The Resolution Function Problem for TOF-GISANS

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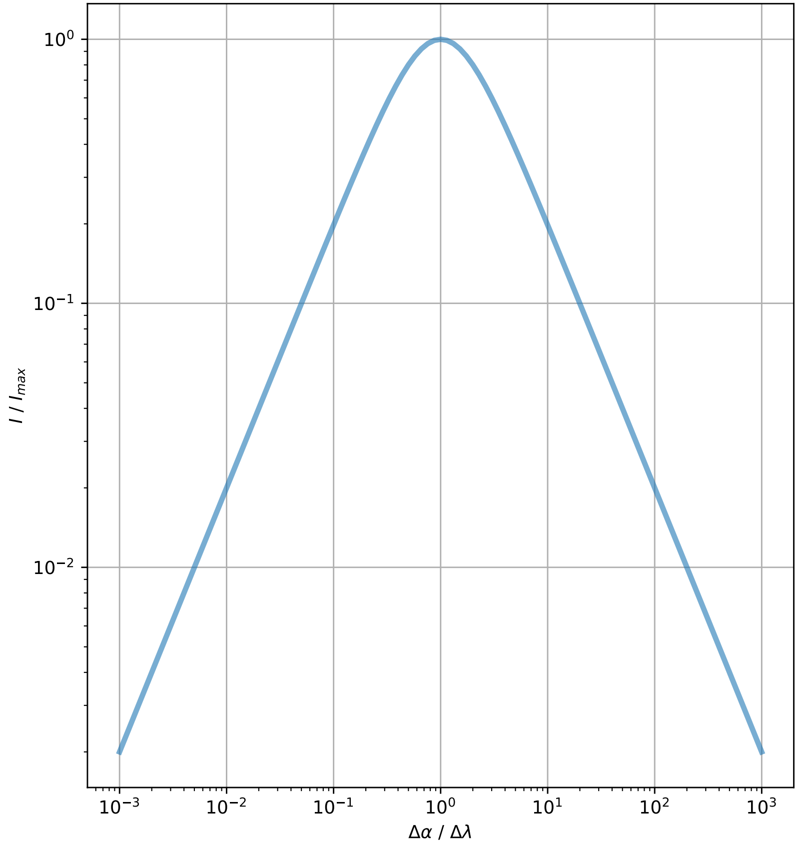
Overview

- Reflectometry : Q_z
- GISANS : Q_y
- Depth resolution ?
- Implementation

Resolution function for specular reflectometry

$$\frac{\Delta Q_z}{Q_z} = \sqrt{\left(\frac{\Delta \alpha_i}{\alpha_i}\right)^2 + \left(\frac{\Delta \lambda}{\lambda}\right)^2}$$

$$I \propto \Delta \alpha_i \, \Delta \lambda$$



Maximized intensity when:

$$\frac{\Delta \alpha_i}{\alpha_i} = \frac{\Delta \lambda}{\lambda}$$

- at 0.5°, with $10m$ collimation and 10% $\Delta\theta$, footprint = 1000 mm
  $\Rightarrow$ Reflectometry is **divergence starved**
  $\Rightarrow$ "we wish to overilluminate !" (bad idea)

For GISANS

$$I \propto \Delta\alpha_i \; \Delta\Psi_i \; \Delta\lambda$$

$$\left(\frac{\Delta Q_z}{Q_z}\right)^2 = \frac{(\Delta\alpha_i)^2 + (\Delta\alpha_f)^2}{(\alpha_i + \alpha_f)^2} + \left(\frac{\Delta\lambda}{\lambda}\right)^2$$

$$\left(\frac{\Delta Q_y}{Q_y}\right)^2 = \frac{(\Delta\psi_i)^2 + (\Delta\psi_f)^2}{(\psi_i - \psi_f)^2} + \left(\frac{\Delta\lambda}{\lambda}\right)^2$$

Close to in-plane forward scattering $\Delta Q_y / Q_y$ diverges, but ΔQ_y is finite:

$$(\Delta Q_y)^2 = k^2[(\Delta\Psi_i)^2 \; + \; (\Delta\Psi_f)^2] + \left(\frac{Q_y \Delta\lambda}{\lambda}\right)^2$$

which becomes function of only the divergence at very low Q_y

Divergence starvation?

