Jülich Centre for Neutron Science

Heinz Maier-Leibnitz Zentrum

MSCA3

Multiple scattering simulation

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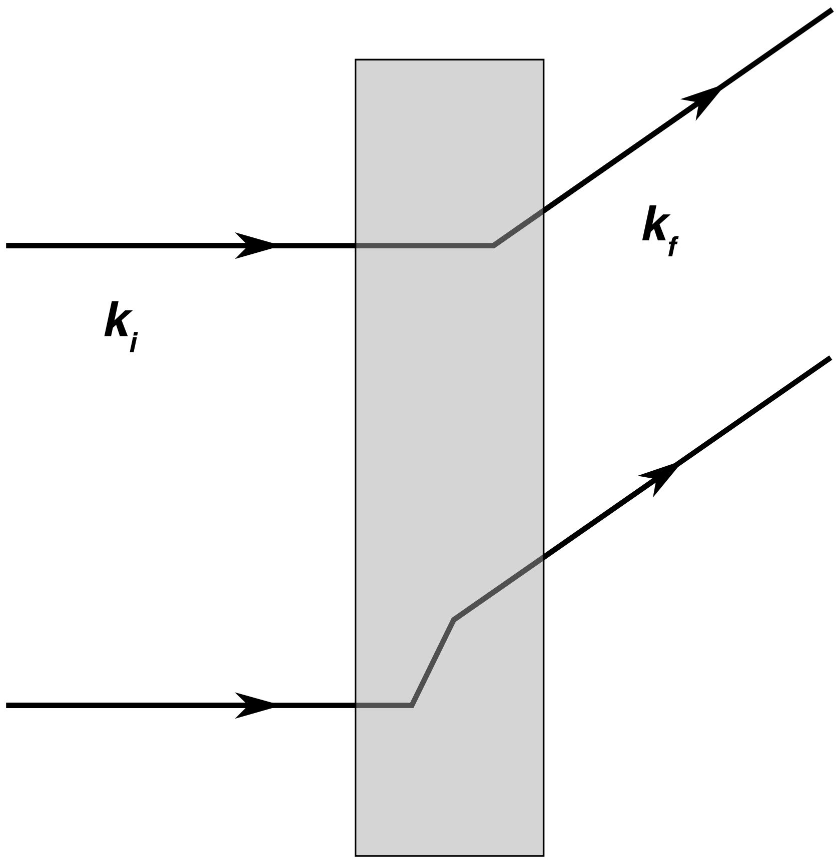
Multiple scattering

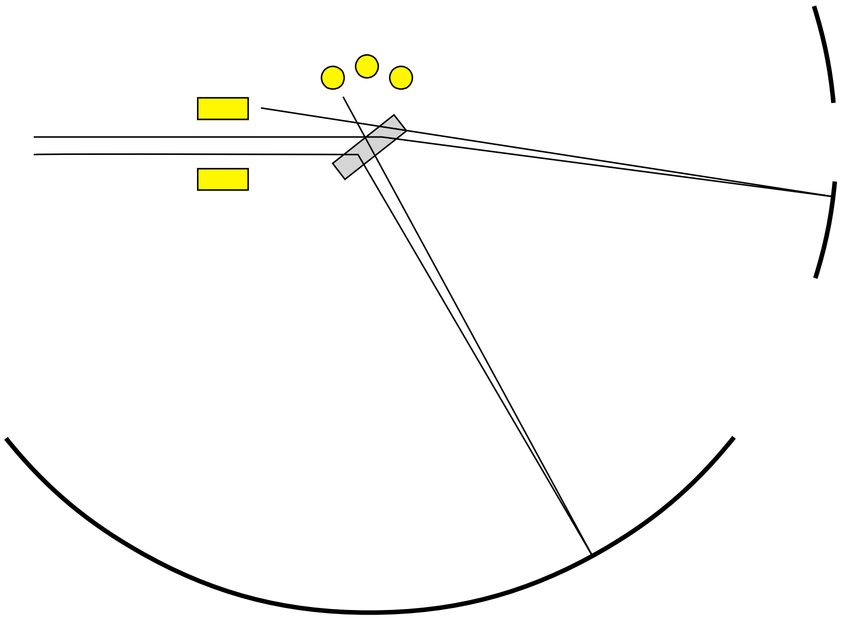


~90% transmission:
~10% single scattering
~1% multiple scattering

Available multiple scattering simulators

- MSCAT by Copley (1974), based on MSC by Bischoff (1970)
- DISCUS by Johnson (1974)
- SPEC_SIM by Blasdell et al. (1998)
- DINSMS by Mayers et al. (2002)

