Multiple scattering in GISANS experiments
the different cases
and their consequences

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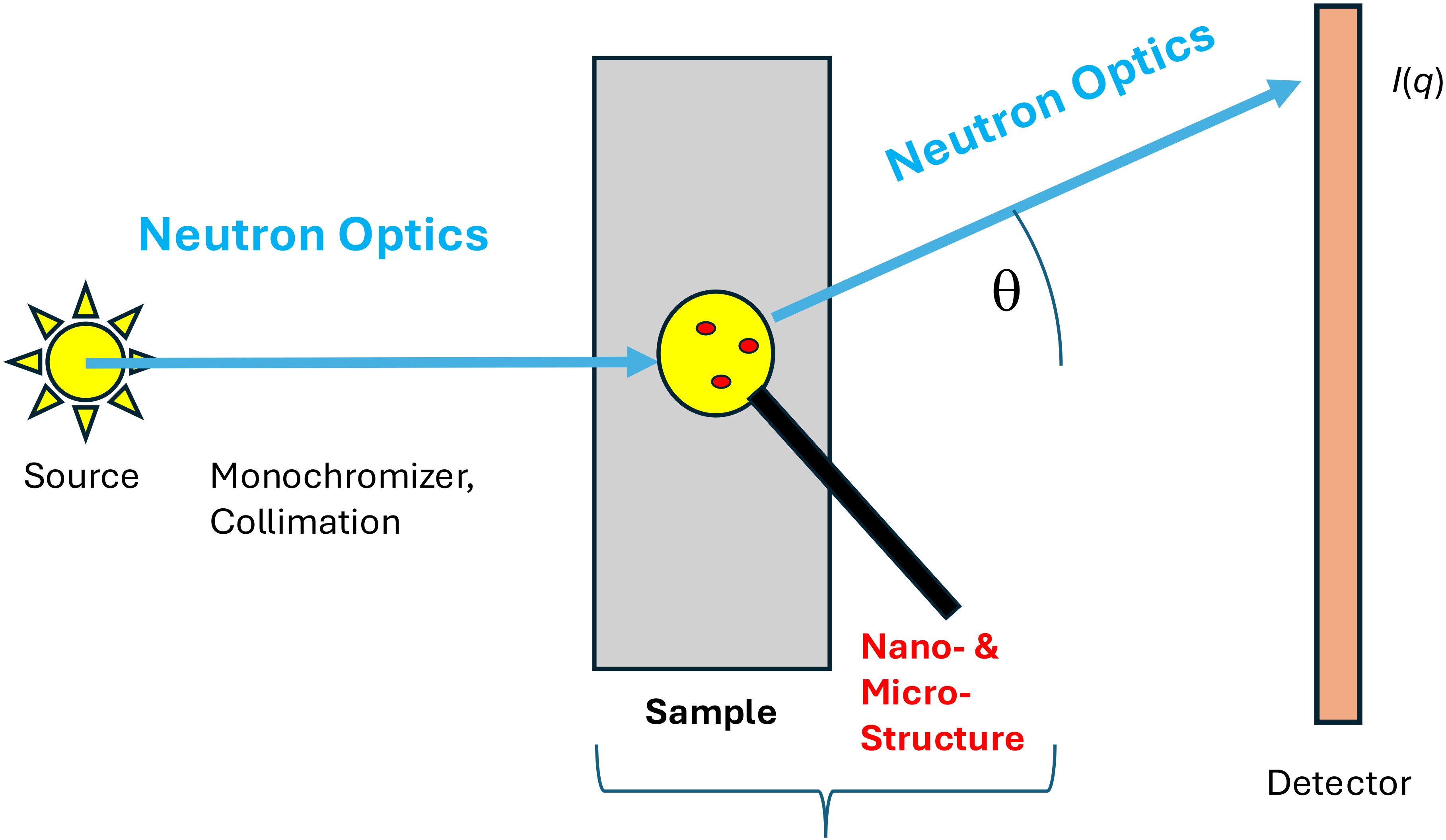
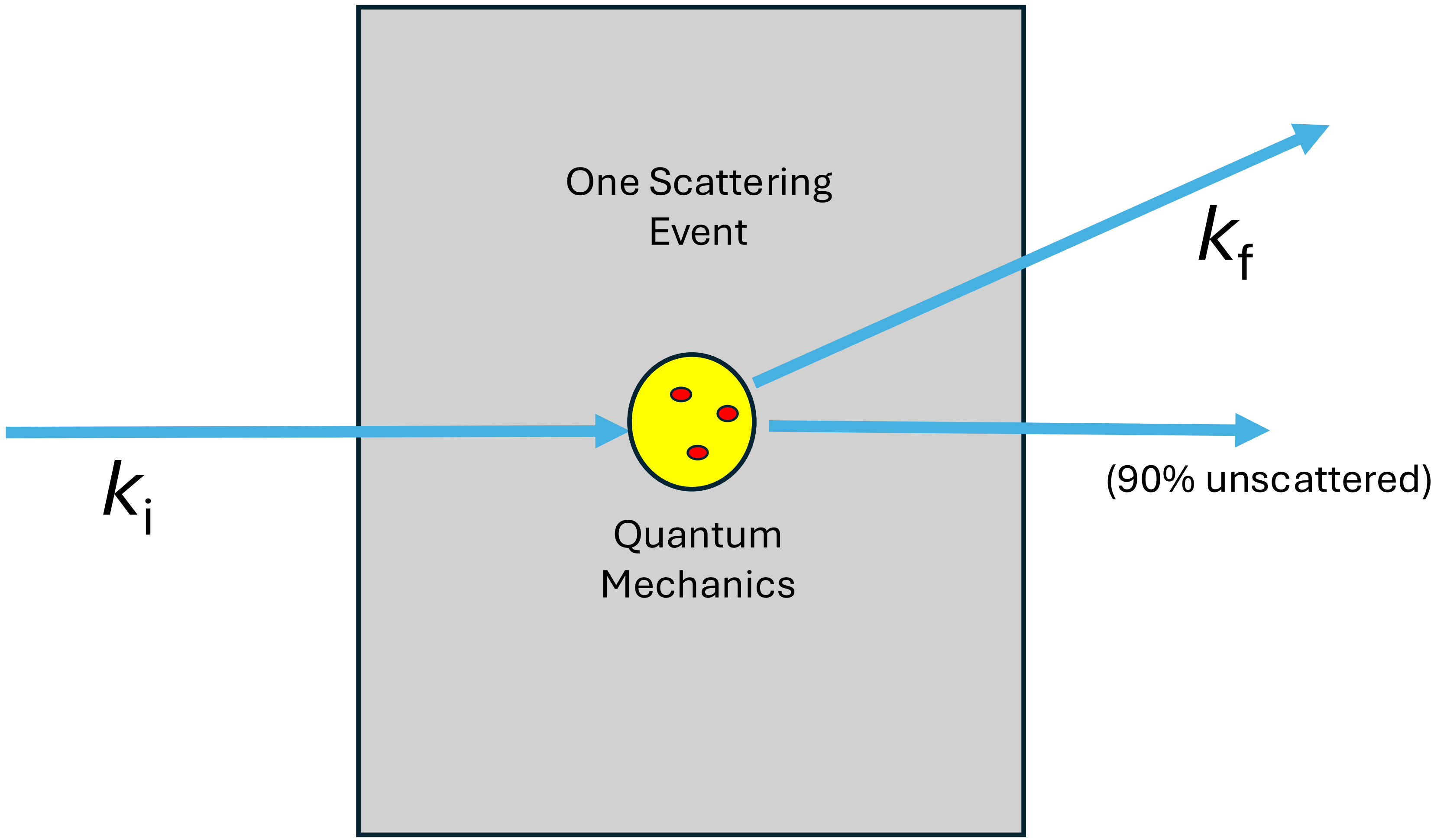
INTRO: Small angle scattering experiment



