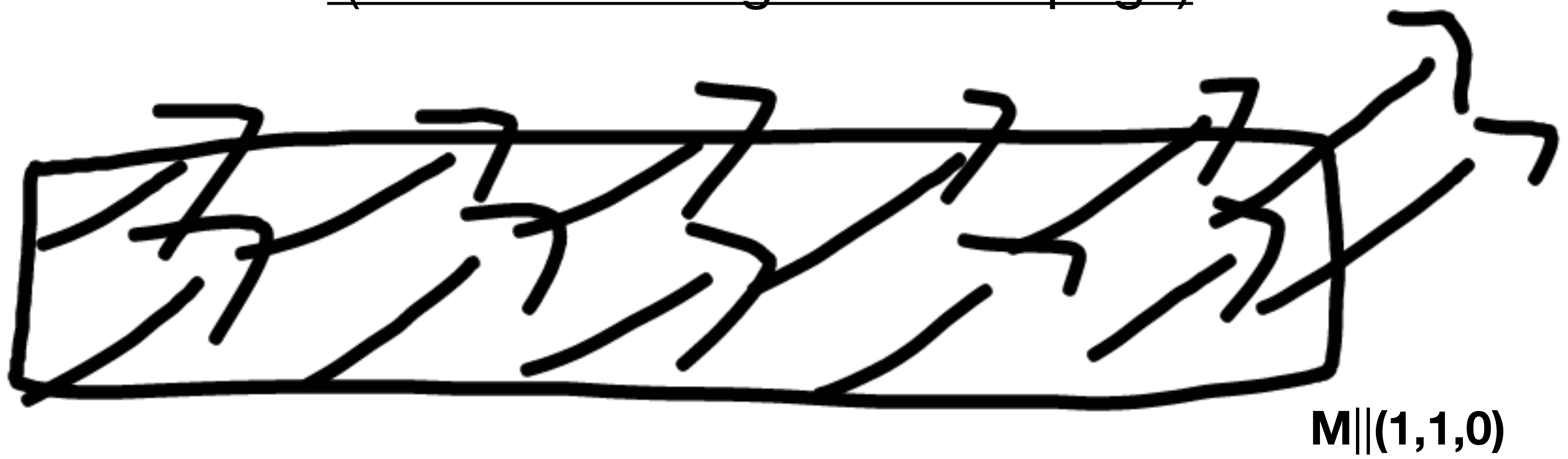


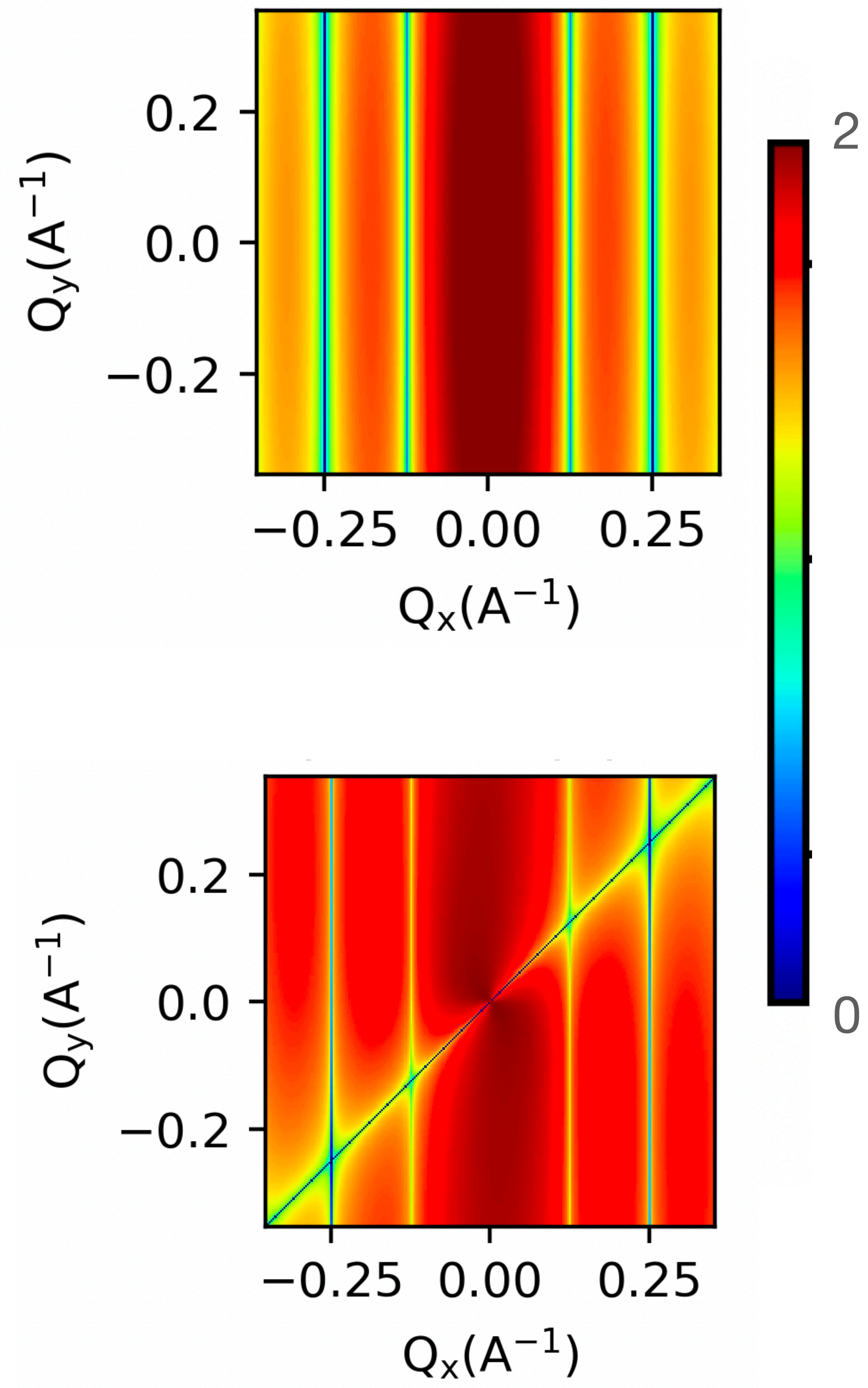
Example:Unpolarized SANS of a magnetic slab

Non-magnetic slab in the beam
(neutron beam goes in the page)

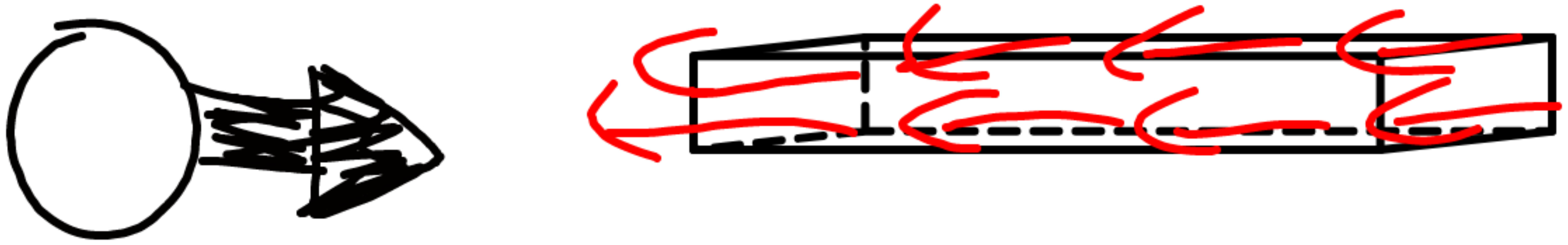


Magnetic slab in the beam
(neutron beam goes in the page)