MSCA3 – Monte Carlo multiple scattering for backscattering instruments



MSCA3 design details

- C++
- OpenMP for parallel processing
- YAML for config file parsing
- Histogram lookup using the alias method (O(1) vs. binary search's O(log n))

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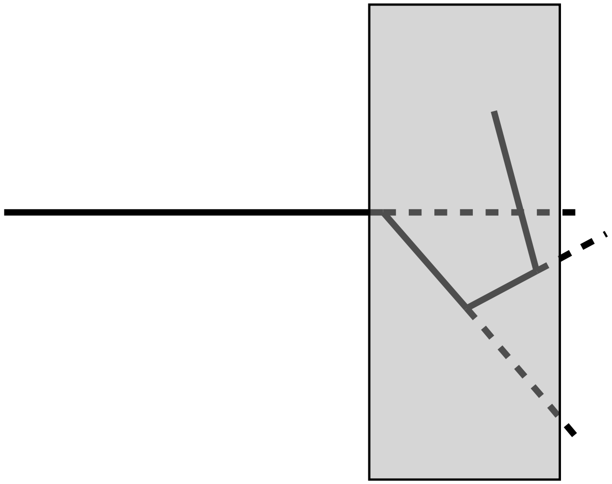
Basic simulation loop

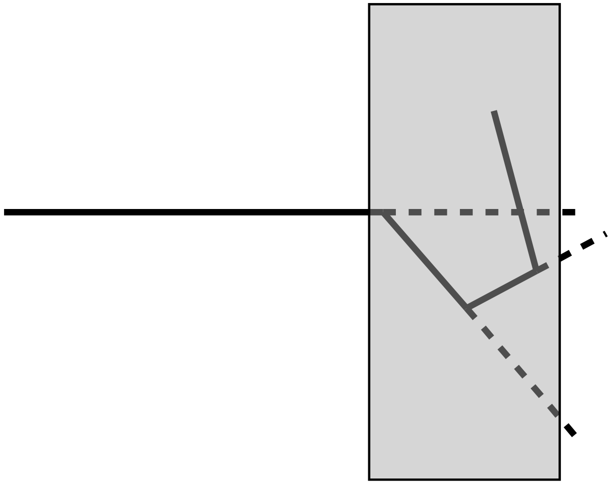
- Generate neutron
- Scattering loop:
  - Draw interaction point
  - Score detectors
  - Draw new direction, energy
  - Russian roulette (continue loop or break)



Mitglied der Helmholtz-Gemeinschaft

Forced scattering – every neutron counts

Transmission probability: $t = e^{-\mu d}$



Probability that interaction takes place at *d* if it takes place at all:

$$p_l = \frac{1 - t(d)}{1 - t(D)}$$

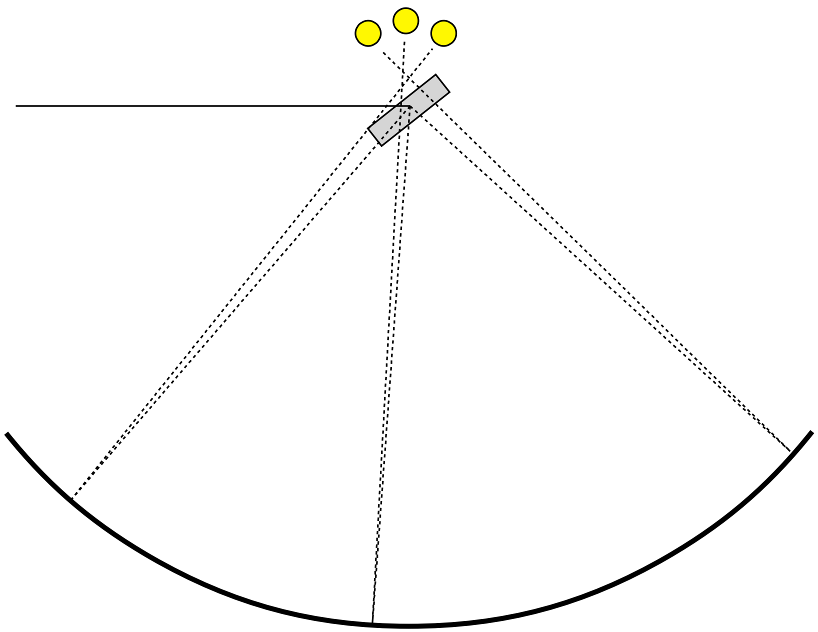
Compensate by multiplying neutron weight *w* by 1-*t* (*d*)