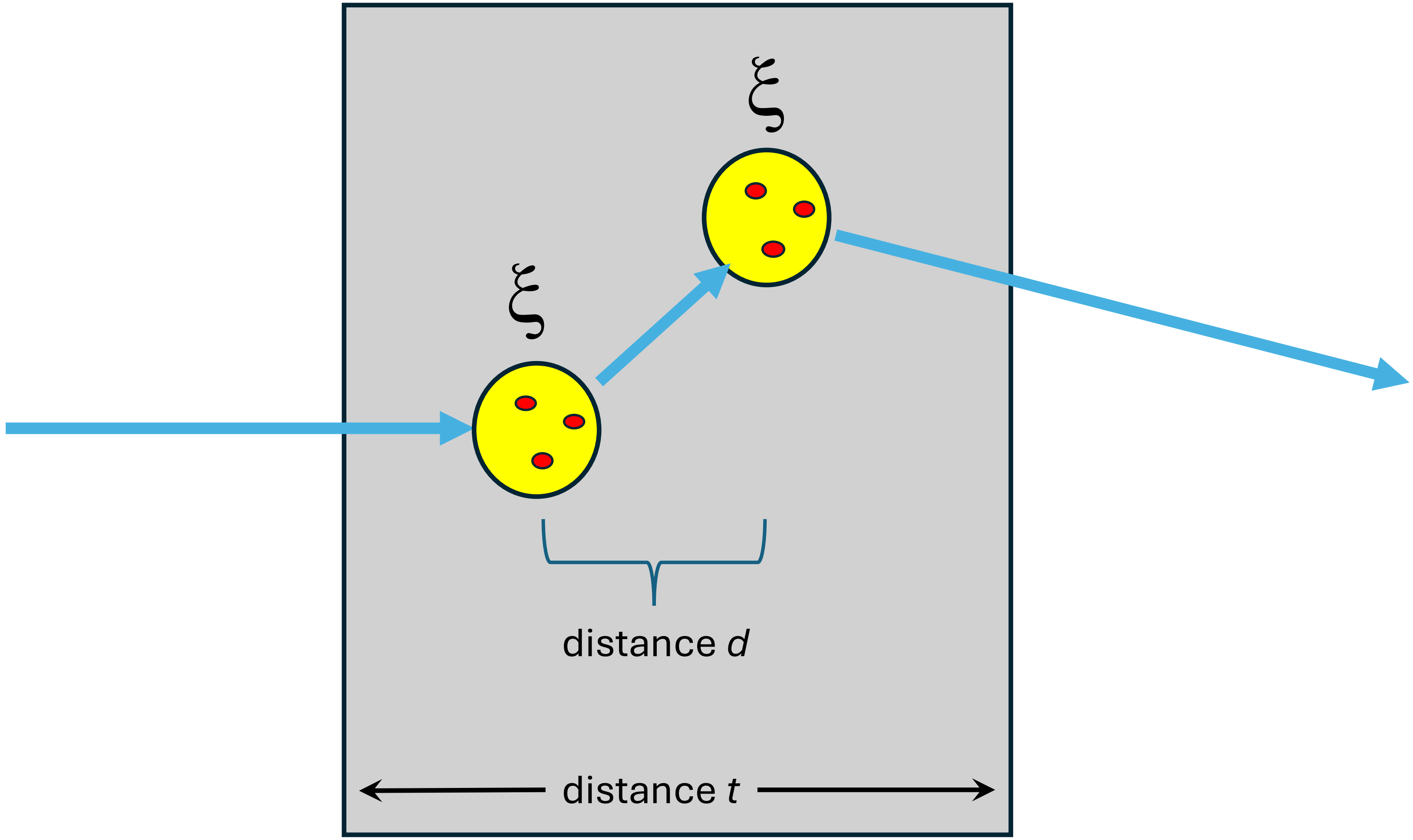
This is the topic of the talk

The (1st order) Born Approximation



$$I(\boldsymbol{k}_{\mathrm{f}} - \boldsymbol{k}_{\mathrm{i}}) \sim |\langle \boldsymbol{k}_{\mathrm{i}} | V(\boldsymbol{r}) | \boldsymbol{k}_{\mathrm{f}} \rangle|^2$$