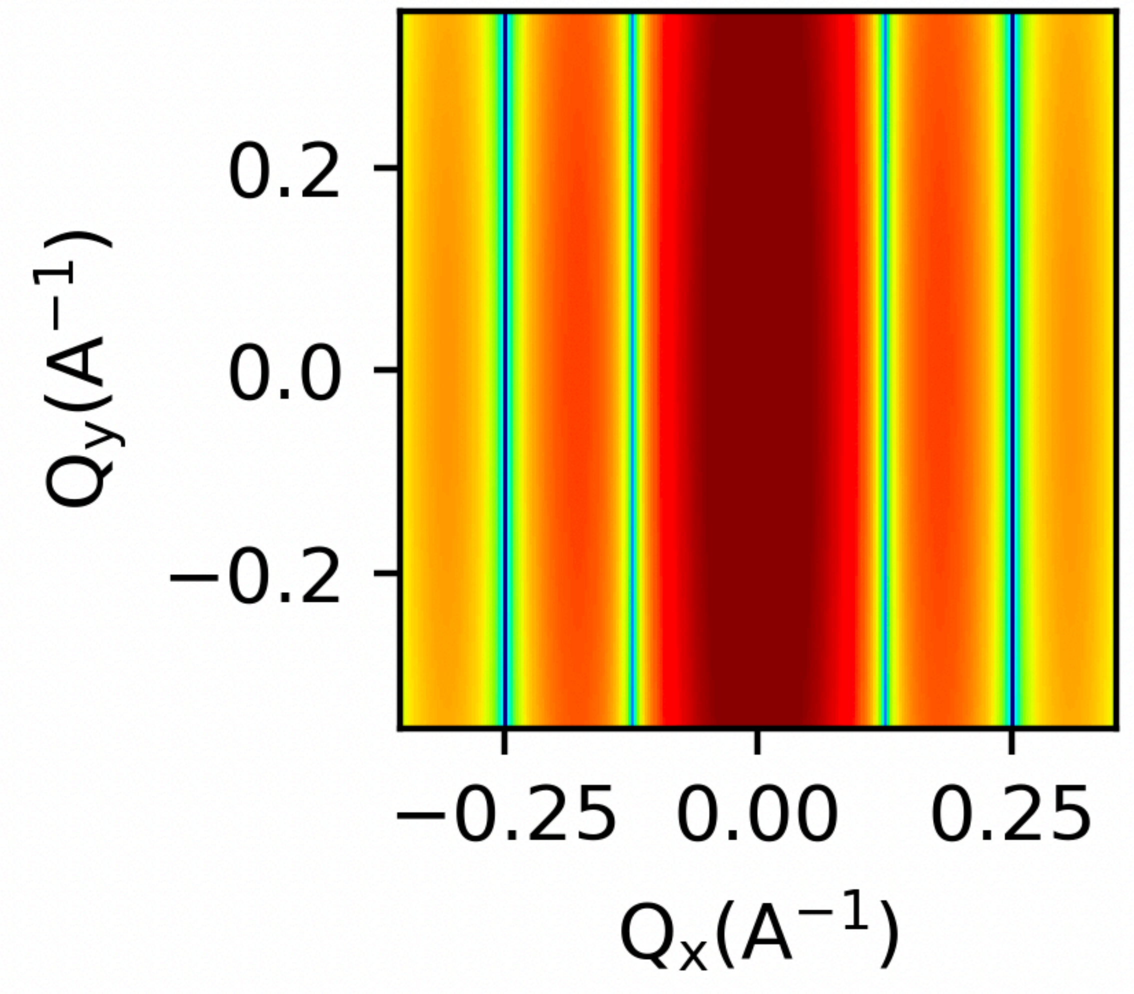




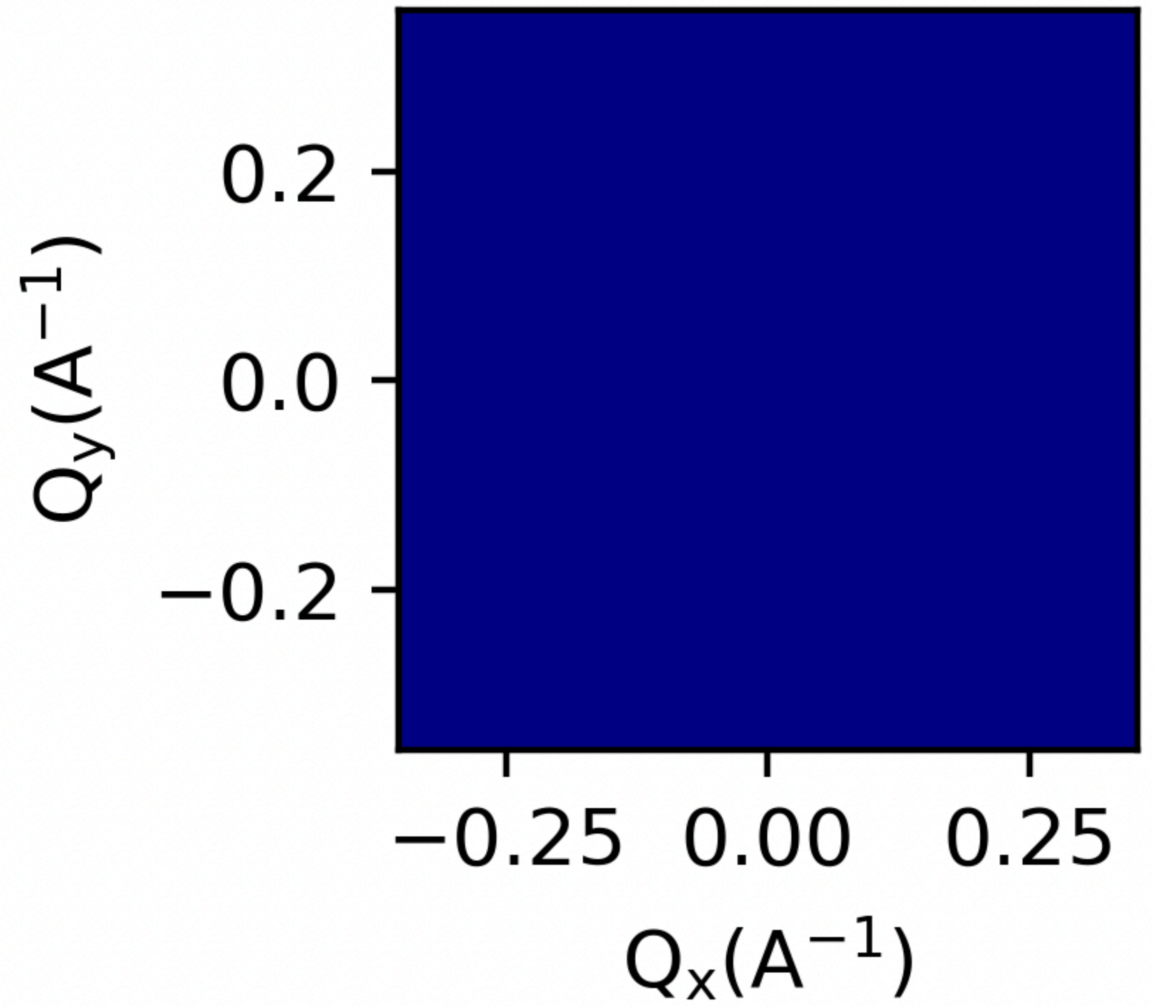
Example:Unpolarized SANS of a magnetic slab



Non Spin-Flip (NSF)



Spin-Flip (SF)



Uniaxial Polarization Analysis : General Rules

1) Nuclear scattering is always non-spin-flip (NSF)

2) The magnetization parallel to the scattering momentum vector **Q** cannot be observed.

3) and 4) Magnetic scattering is both spin-flip (SF) and NSF. The NSF is given by the magnetization *parallel* to the neutron spin, while the SF is given by the magnetization *perpendicular* to the neutron spin.

Nuclear Scattering

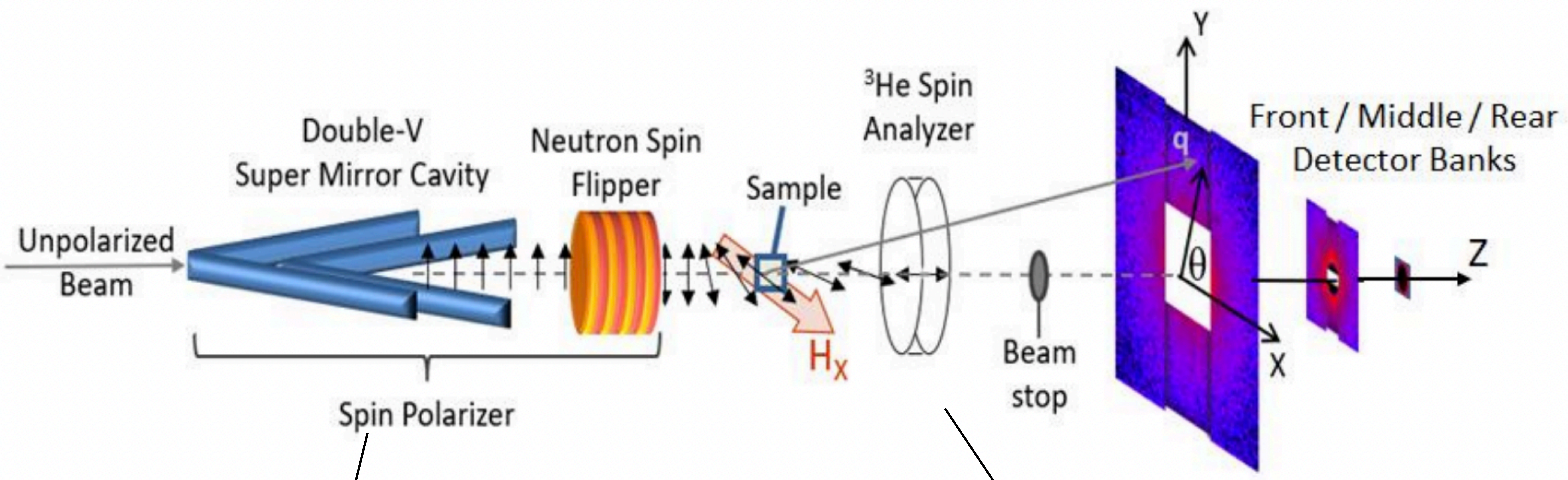
$$\langle \mathbf{S}' | b | \mathbf{S} \rangle = b \langle \mathbf{S}' | \mathbf{S} \rangle = \begin{cases} b \begin{cases} |\uparrow\rangle \rightarrow |\uparrow\rangle \\ |\downarrow\rangle \rightarrow |\downarrow\rangle \end{cases} \text{Non-spin-flip} \\ 0 \begin{cases} |\uparrow\rangle \rightarrow |\downarrow\rangle \\ |\downarrow\rangle \rightarrow |\uparrow\rangle \end{cases} \text{Spin-flip} \end{cases}$$

Magnetic Scattering

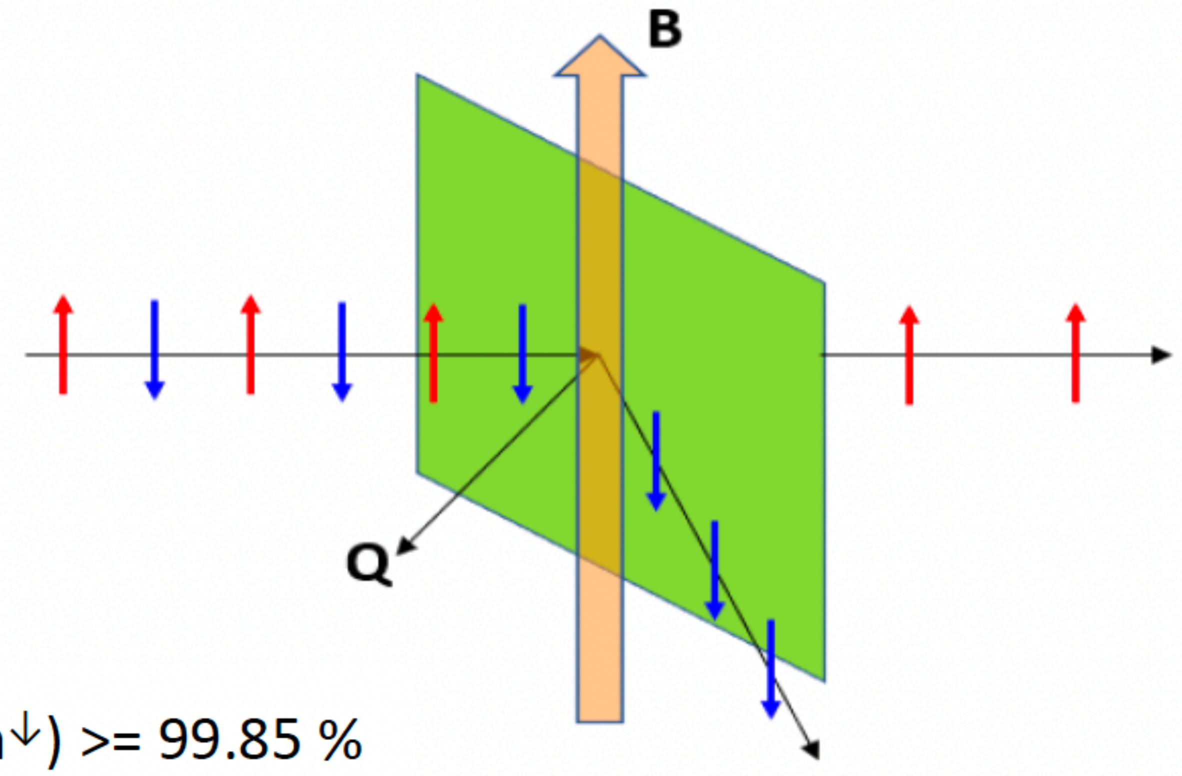
$$\langle \mathbf{S}' | V_m(\mathbf{Q}) | \mathbf{S} \rangle = -\frac{\gamma_n r_0}{2\mu_B} \begin{cases} M_{\perp z}(\mathbf{Q}) & |\uparrow\rangle \rightarrow |\uparrow\rangle \\ -M_{\perp z}(\mathbf{Q}) & |\downarrow\rangle \rightarrow |\downarrow\rangle \\ M_{\perp x}(\mathbf{Q}) - iM_{\perp y}(\mathbf{Q}) & |\uparrow\rangle \rightarrow |\downarrow\rangle \\ M_{\perp x}(\mathbf{Q}) + iM_{\perp y}(\mathbf{Q}) & |\downarrow\rangle \rightarrow |\uparrow\rangle \end{cases}$$