Scoring

For each detector draw random impact point on analyzer and for each energy channel calculate:

- Scattering probability *s*
- Transmission probability *t*

Increment channel by *wst*



Scattering probability

$$s = \frac{\sigma_{bound}}{\sigma_{total}} \frac{k_f}{k_i} \frac{\Delta\Omega}{4\pi} \Delta\omega_i S(q,\omega)$$

Scattering law S supplied by user.
Simplification due to $\omega << E_i$: $k_f \approx k_i$

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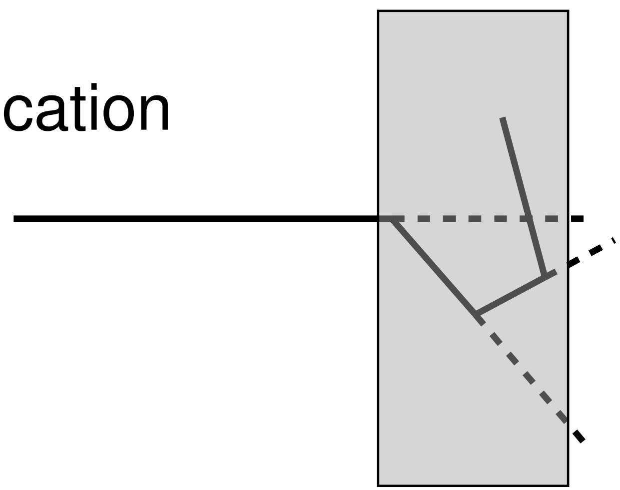
Drawing new energy

$$F(q,\omega)=\int_0^q dq'\,q'\,S(q',\omega)$$

Marginal ω distribution with simplification due to ω << E_i: $k_f = k_i$:

$$\frac{\int_{-\infty}^{\omega} d\omega'\,F(2k_i,\omega')}{\int_{-\infty}^{E_i} d\omega'\,F(2k_i,\omega')}=\xi$$



Drawing scattering angle

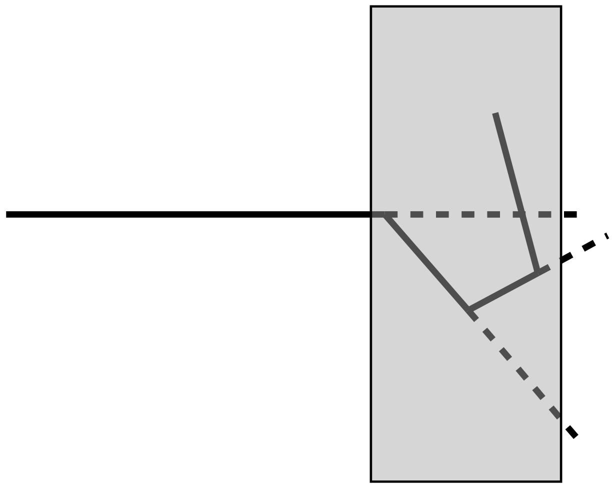
$$F(q,\omega)=\int_0^q dq'\,q'\,S(q',\omega)$$

Marginal *q* distribution

$$\frac{F(q,\omega)}{F(2k_i,\omega)}=\xi$$

$$q^2=k_i^2+k_f^2-2k_ik_f\cos(\theta)\approx k_i^2\sin\left(\frac{\theta}{2}\right)$$