Multiple scattering – independent events

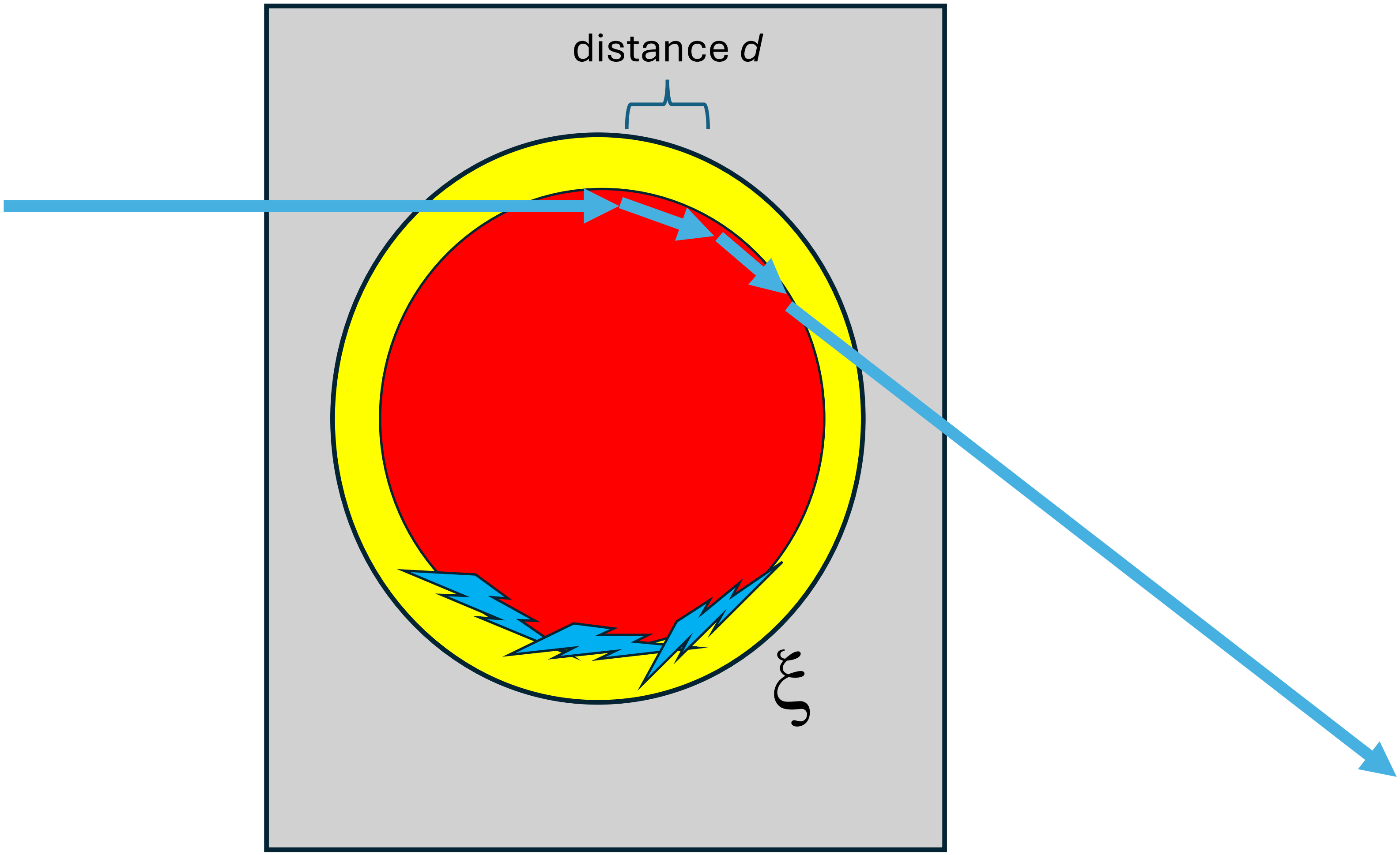


Optics: continuity

$$\operatorname{div} \boldsymbol{j} = \nabla \cdot \boldsymbol{j} = 0$$

$\boldsymbol{j} \sim I$

Coherent multiple scattering



surface resonances – GISANS community knows Yoneda/Vineyard surface resonances

~ „rainbow“ redirection of light rays to spectator

The *early* take home message

scattering event distance d

$d >> t$ sample thickness -> 1st order Born approx.

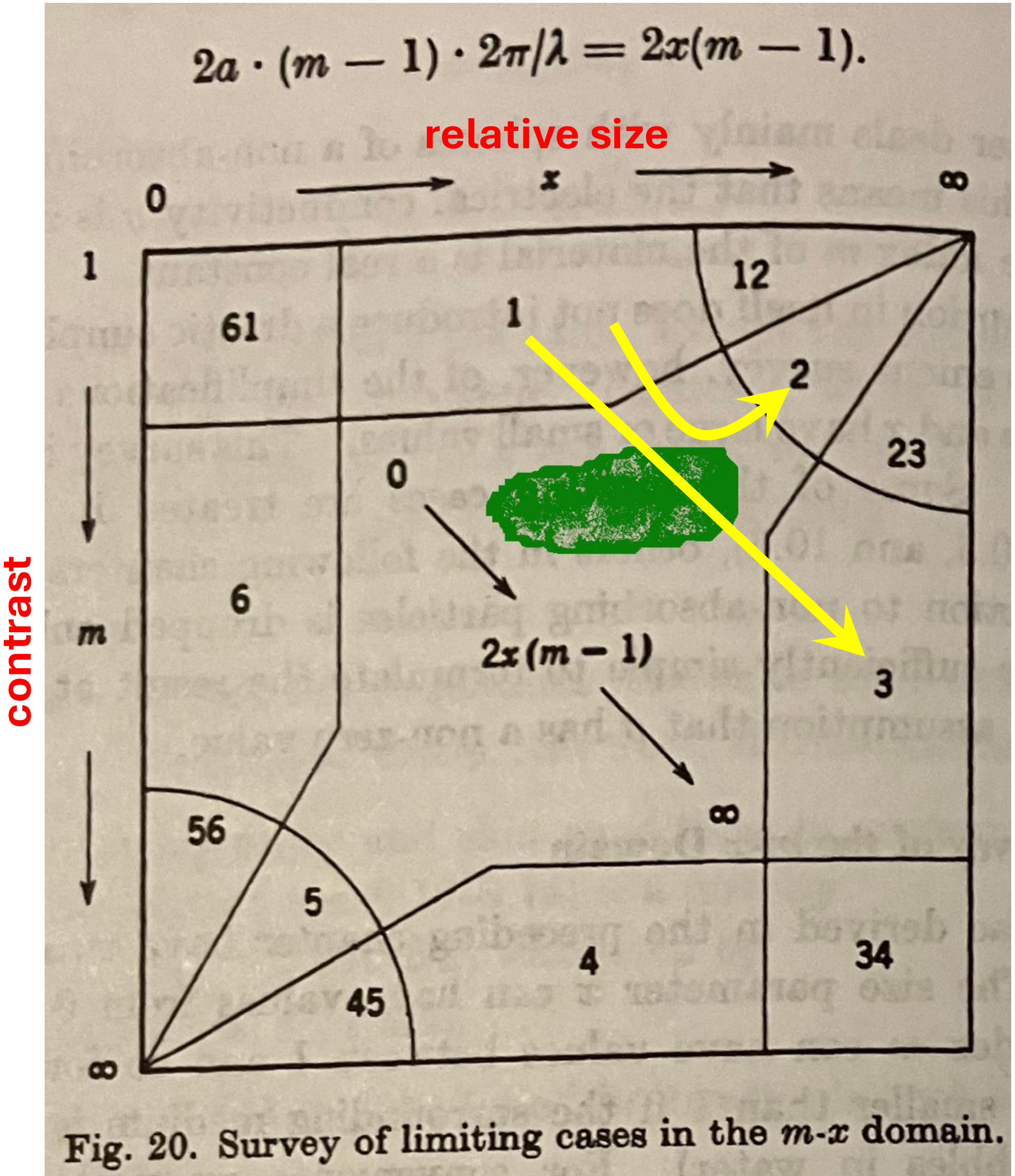
$\xi << d < t$ incoherent multiple scattering