V-SANS : uniaxial polarization analysis can be performed

S. Oberdick et al., Sci. Reports 8, 3425 (2018)

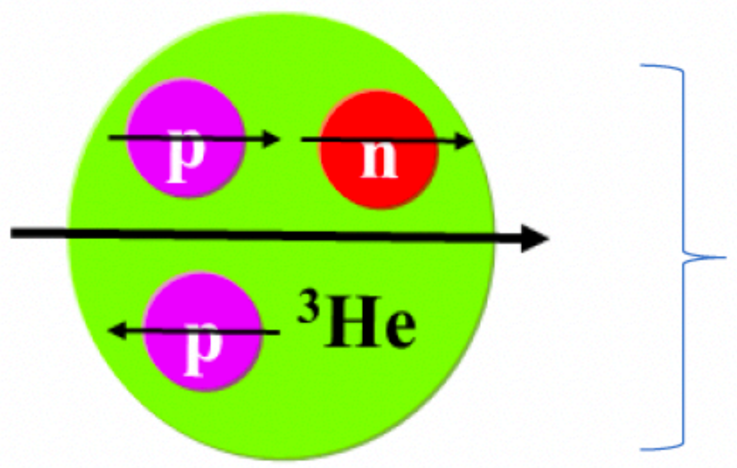


Spin Polarizer



P ≡ (n↑- n↓)/(n↑+ n↓) >= 99.85 %

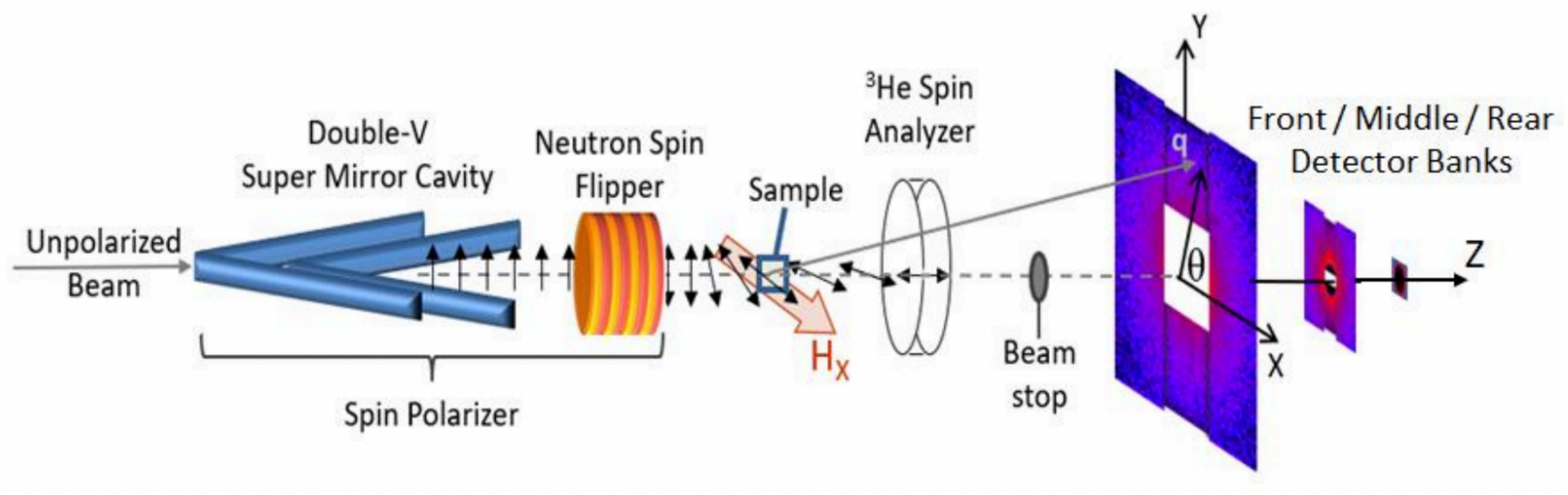
He3 Analyzer



Neurons aligned with ^{3}He pass; otherwise absorbed

V-SANS : Uniaxial polarization analysis can be performed

S. Oberdick et al., Sci. Reports 8, 3425 (2018)



1) Unpolarized

$$I(q) = I_{uu}(q) + I_{ud}(q) + I_{du}(q) + I_{dd}(q)$$

2) Half-polarized (polarizer only)

$$I_u(q) = I_{uu}(q) + I_{ud}(q)$$

$$I_d(q) = I_{du}(q) + I_{dd}(q)$$

3) Full polarized mode (polarizer and analyzer)

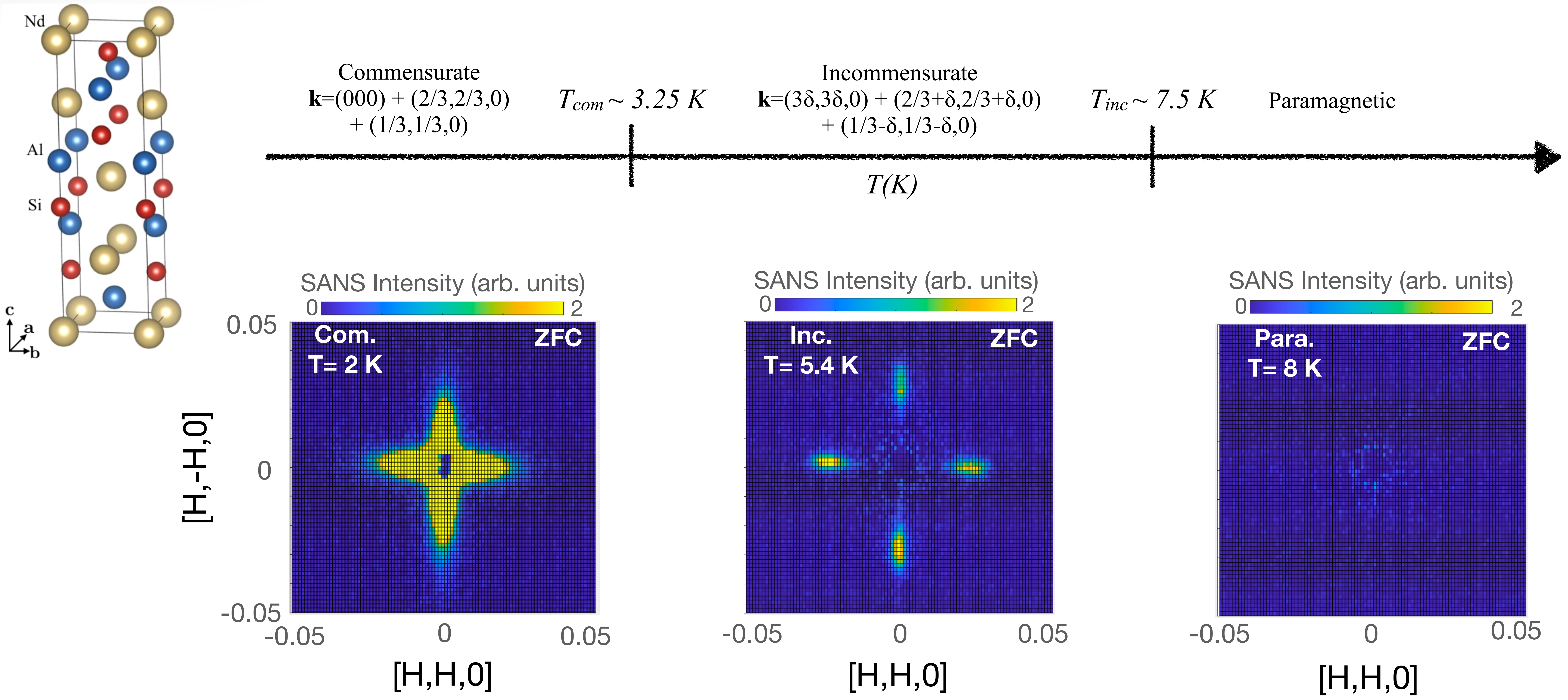
$I_{uu}(q)$

$I_{ud}(q)$

$I_{du}(q)$

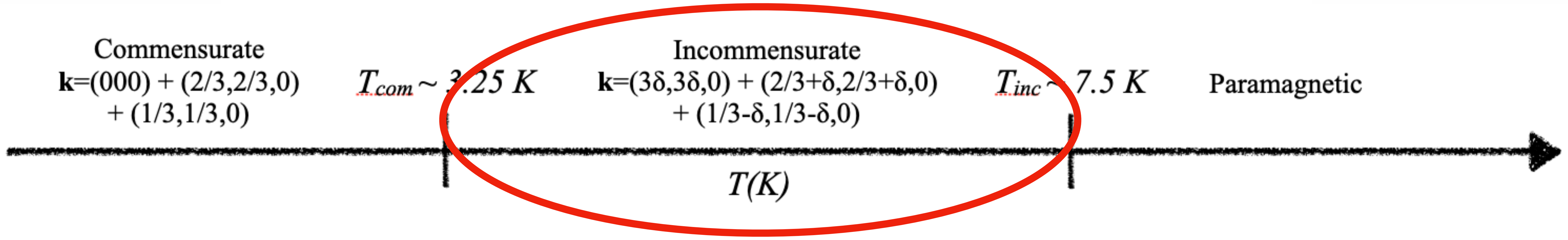
$I_{dd}(q)$

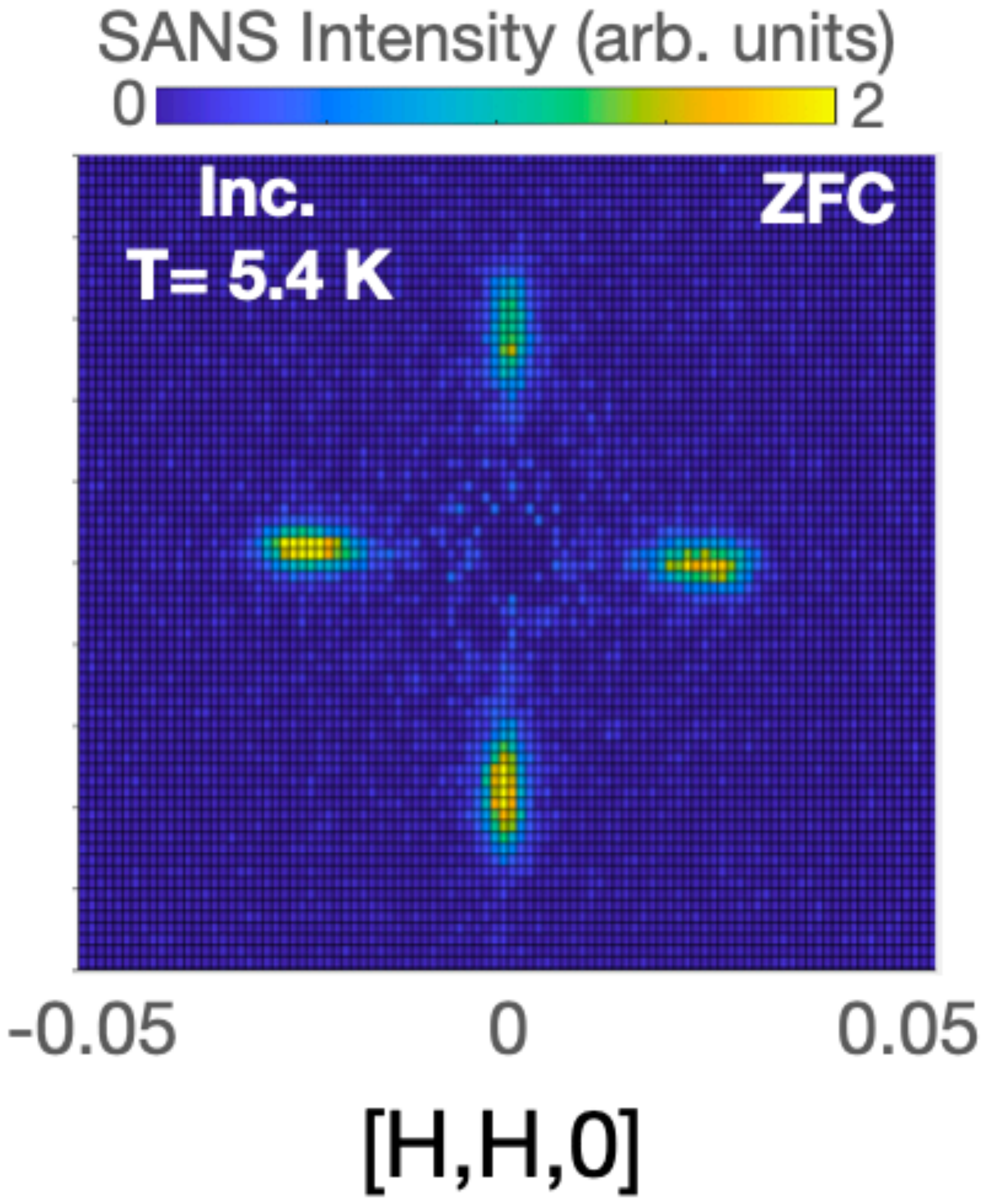
Unpolarized SANS: Weyl-mediated magnetism in NdAlSi