$$\phi=2\pi\xi$$

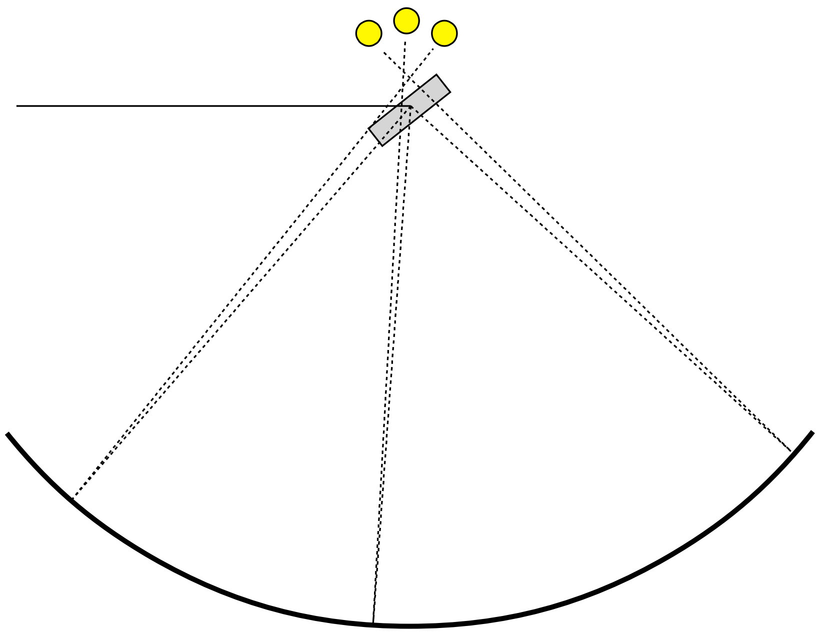


Russian roulette

If neutron weight *w* is less than a set value, there is a probability of p_{finish_him} that the scattering loop will be broken