- Vertically just as bad as reflectometry :
  - sample acts like a virtual slit
  - optimal divergence not reachable
- Horizontally, not as bad as Vertically:
  - footprint effect much less severe

Long tails of the distribution functions of $(\alpha_i, \Psi_i, \lambda)$ are important:

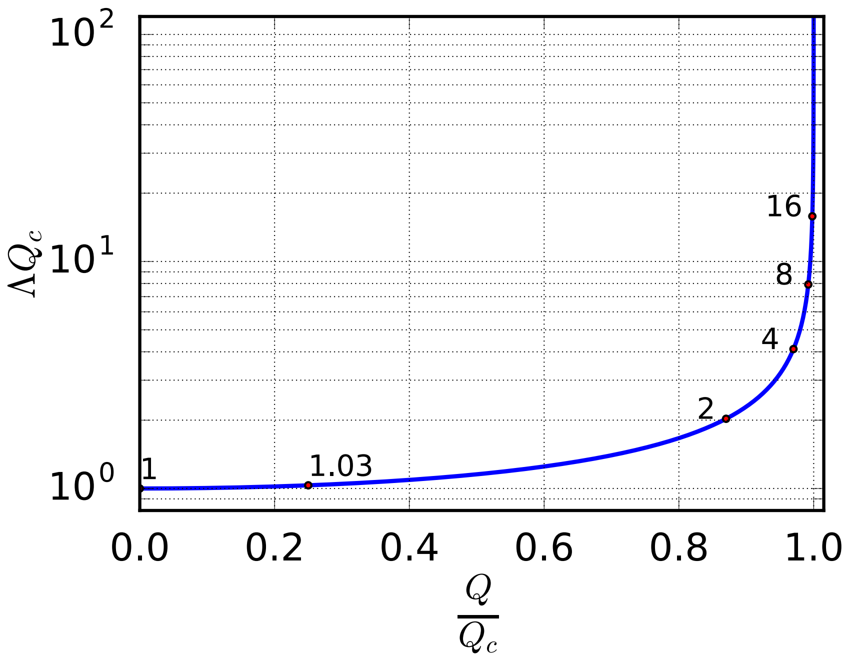
Penetration depth catastrophy:

$\Lambda|_{\alpha_c} \rightarrow \infty$: tails kill the depth-sensitivity

Coupling to DWBA intensity:

$$\left(\frac{d\sigma}{d\Omega}\right) \propto |T(\alpha_i)|^2 \;.\; |S(Q_y, Q_z)|^2 \;.\; |T(\alpha_f)|^2$$

$\left.\frac{d|T|^2}{d\alpha}\right|_{\alpha_c} \rightarrow \infty$: tails smear the Yoneda enhancement