$d < \xi$ coherent multiple scattering

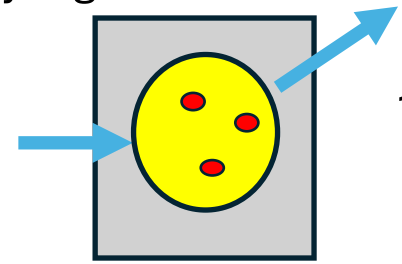
$$d = \Sigma^{-1}$$ total scattering probability

Comparison to SALS (light scattering)

H.C. van de Hulst, p. 132

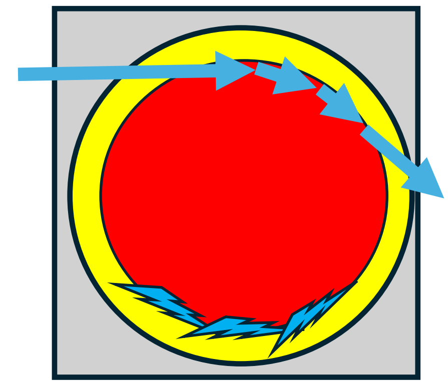


1: Rayleigh-Gans



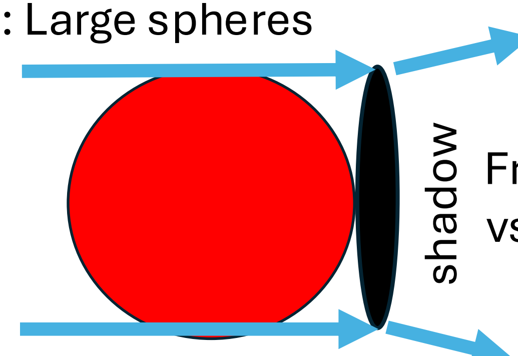
1st order Born

1 --> 3(2): No mans land



Coherent multiple scattering

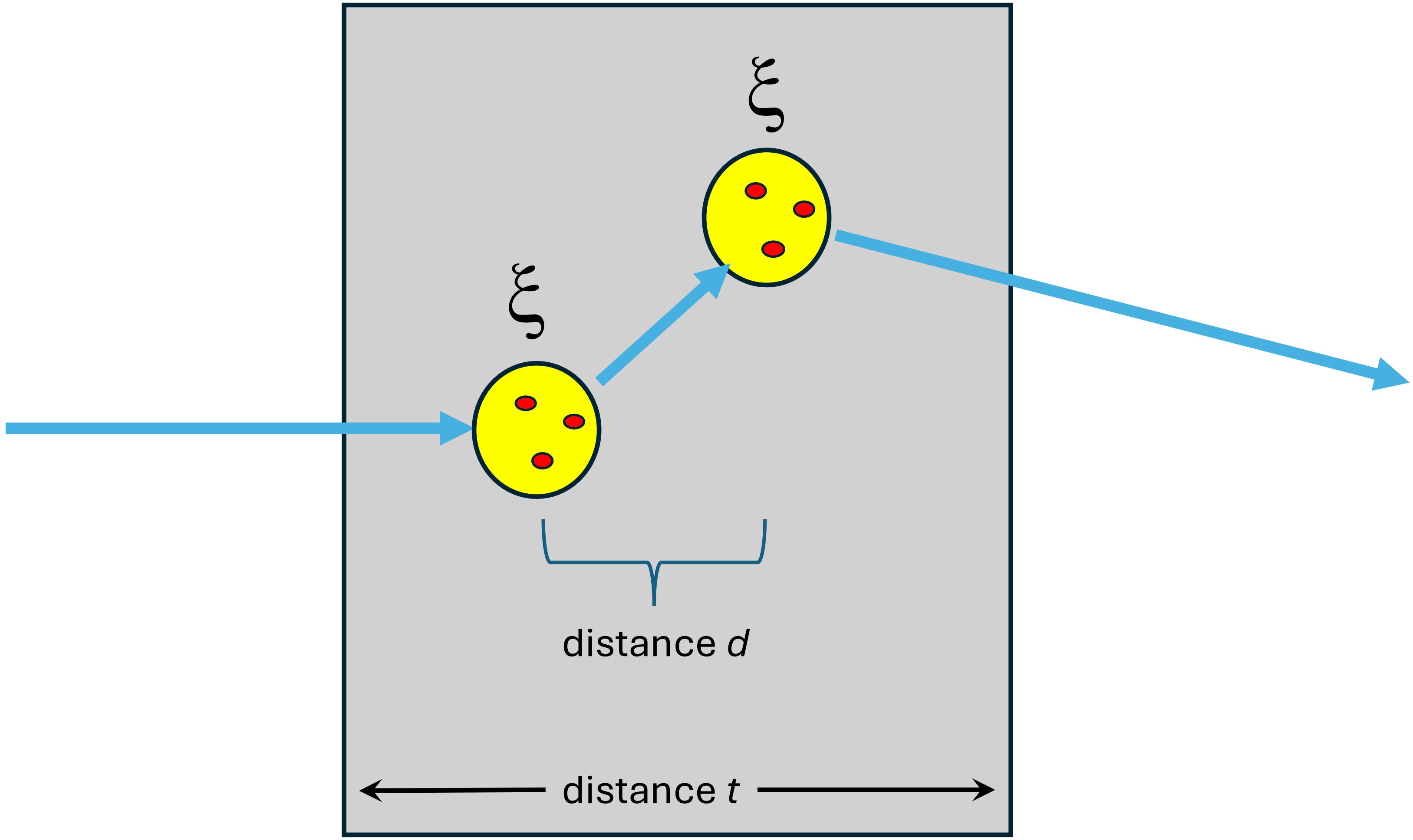
3: Large spheres



Fraunhofer vs. Fresnel

For SANS and GISANS: Focus on this case:

(incoherent multiple scattering)



Optics: continuity $\operatorname{div} \boldsymbol{j} = \nabla \cdot \boldsymbol{j} = 0$ $\boldsymbol{j} \sim I$

For the talk

$$\frac{d\Sigma_{coh}}{d\Omega}(q)$$ nano- (micro) structure

Σ_{inc} (spin-) incoherent

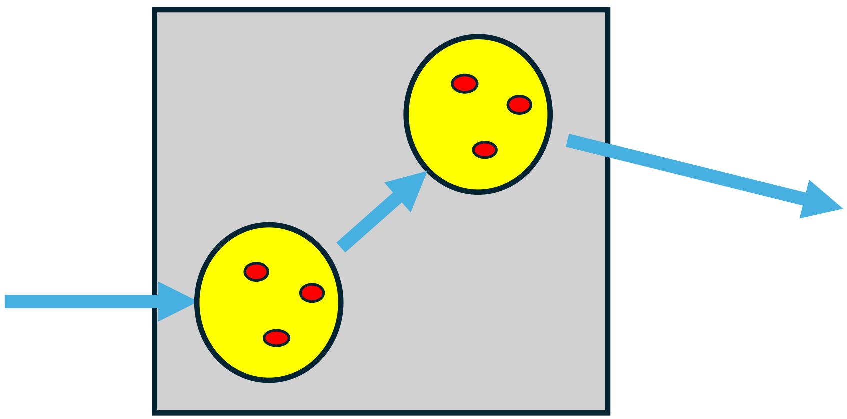
- ideal, theoretical cross sections

- small / large angles
- term incoherent

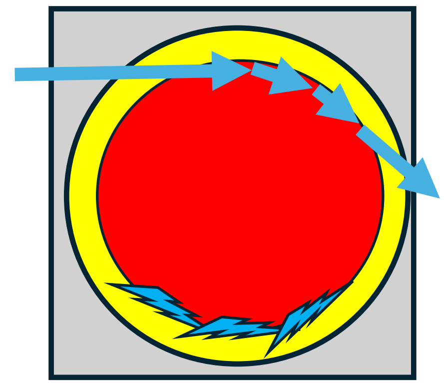
- for the treatment inc / coh needs to be distinguished !