If neutron survives, *w* is compensated by p_{finish_him}

Second passage of neutrons

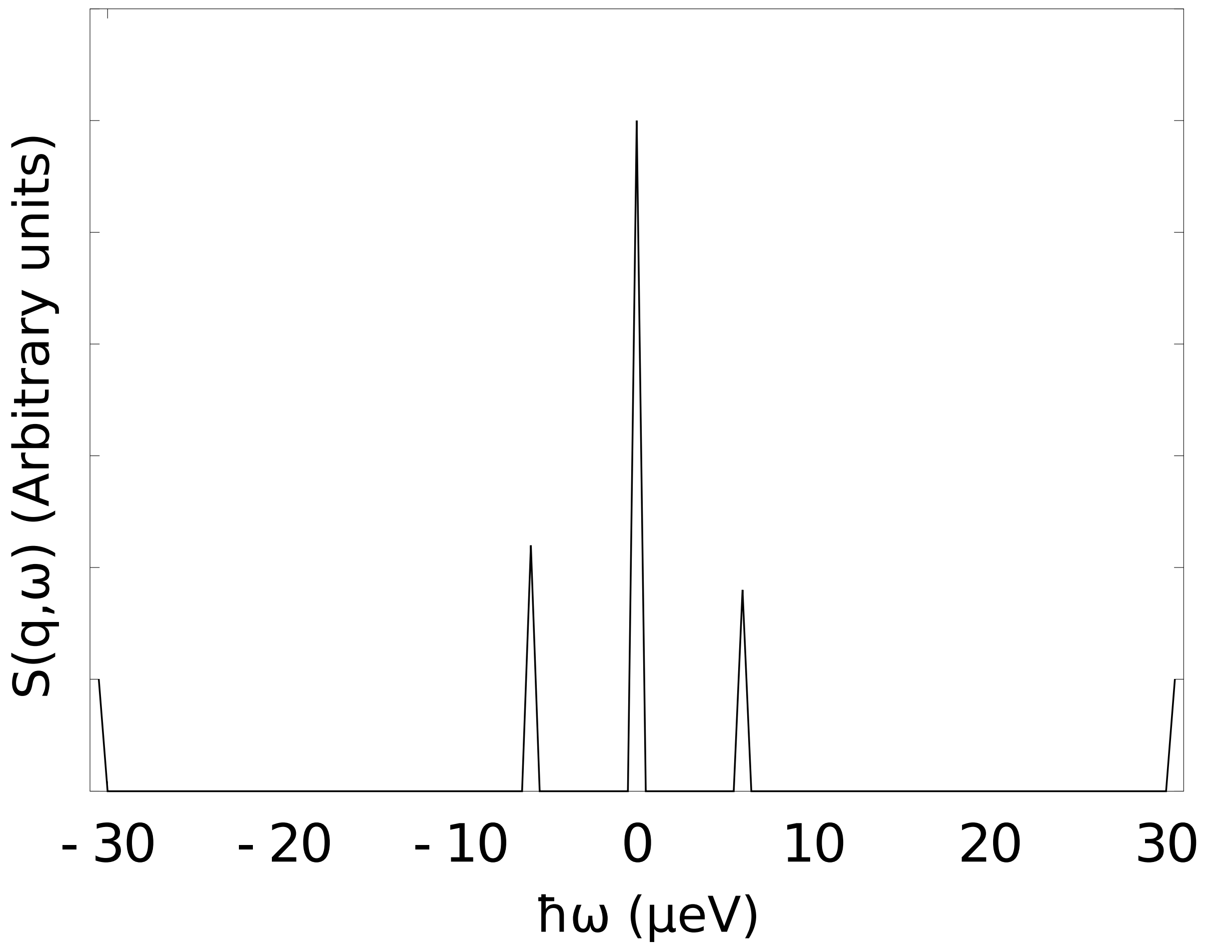


Randomly force neutrons to undergo second passage scattering

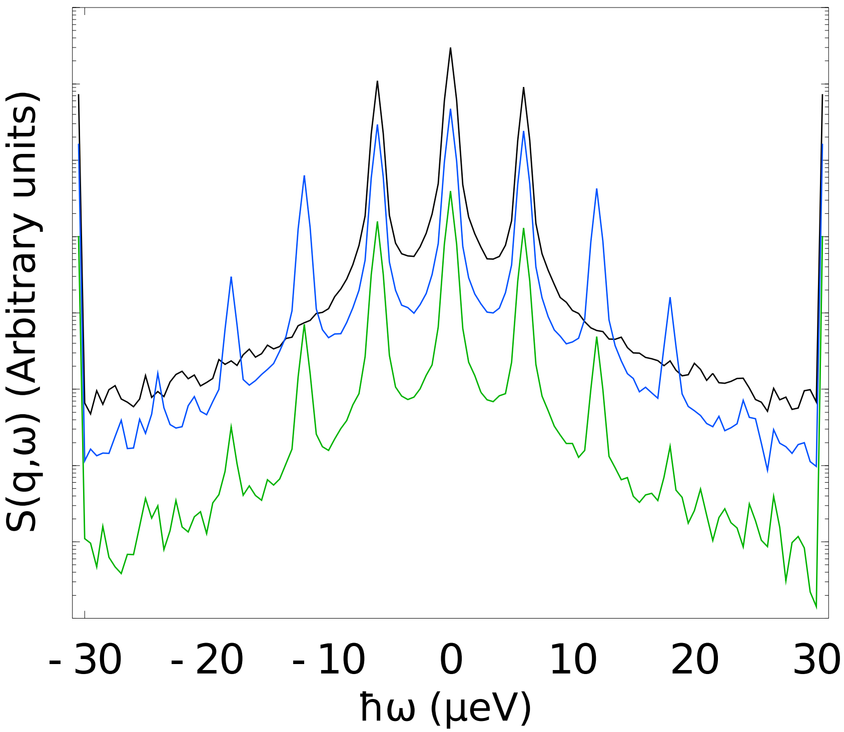
Second passage simulation

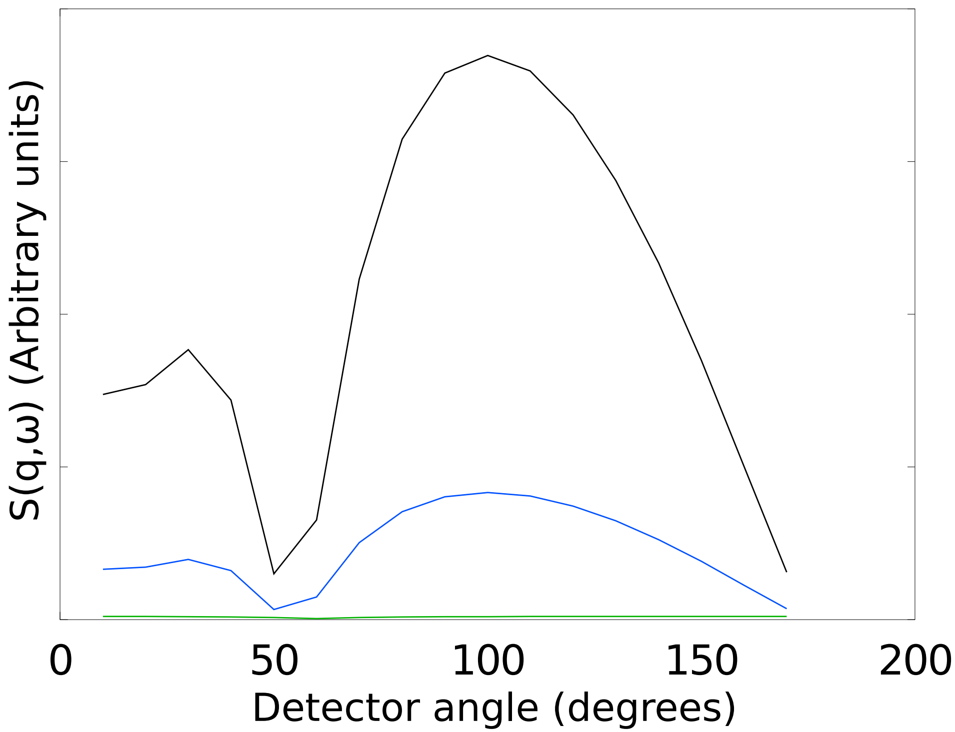
- Draw random reflection point on analyzer
- „Freeze neutron energy“; record scattering probabilities to different energy channels
- Scatter directly to detectors