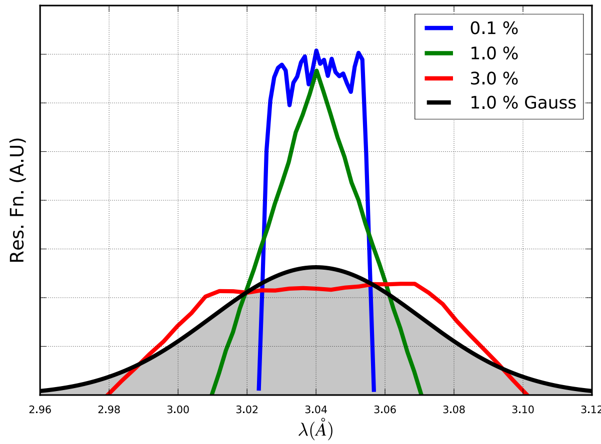


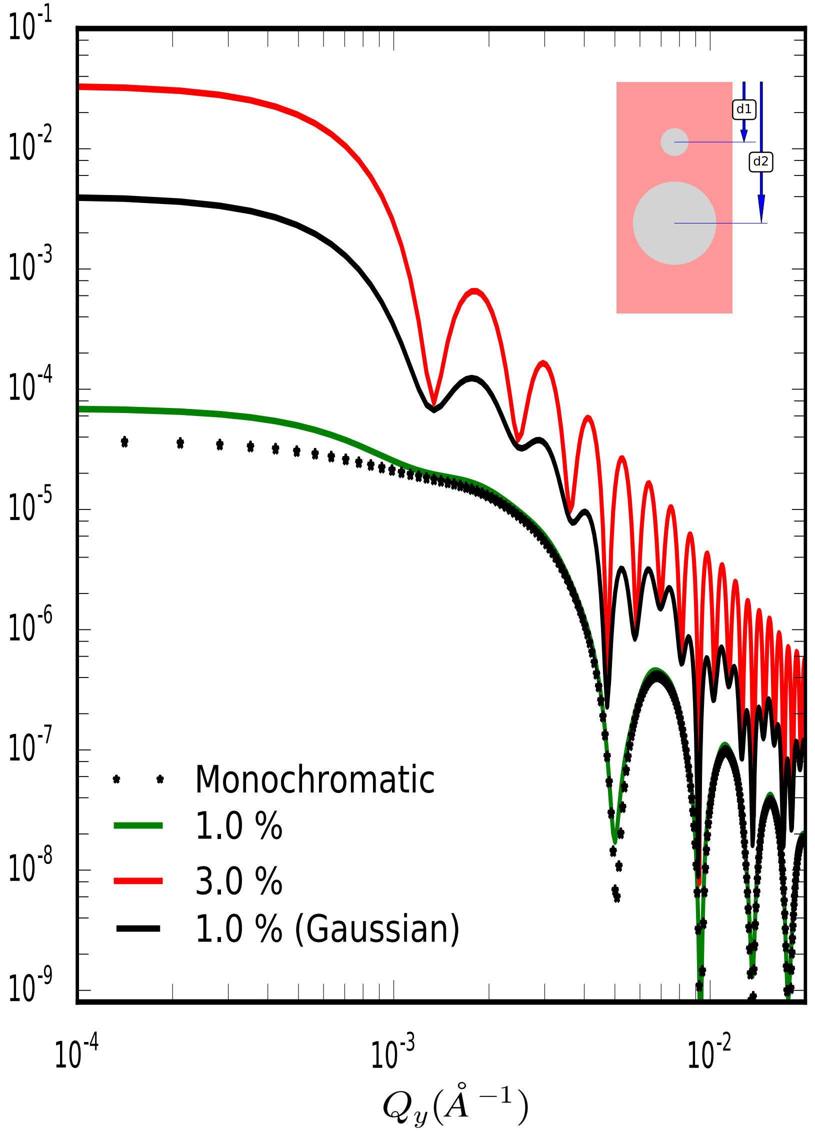
What are the Constraints?

- Vertically very strong! We need to to resolve angle *wrt* α_c!
- Horizontally often less stringent (except at very lowest Q_y)

Some practical consequence:

- TOF binning shapes $\Delta\lambda(\lambda)$ (exple for 1% chopper)
- Gaussian should not be *assumed*





- For TOF: gravitation effect is important
  - $\alpha_i = \alpha_i(\lambda)$
  - $\Delta\lambda$ creates additional divergence
  - footprint / overillumination strongly affected: might truncate your divergence *tails*
- Path length differences couple divergence with wavelength: significant when highest λ resolution is desired
  - At ~5° scatt angle, the sample to pixel distance has to replace SDD for 1% TOF resolution.
  - Chopping time, moderator geometry become relevant.
- For large samples, uniformity becomes a (more) serious issue
- The optimal Intensity/Resolution tradeoff is not straightforward
- Simulations need higher resolution where $I_0(\lambda)$ varies strongly, do not assume your bins are filled uniformly

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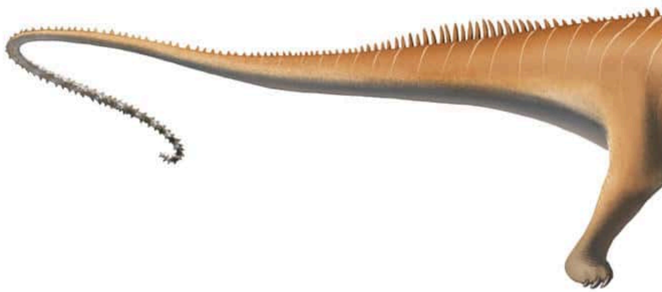
tails...



Implementation of the Resolution Function

Analytical models are not good enough / convenient here:

$\Rightarrow$ MC sampling over fine $(\alpha_i, \Psi_i, \lambda)$ grid

Either:

- Very good *McStas* model (but, is "good enough" achievable?)

Or:

- Actual high resolution beam diagnostics (*TimePix* camera!)
- *TimePix* from various configurations can be used to train a ML model of the instrument
- Cheap validity check with "standard" samples ($Si, Ti/Ni$ nanostructures) can then be used to infer $\Delta Q/Q$ without new *TimePix* acquisition

Implication for fitting

BornAgain simulation is the bottleneck:

direct evaluation of all the MC simulated rays not practical (ms to s per incident neutron)
$\Rightarrow$ Lookup table for $\frac{d\sigma}{d\Omega}(\alpha_f, \Psi_f | \alpha_i, \Psi_i, \lambda)$

- 1 sample structure needs typ. 125000 pixels from *BornAgain*
- $50_\lambda \times 50_\alpha \times 50_\Psi \times 200_{xpix} \times 200_{ypix} = 5 \times 10^9 floats \approx 20GB$ at float32

$\Rightarrow$ mitigation?

- sparser lookup along ψ_i (slower variation of the cross section, no nasty effects as for α_i)
- Fit over a sparse grid of cuts first (multiple coupled 1D fits)
- Complement the lookup with a surrogate model (neural network or Gaussian process)... it needs to be built...

Questions ?