Terminology

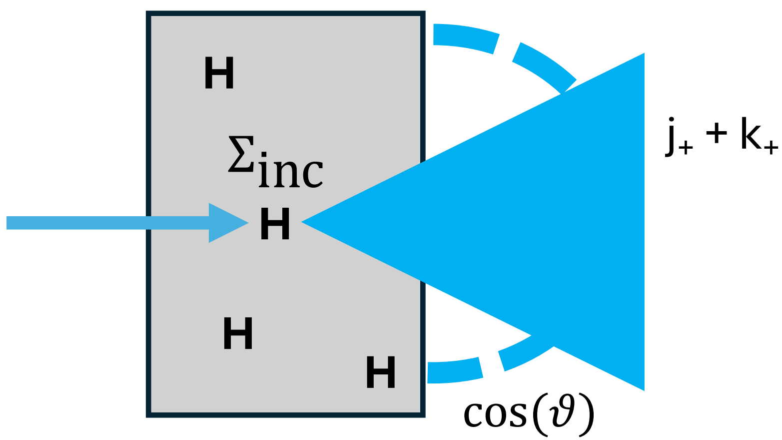
Incoherent multiple scattering



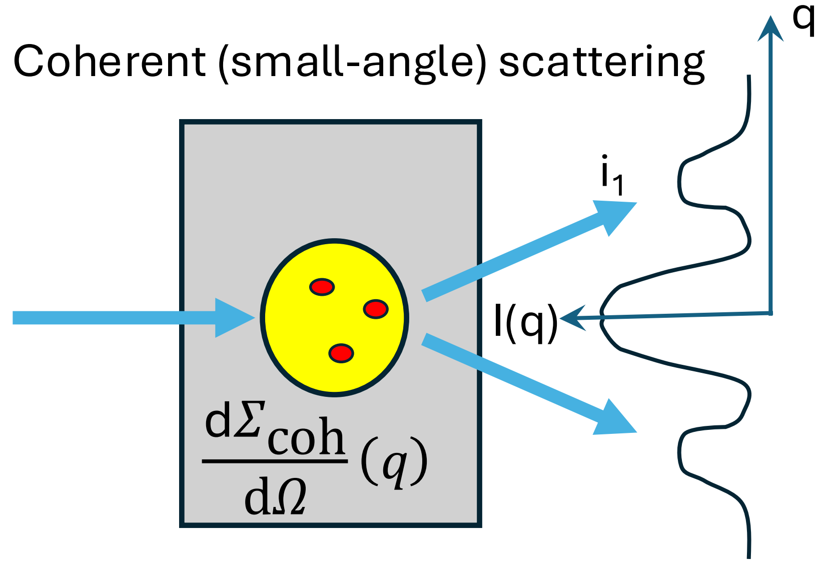
Coherent multiple scattering



Spin incoherent scattering



Coherent (small-angle) scattering



Incoherent multiple scattering

$$\frac{\partial I_0(z)}{\partial z} = -\Sigma_t I_0(z), \tag{1}$$

$$\frac{\partial i_1(z,\mathbf{Q})}{\partial z} = \frac{\mathrm{d}\Sigma_c}{\mathrm{d}\Omega}(\mathbf{Q}) I_0(z) + \int \frac{\mathrm{d}\Sigma_c}{\mathrm{d}\Omega}(\mathbf{Q}' - \mathbf{Q}) i_1(z,\mathbf{Q}')\,\mathrm{d}\Omega' - \Sigma_t i_1(z,\mathbf{Q}), \tag{2}$$

$$\frac{\partial j_+(z,\vartheta)}{\partial z} = \frac{\Sigma_i}{4\pi}\left[I_0(z) + I_1(z) + \int \frac{j_+ + j_-}{\cos\vartheta}\,\mathrm{d}\Omega\right] - \Sigma_{iia}\frac{j_+(z,\vartheta)}{\cos\vartheta}, \tag{3}$$

$$-\frac{\partial j_-(z,\vartheta)}{\partial z} = \frac{\Sigma_i}{4\pi}\left[I_0(z) + I_1(z) + \int \frac{j_+ + j_-}{\cos\vartheta}\,\mathrm{d}\Omega\right] - \Sigma_{iia}\frac{j_-(z,\vartheta)}{\cos\vartheta}, \tag{4}$$

$$\mathrm{div}\,\boldsymbol{j} = 0$$

small angles

elastic incoherent

Jaksch, S., Pipich, V., & Frielinghaus, H. (2021). Multiple scattering and resolution effects in small-angle neutron scattering experiments calculated and corrected by the software package MuScatt. Applied Crystallography, 54(6), 1580-1593.

Incoherent multiple scattering

$$\frac{\partial I_0(z)}{\partial z} = -\Sigma_t I_0(z), \quad (1)$$

$$\frac{\partial i_1(z,\mathbf{Q})}{\partial z} = \frac{d\Sigma_c}{d\Omega}(\mathbf{Q}) I_0(z) + \int \frac{d\Sigma_c}{d\Omega}(\mathbf{Q}'-\mathbf{Q}) i_1(z,\mathbf{Q}')\, d\Omega' - \Sigma_t i_1(z,\mathbf{Q}), \quad (2)$$

$$\frac{\partial j_+(z,\vartheta)}{\partial z} = \frac{\Sigma_i}{4\pi}\left[I_0(z) + I_1(z) + \int \frac{j_+ + j_-}{\cos\vartheta}\, d\Omega\right] - \Sigma_{iia}\frac{j_+(z,\vartheta)}{\cos\vartheta}, \quad (3)$$

$$-\frac{\partial j_-(z,\vartheta)}{\partial z} = \frac{\Sigma_i}{4\pi}\left[I_0(z) + I_1(z) + \int \frac{j_+ + j_-}{\cos\vartheta}\, d\Omega\right] - \Sigma_{iia}\frac{j_-(z,\vartheta)}{\cos\vartheta}, \quad (4)$$

$$\frac{\partial k_+(z,\vartheta)}{\partial z} = \frac{\Sigma_{ii}}{4\pi}\left[I_0(z) + I_1(z) + \int \frac{j_+ + j_-}{\cos\vartheta}\, d\Omega\right] + \frac{\Sigma_{i2}}{4\pi}\int \frac{k_+ + k_-}{\cos\vartheta}\, d\Omega - \Sigma_{ia2}\frac{k_+(z,\vartheta)}{\cos\vartheta}, \quad (5)$$

$$-\frac{\partial k_-(z,\vartheta)}{\partial z} = \frac{\Sigma_{ii}}{4\pi}\left[I_0(z) + I_1(z) + \int \frac{j_+ + j_-}{\cos\vartheta}\, d\Omega\right] + \frac{\Sigma_{i2}}{4\pi}\int \frac{k_+ + k_-}{\cos\vartheta}\, d\Omega - \Sigma_{ia2}\frac{k_-(z,\vartheta)}{\cos\vartheta}, \quad (6)$$

with

$$\Sigma_t = \Sigma_c + \Sigma_i + \Sigma_{ii} + \Sigma_a, \quad \Sigma_{iia} = \Sigma_i + \Sigma_{ii} + \Sigma_a \quad (7)$$