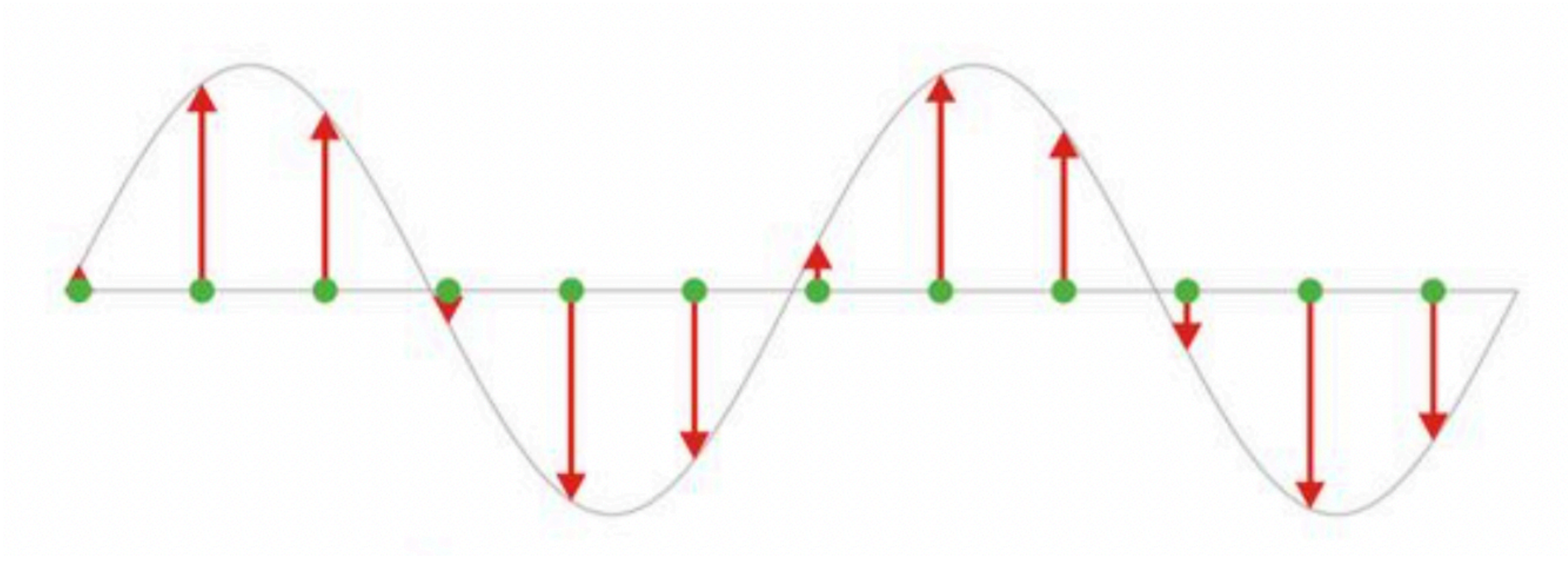
- J. Gaudet al., Nature Materials 20, 1650-1656 (2021)

Unpolarized SANS: Weyl-mediated magnetism in NdAlSi



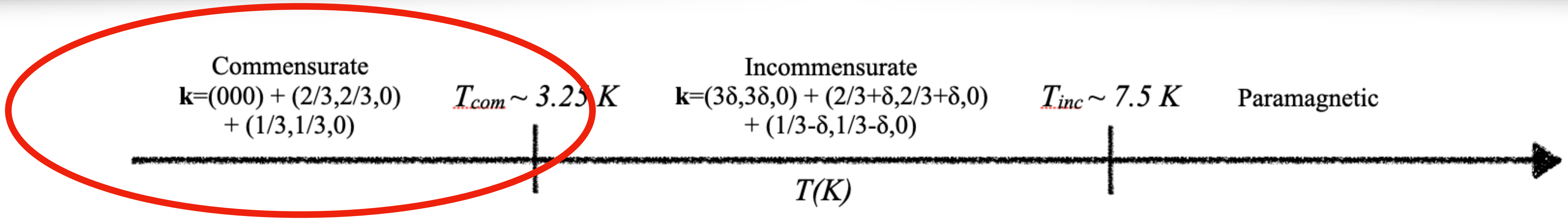


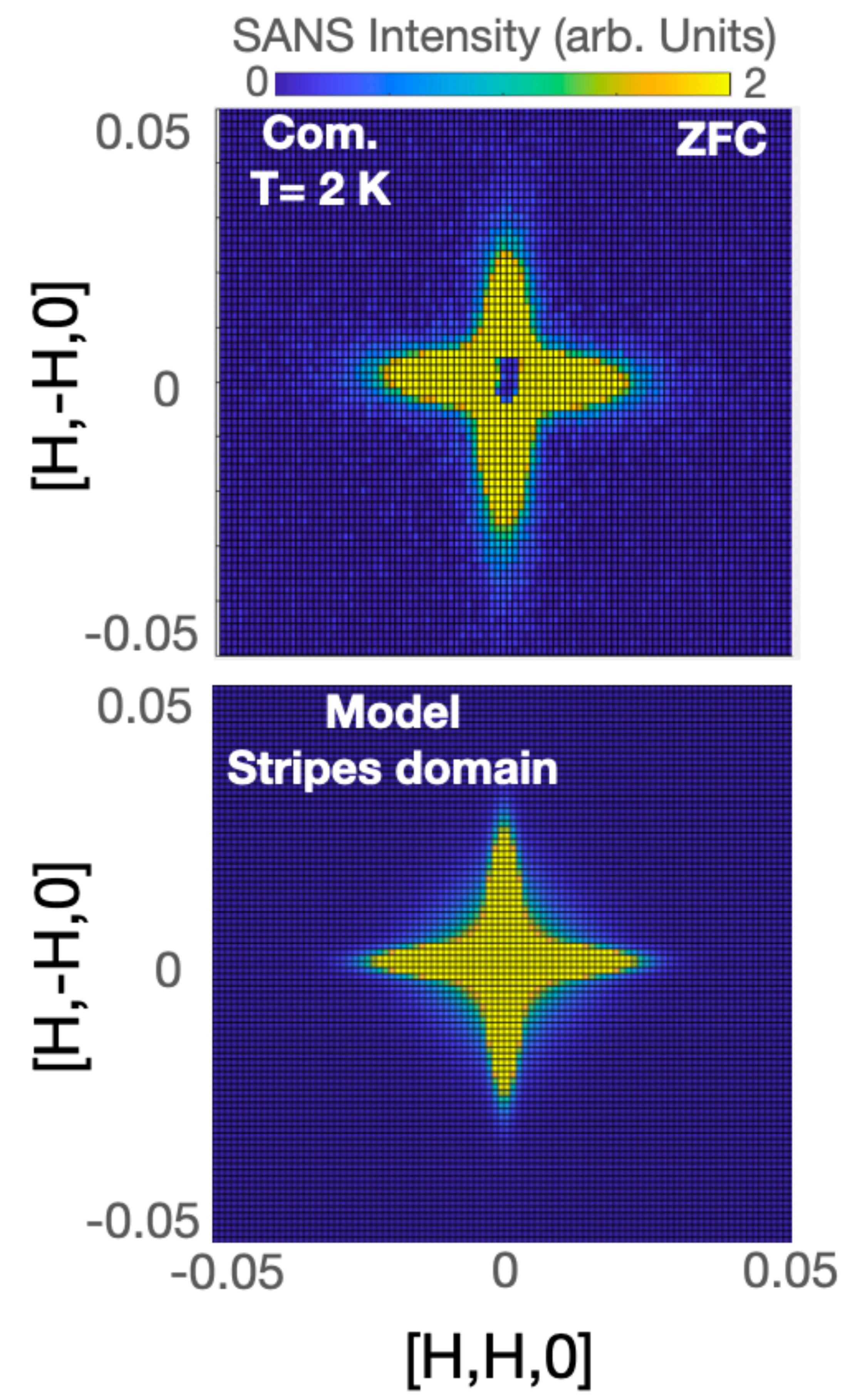
Modulated spin density wave



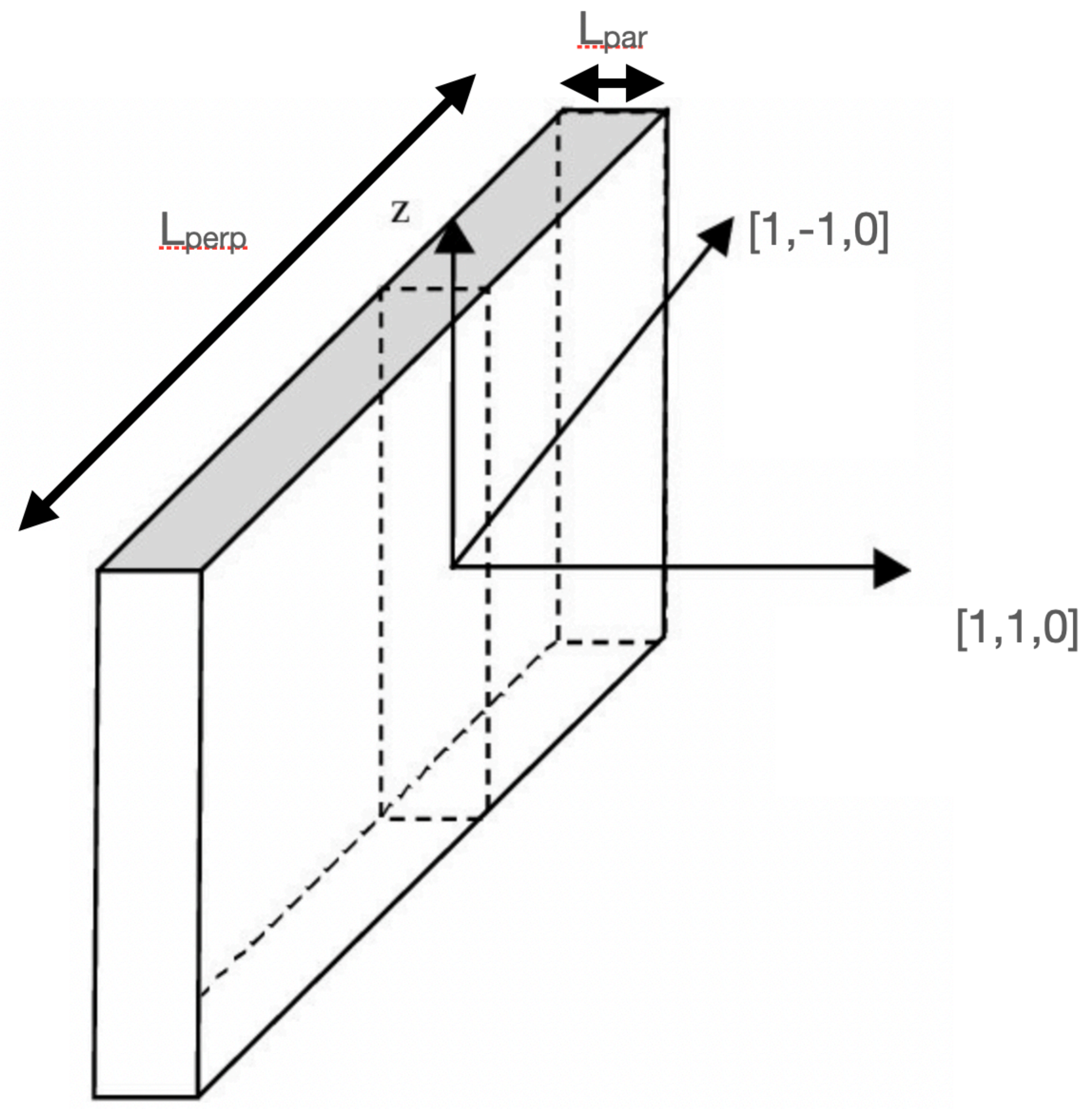
- J. Gaudet al., Nature Materials 20, 1650-1656 (2021)