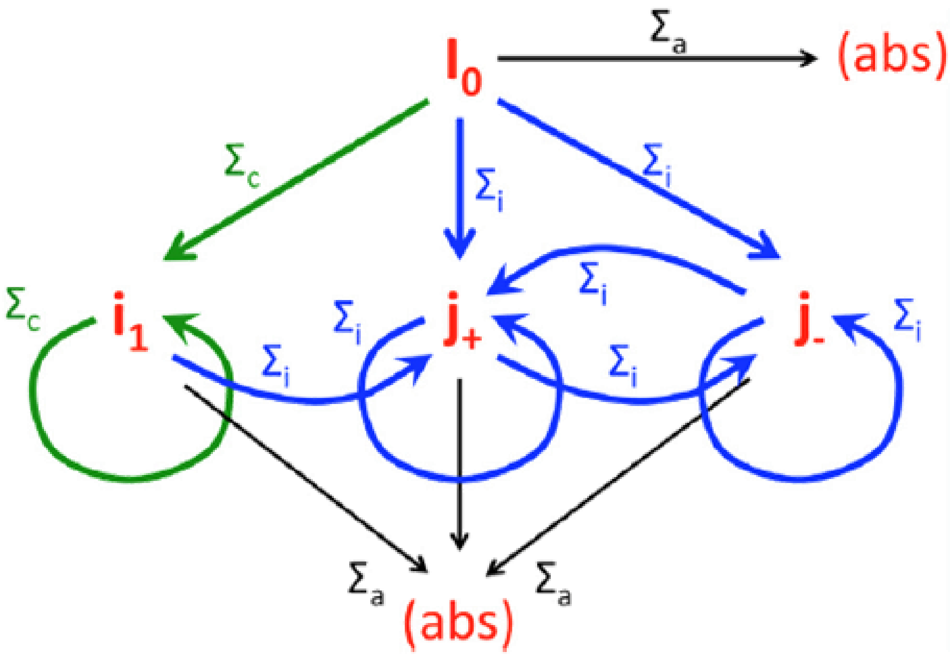
and

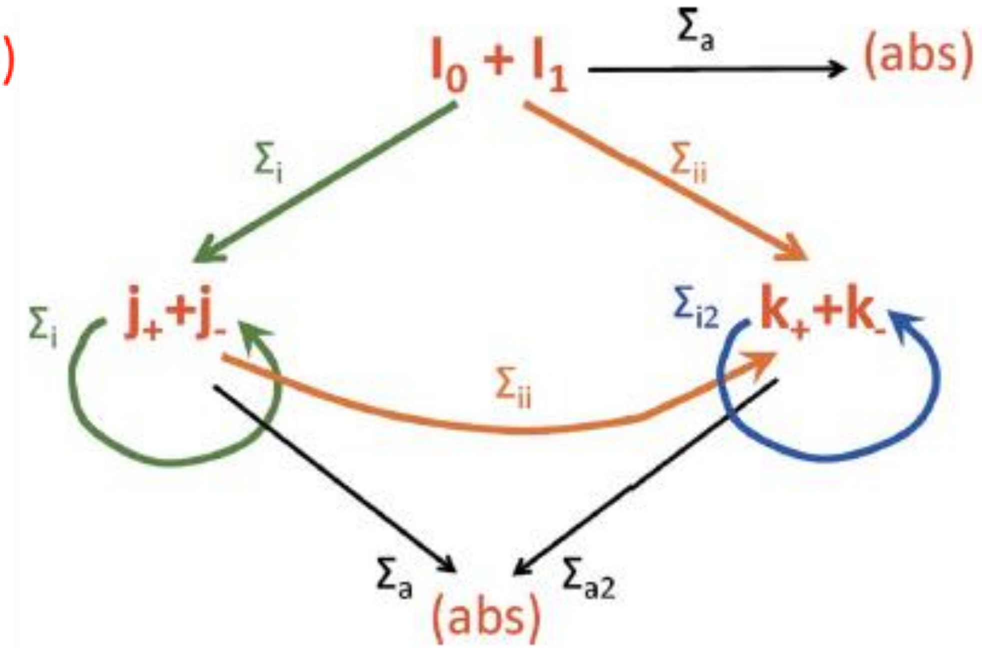
$$\Sigma_{ia2} = \Sigma_{i2} + \Sigma_{a2}, \quad \Sigma_{i2} = \Sigma_i, \quad \Sigma_{a2} = \Sigma_a \lambda_2/\lambda. \quad (8)$$

k_+, k_- inelastic incoherent, vibrations

Arbe, A., Nilsen, G. J., Stewart, J. R., Alvarez, F., Sakai, V. G., & Colmenero, J. (2020). Coherent structural relaxation of water from meso-to intermolecular scales measured using neutron spectroscopy with polarization analysis. Physical Review Research, 2(2), 022015.

The scattering cross sections





Frielinghaus, H. (2018). Strategies for removing multiple scattering effects revisited. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 904, 9-14.

Solutions for SANS

Coherent signal: Schmatz & Schelten

Elastic incoherent: Chandrasekhar

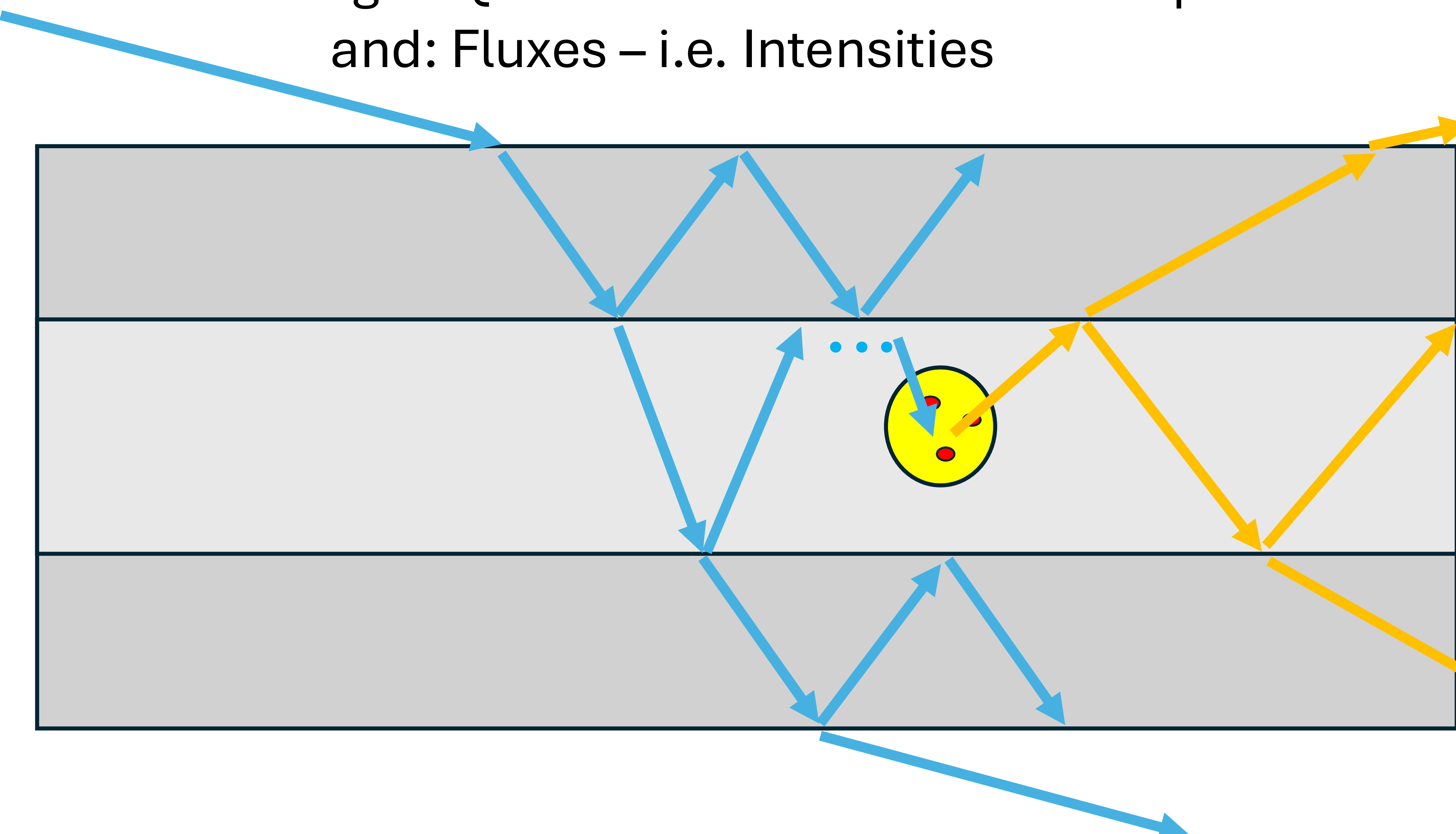
Inelastic incoherent: modified Chandrasekhar (approx.)