Unpolarized SANS: Weyl-mediated magnetism in NdAlSi





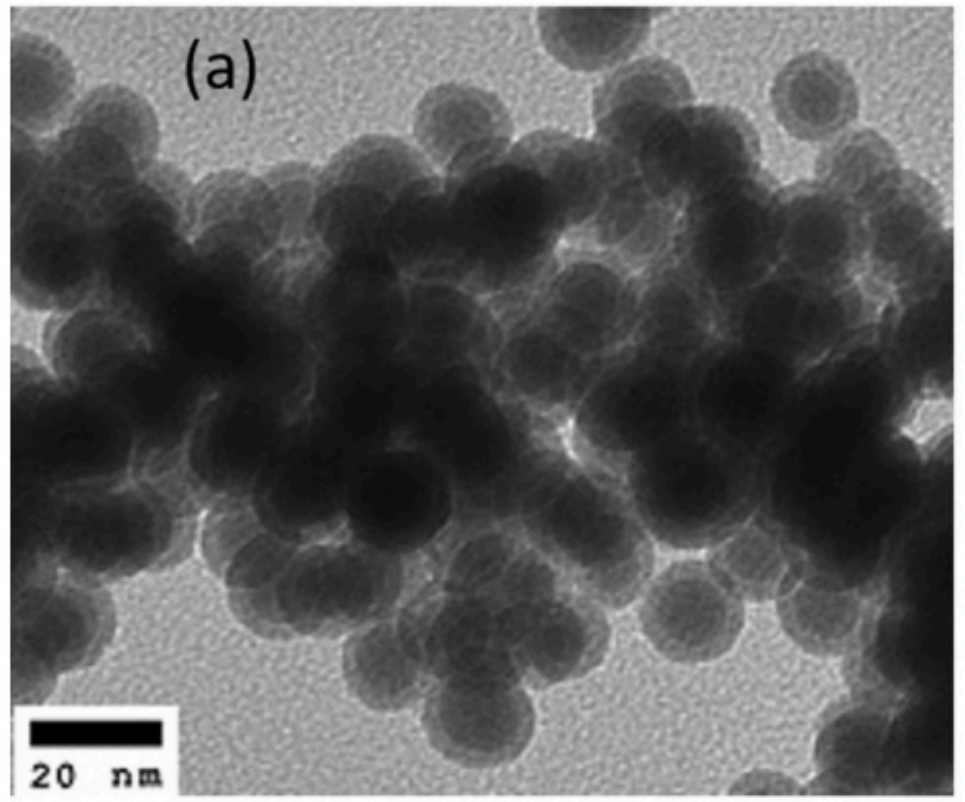
Stripe ferromagnetic domains

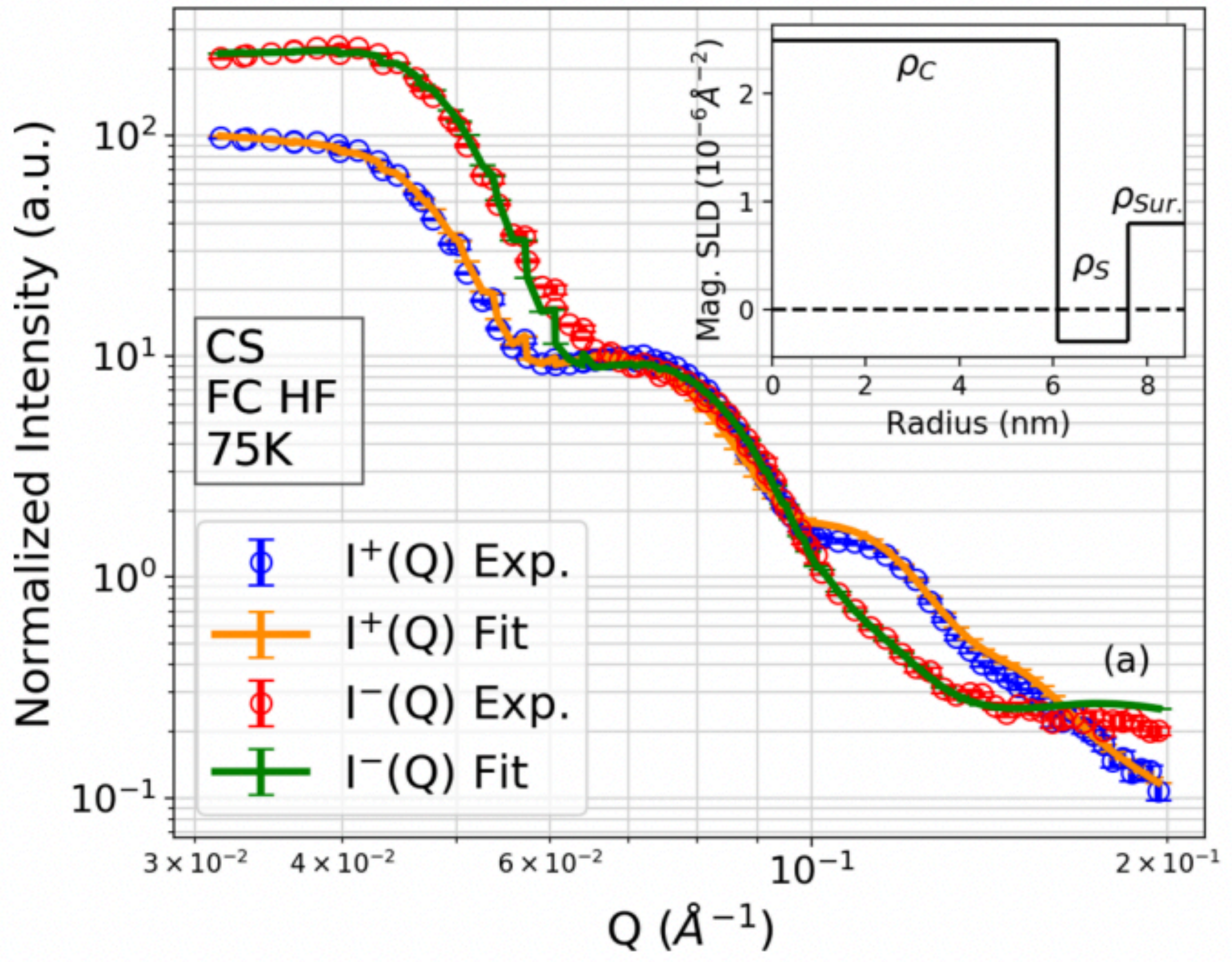


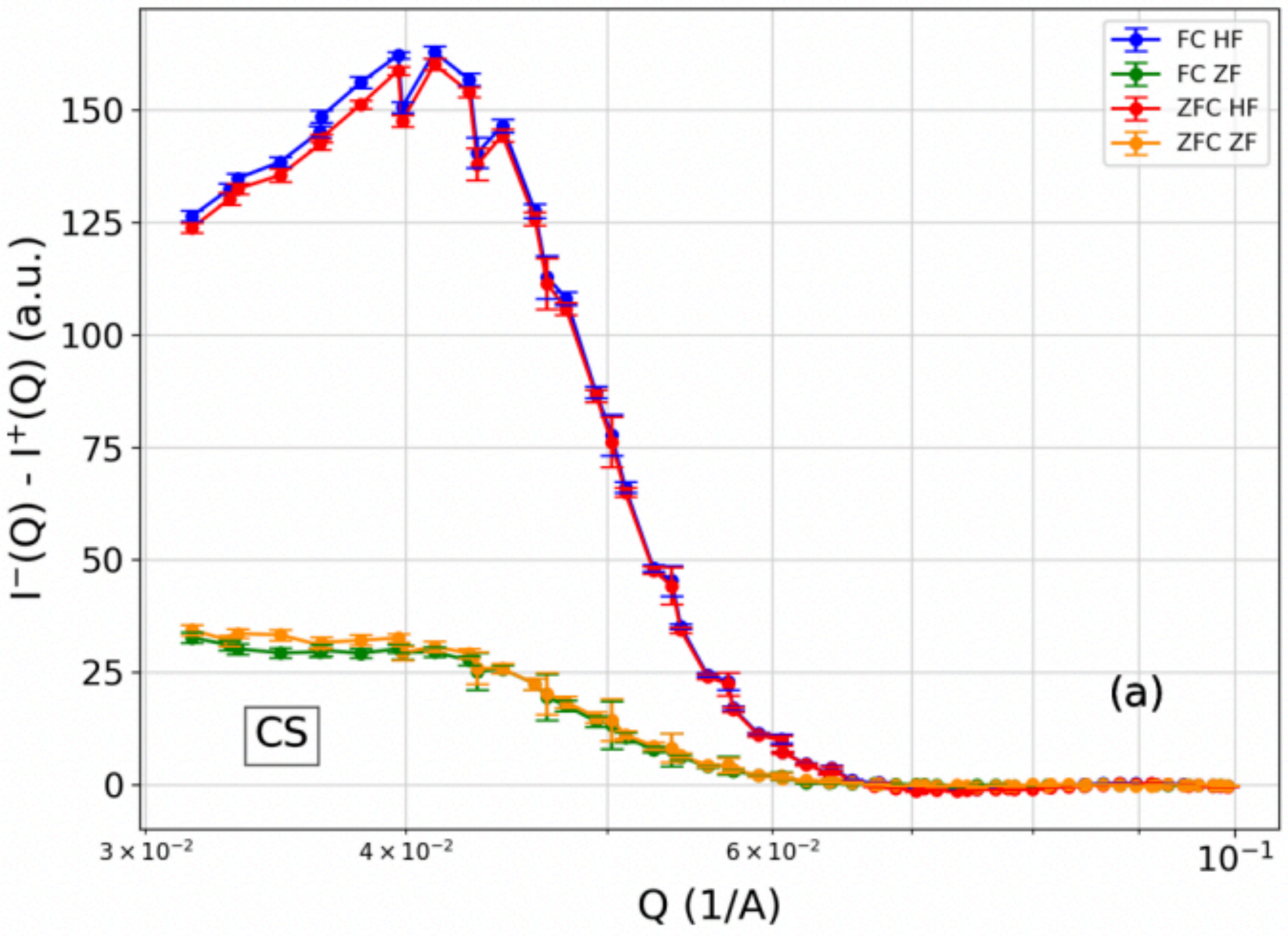
- J. Gaudet al., Nature Materials 20, 1650-1656 (2021)

Example of Half-polarized SANS:
Identifying the weak magnetic scattering in nanoparticles (NPs) system

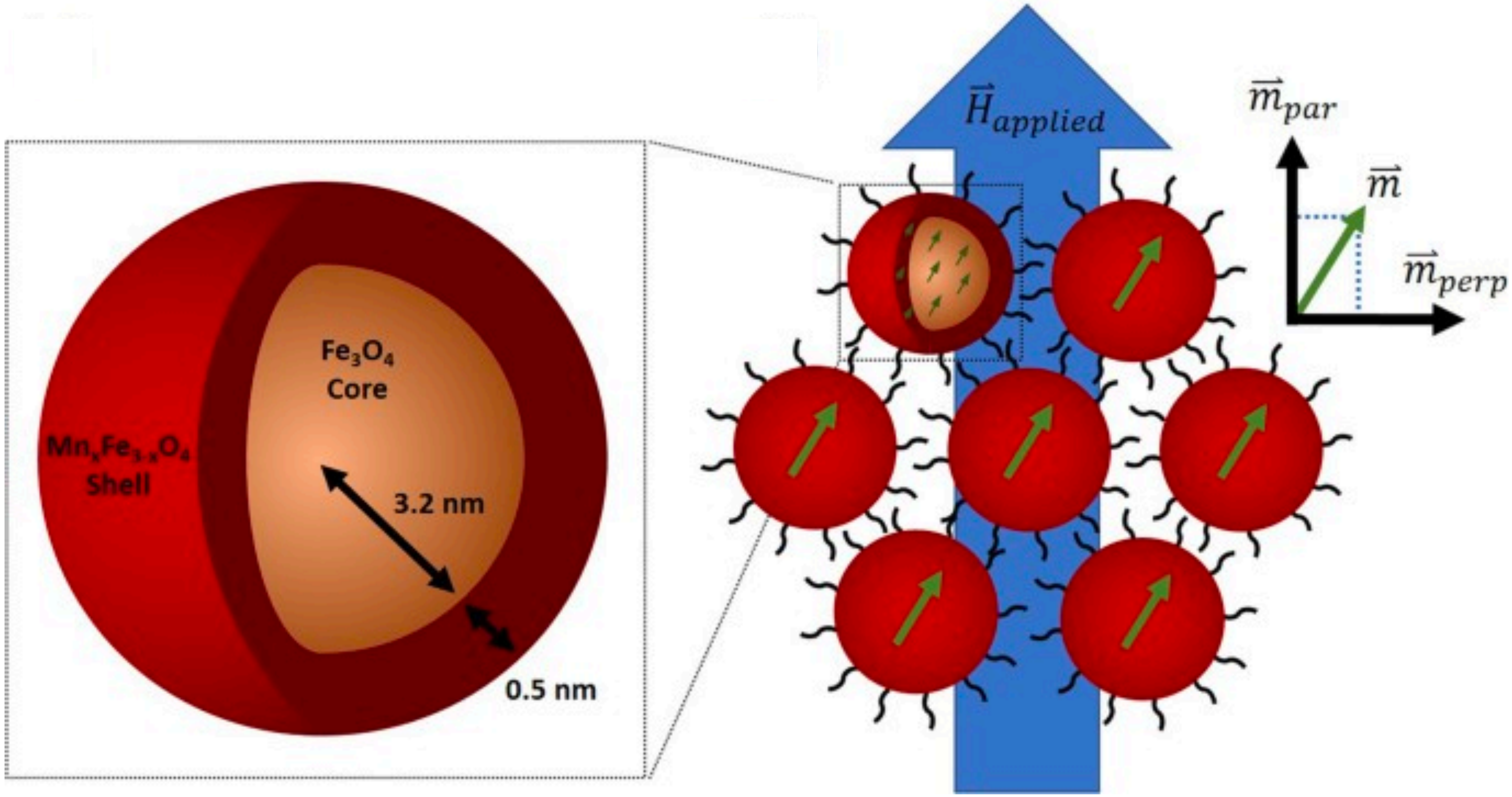
C. Kons et al., PRM **4**, 034408 (2020)







Full-polarized SANS:
Characterizing the in-field 3D magnetization profile of NP's



S. Oberdick et al., Sci. Reports 8, 3425 (2018)

Full-polarized SANS:
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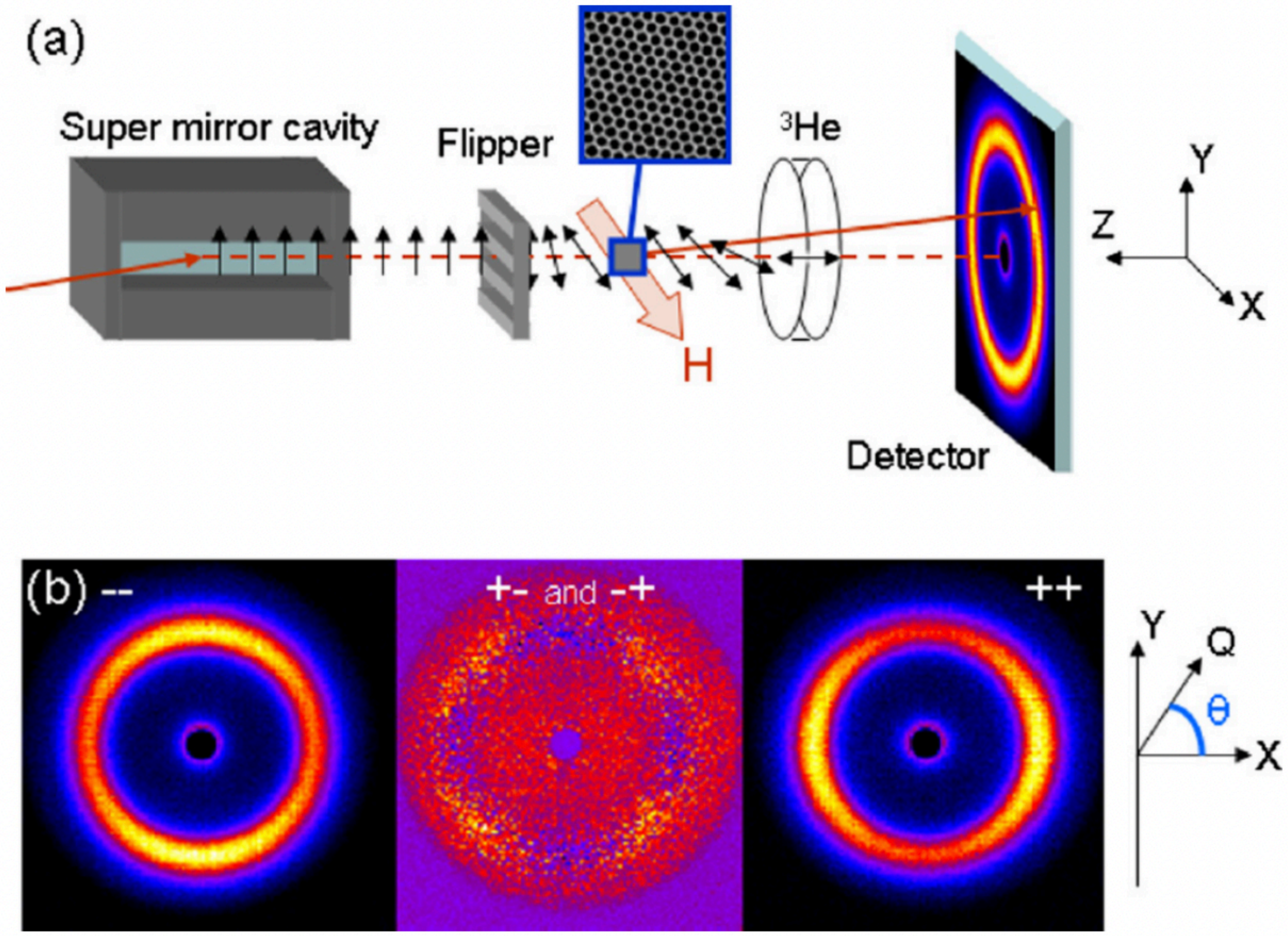


K. L. Krycka et al., PRB **90**, 180405(R) (2014)

$$I^{++,--}_{\phi=0^\circ} = N^2,$$

$$I^{++,--}_{\phi=90^\circ} = N^2 + M_X^2 \mp 2NM_X,$$

$$I^{+-,-+}_{\phi=0^\circ} = M_Y^2 + M_Z^2 = 2M^2_{\mathrm{PERP}},$$

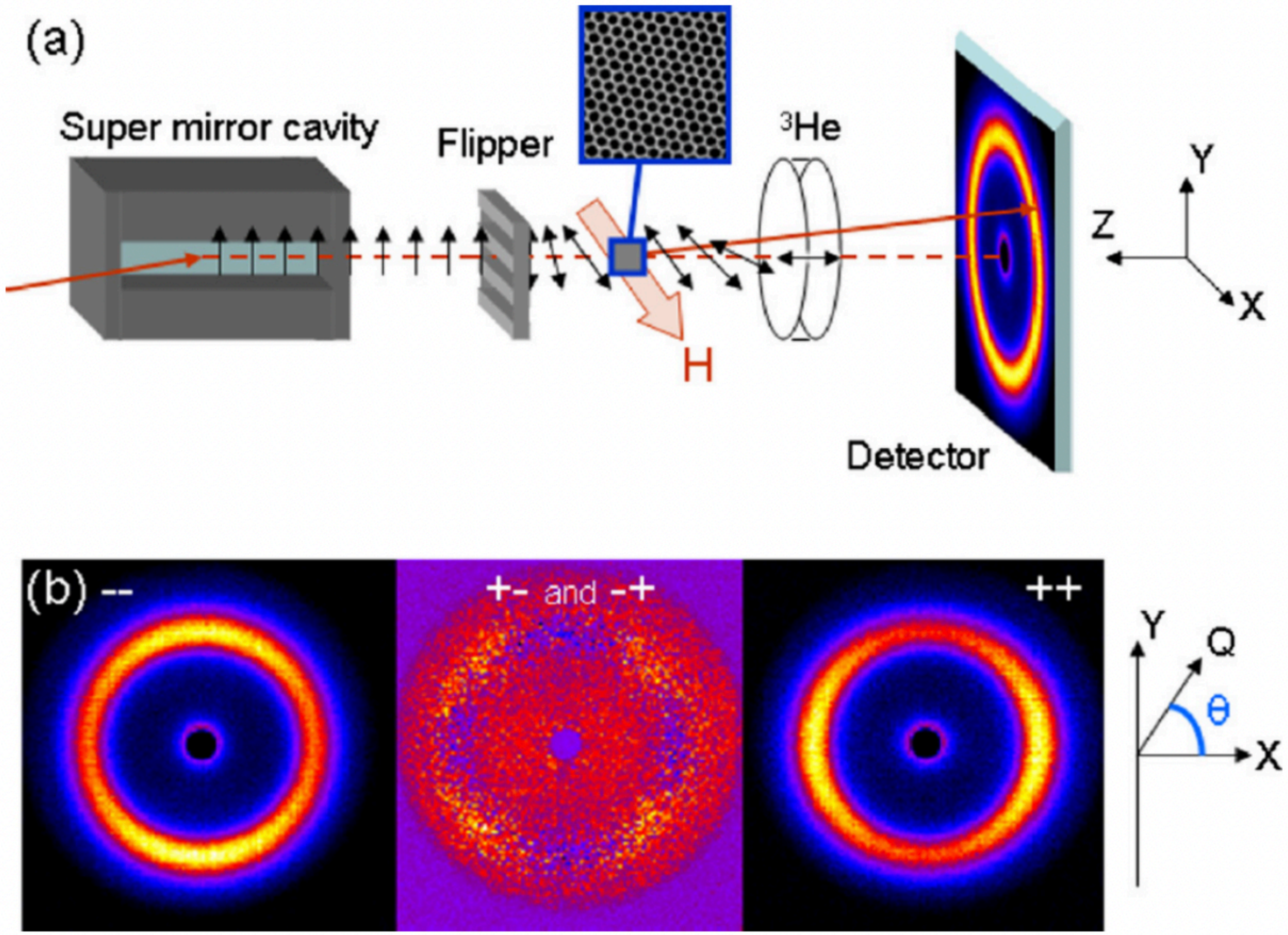
$$I^{+-,-+}_{\phi=90^\circ} = M_Z^2 = M^2_{\mathrm{PERP}},$$

K. L. Krycka, et al., J Appl Cryst **45**, 554–565 (2012)

*Assuming isotropic system with only the X (field) direction being unique

$M^2_x = M^2_{parl}$ $M^2_y = M^2_Z = M^2_{perp}$

Full-polarized SANS:
Characterizing the in-field 3D magnetization profile of NP's



$$N^2(Q) = \frac{1}{2}(I^{++}_{\theta=0^\circ} + I^{--}_{\theta=0^\circ}),$$

$$M^2_{\mathrm{PARL}}(Q) = \frac{(I^{--}_{\theta=90^\circ} - I^{++}_{\theta=90^\circ})^2}{16N^2},$$

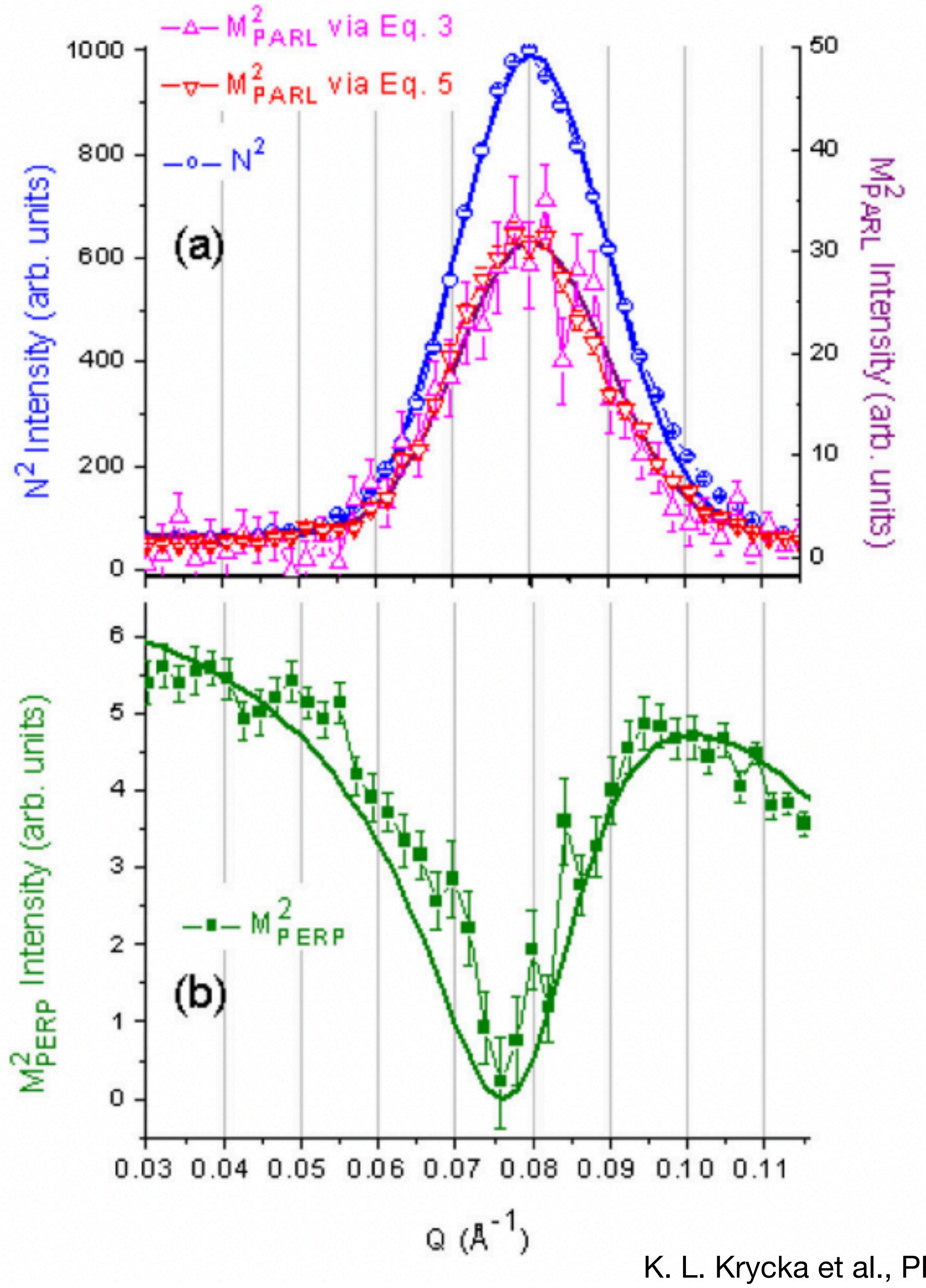
$$M^2_{\mathrm{PERP}}(Q) = \frac{1}{6}(I^{+-}_{\theta=0^\circ,90^\circ} + I^{-+}_{\theta=0^\circ,90^\circ}),$$