MuScatt package can calculate this for SANS

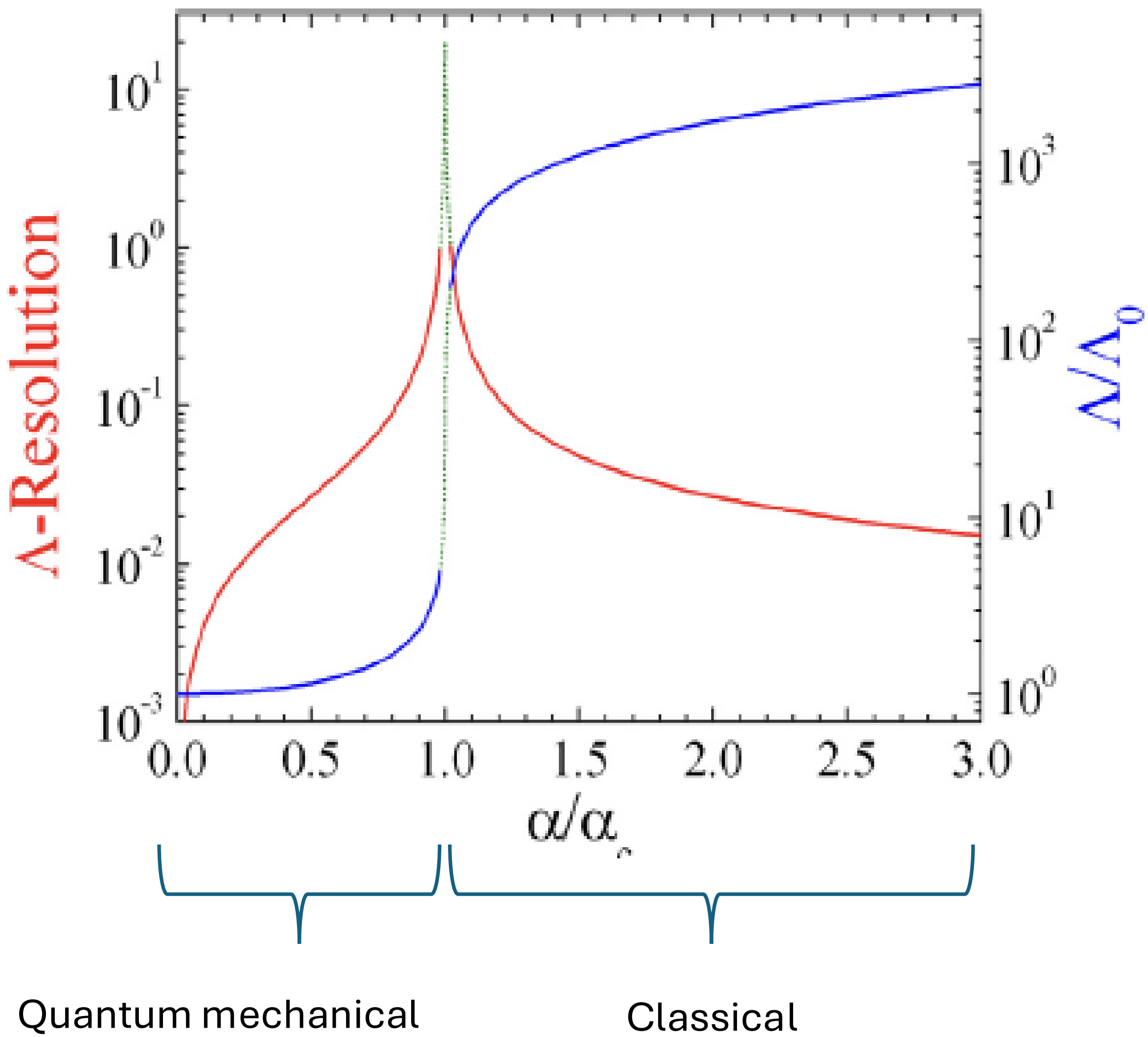
Can also be simulated by McStas

Simulations for GISANS

Disentangle: Quantum Mechanics - i.e. Amplitudes
and: Fluxes – i.e. Intensities



Simulations for GISANS



Simulations for GISANS

- So far: Collective scattering from all layers in whole (single scattering – compares to BornAgain)

- To do: Put single scattering events in sample
  Disentangle: amplitudes and intensities
  About to be done – requires also testing

  Expected: Blurring of signal for long wavelengths

- Currently not forseen: inelastic incoherent – can be done, but requires another level of testing.

Summary

- There are different levels of multiple scattering
- In SANS the cases are clearly described and resolved
- In GISANS this is new.
  Difficulty: disentangle amplitudes and intensities
- Inelastic incoherent surely remains for future

THANK YOU FOR YOUR ATTENTION !