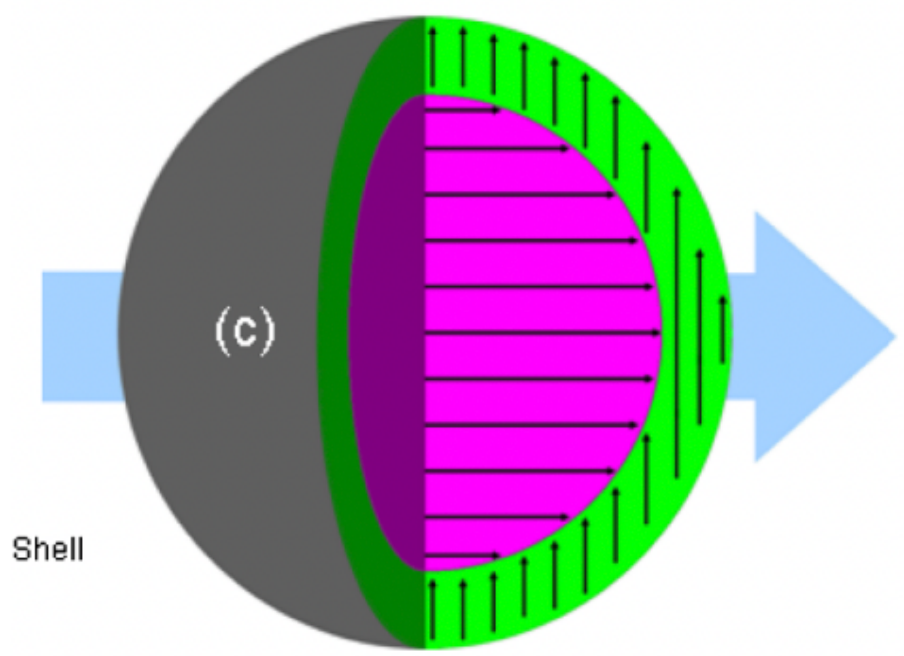
*Assuming isotropic system with only the X (field) direction being unique

$M^2_x = M^2_{parl}$ $M^2_y = M^2_Z = M^2_{perp}$

K. L. Krycka et al., PRB **90**, 180405(R) (2014)

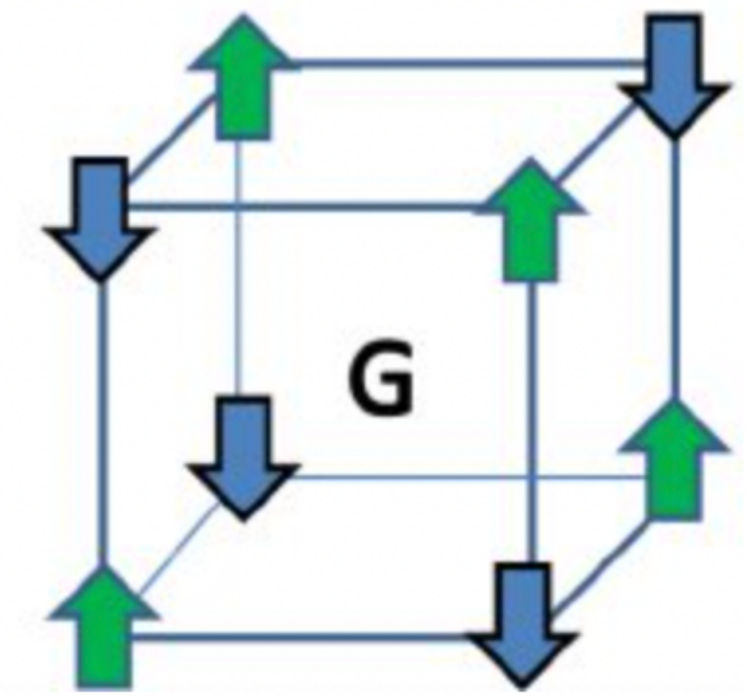
Full-polarized SANS:
Characterizing the in-field 3D magnetization profile of NP's

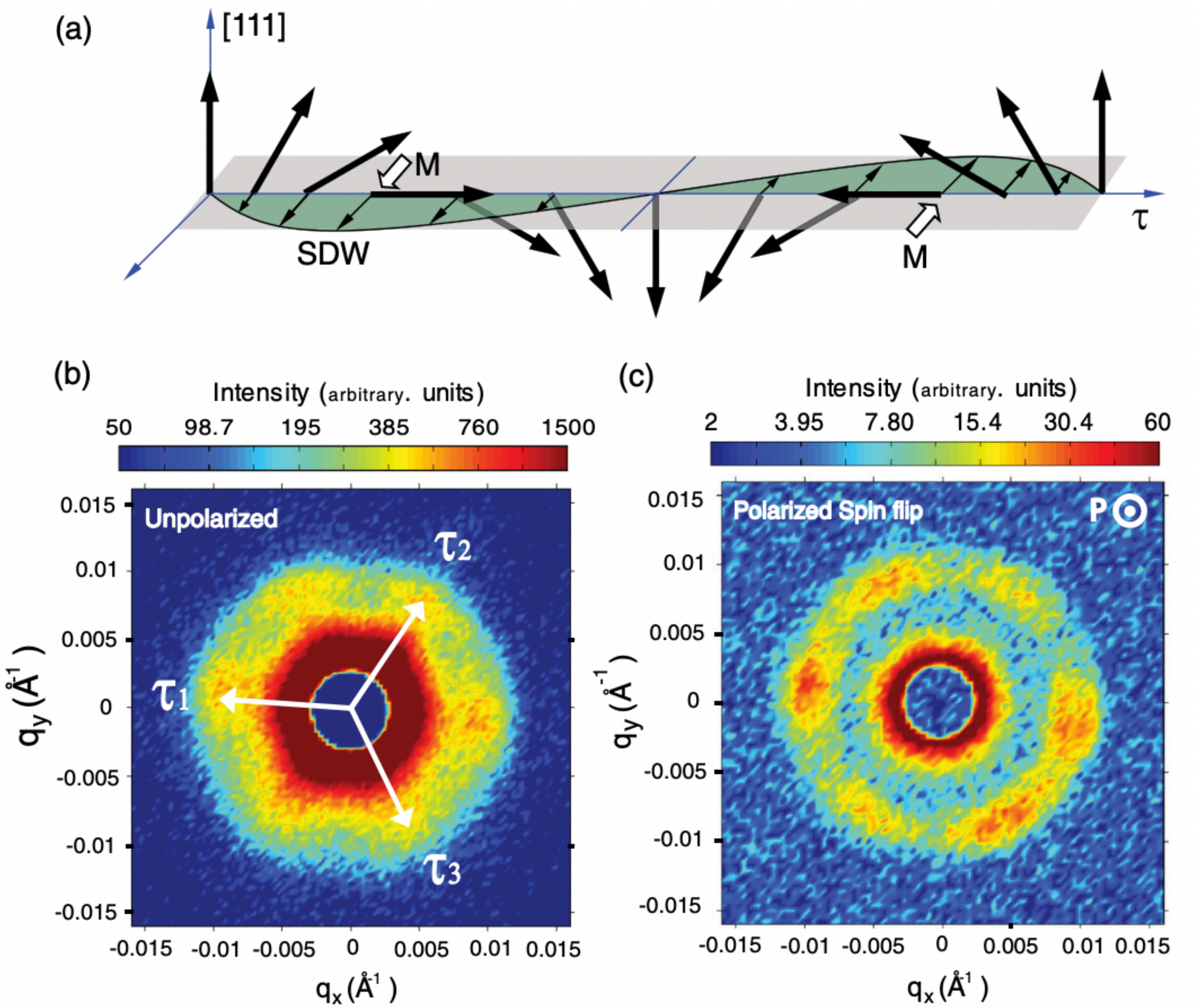




K. L. Krycka et al., PRL **104**, 207203 (2010)

Full-polarized SANS:
Characterizing the long-wavelength spin density wave in $BiFeO_3$





Ramazanoglu, M. et al., PRL **107**, 207206 (2011)

Full-polarized SANS:
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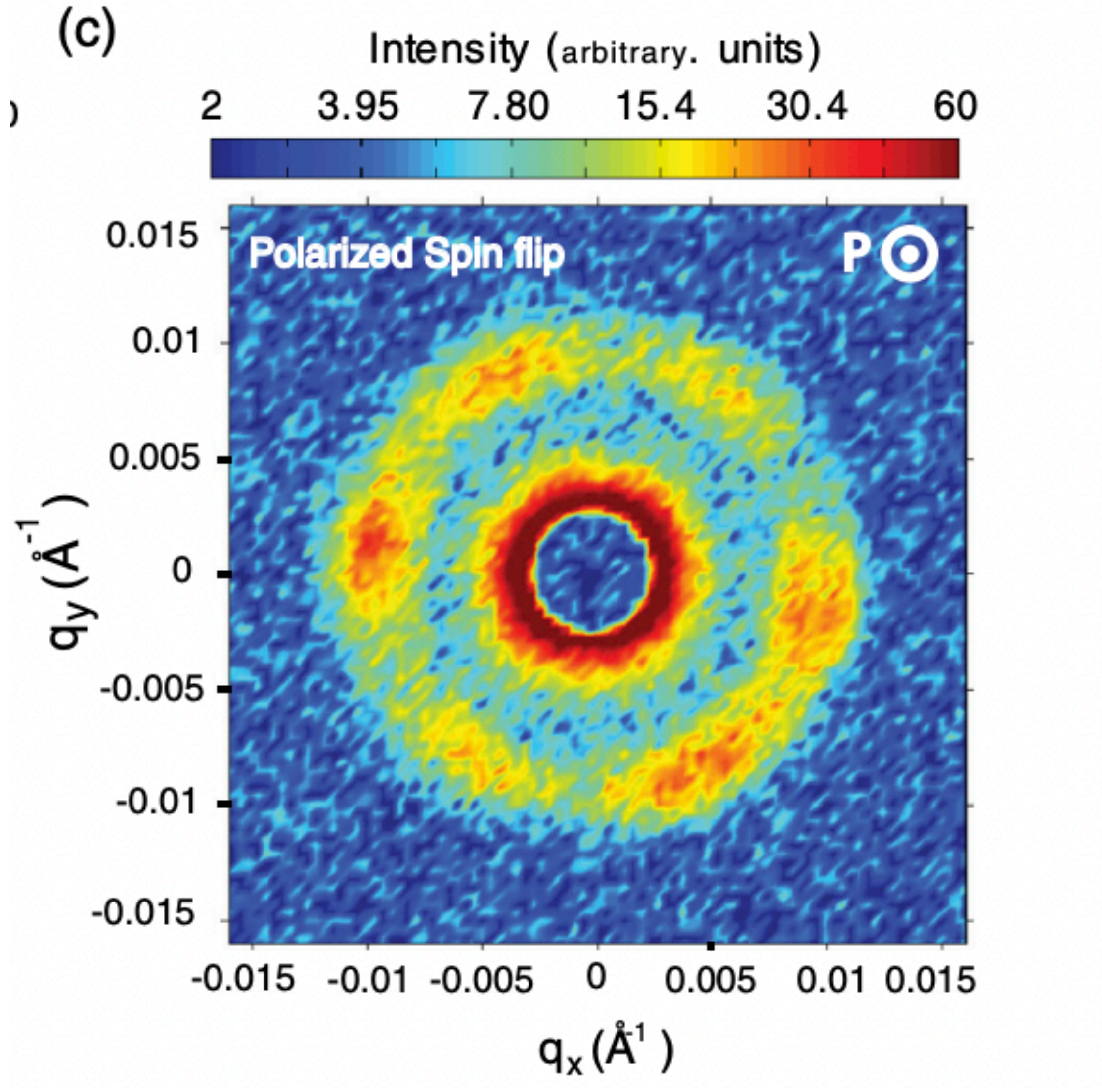
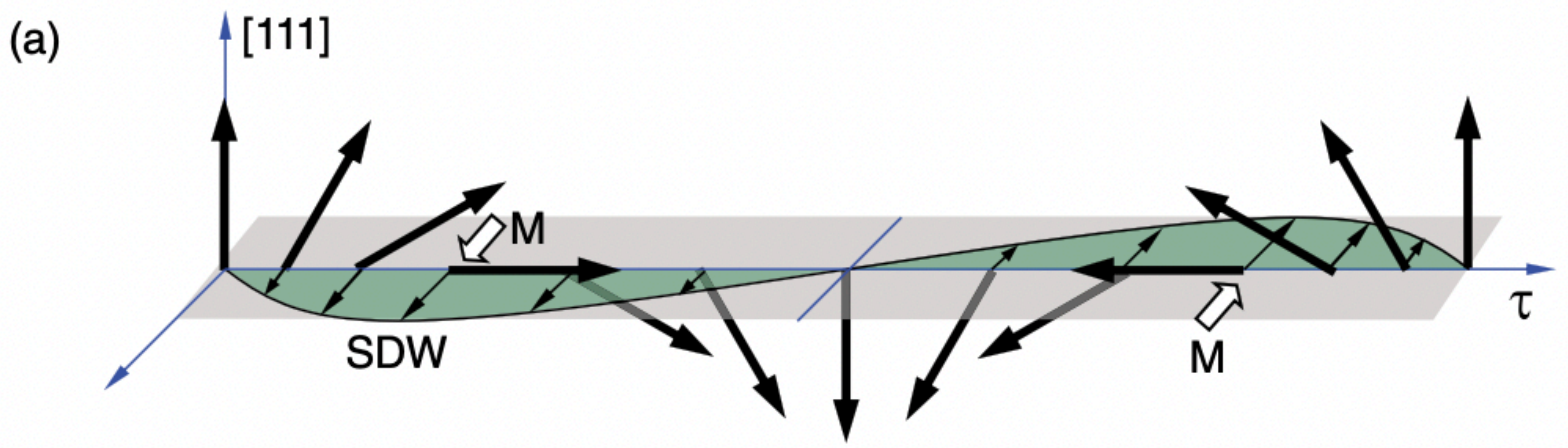
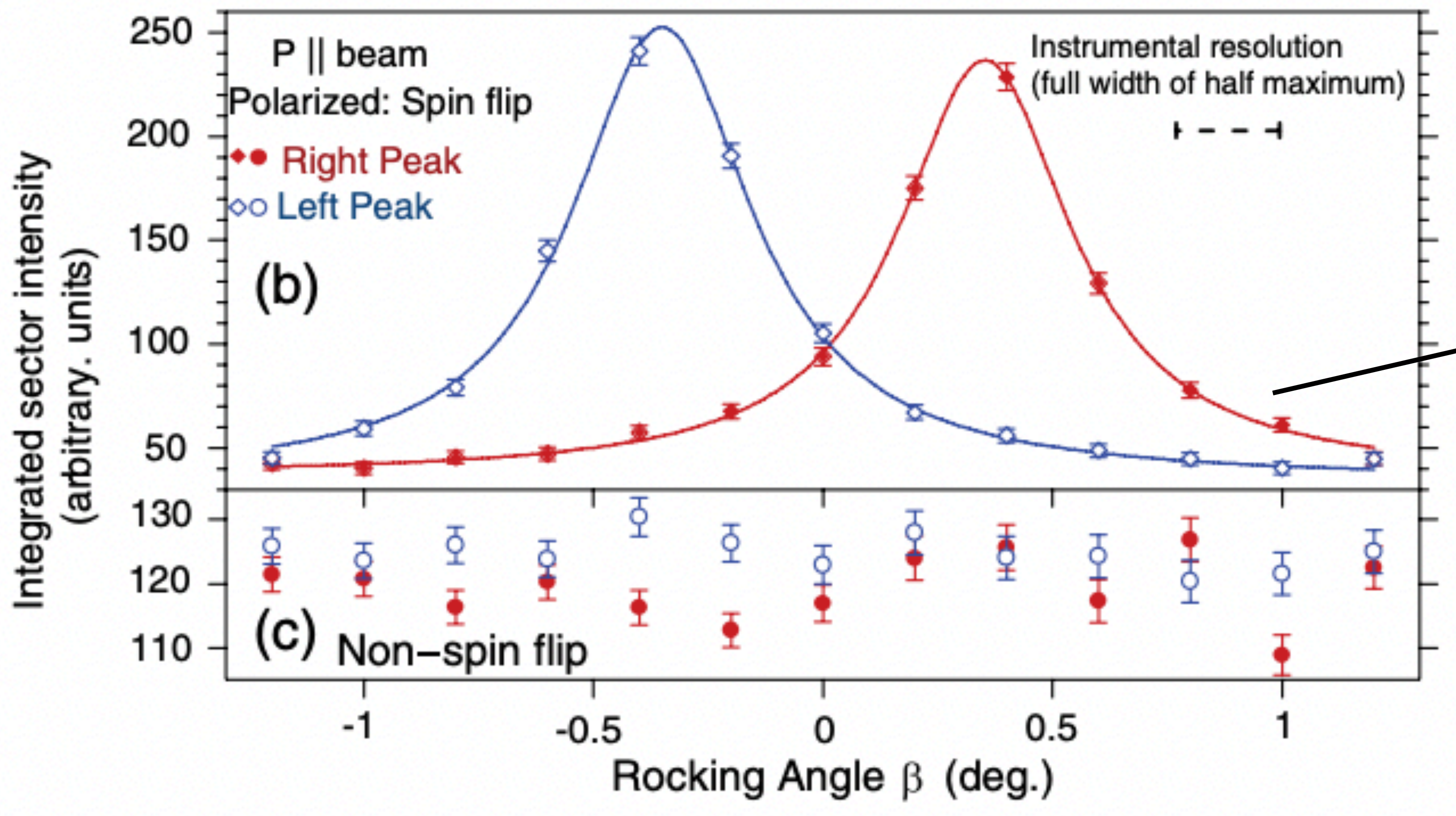






The Bragg peaks only show up in the SF channel for **P**||beam.
This implies:

1) It is magnetic in origin
2) Its spin component is ⊥ to both [111] and **τ**

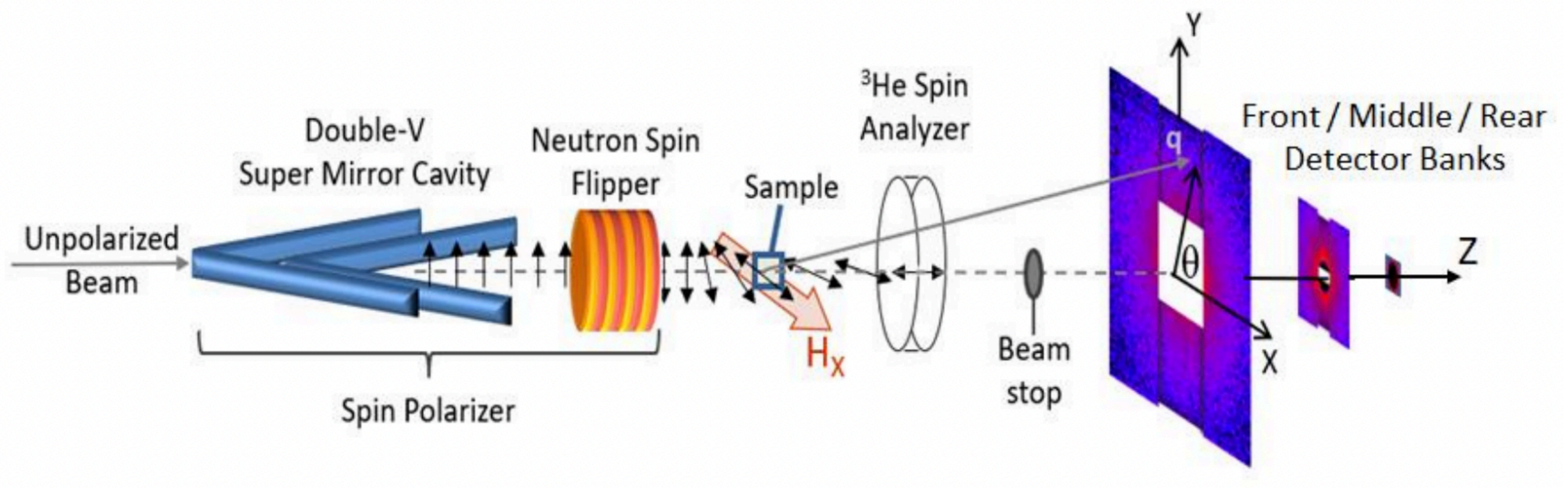
Ramazanoglu, M. et al., PRL **107**, 207206 (2011)

Conclusion

1) Magnetic SANS is used to probe magnetic inhomogeneities on a spatial length scale of ~ 1 to 10 000 nm.

2) NCNR is the host of 5 different SANS instruments including V-SANS, which is a very versatile instrument that also allows for uniaxial polarization analysis.

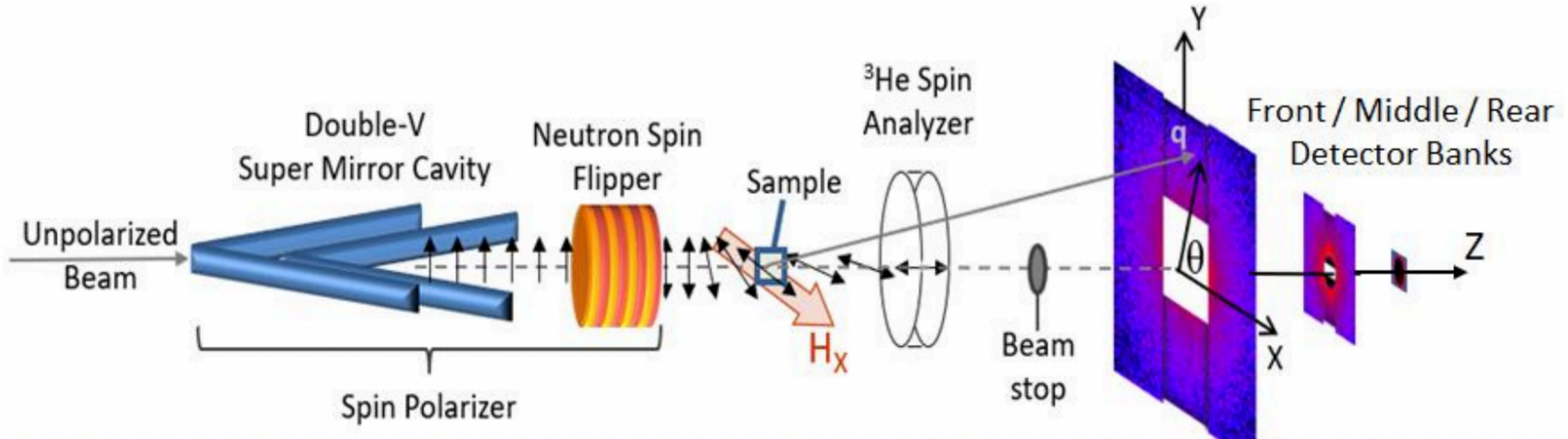
3) Polarized SANS can be used to isolate a weak magnetic signal that lies on top of a huge nuclear scattering signal, to characterize the 3D magnetization profile of NPs, to determine the spin orientation and chirality of spin density wave, and much more…



Conclusion: Please contact us to do polarized SANS at NIST!

Polarized SANS at NIST:

Julie Borchers
Wangchun Chen
Shannon Watson



Thanks to:

Kathryn Krycka
Julie Borchers
Wangchun Chen
Shannon Watson
John Barker
Brian Maranville
Caitlin Wolf
Katie Weigandt
Peter Beaucage

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