Example: simple tunneling model

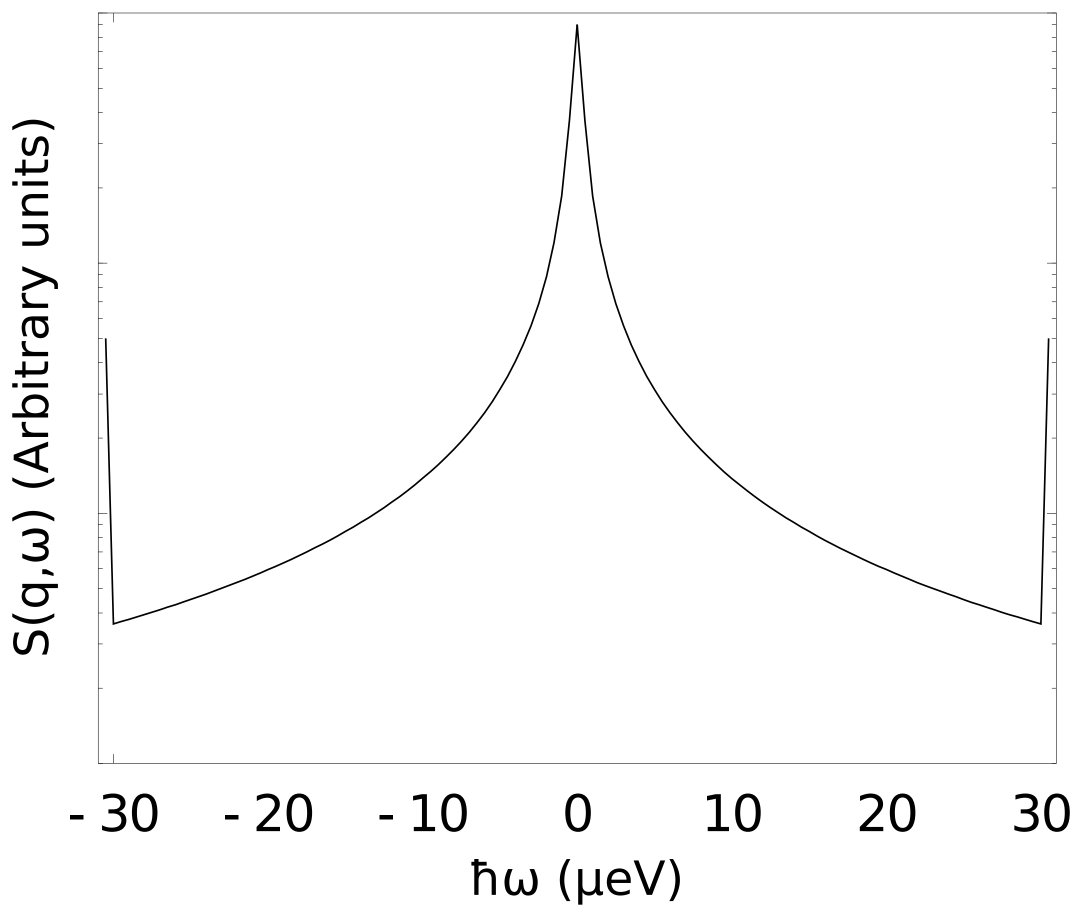


Tunneling model simulation

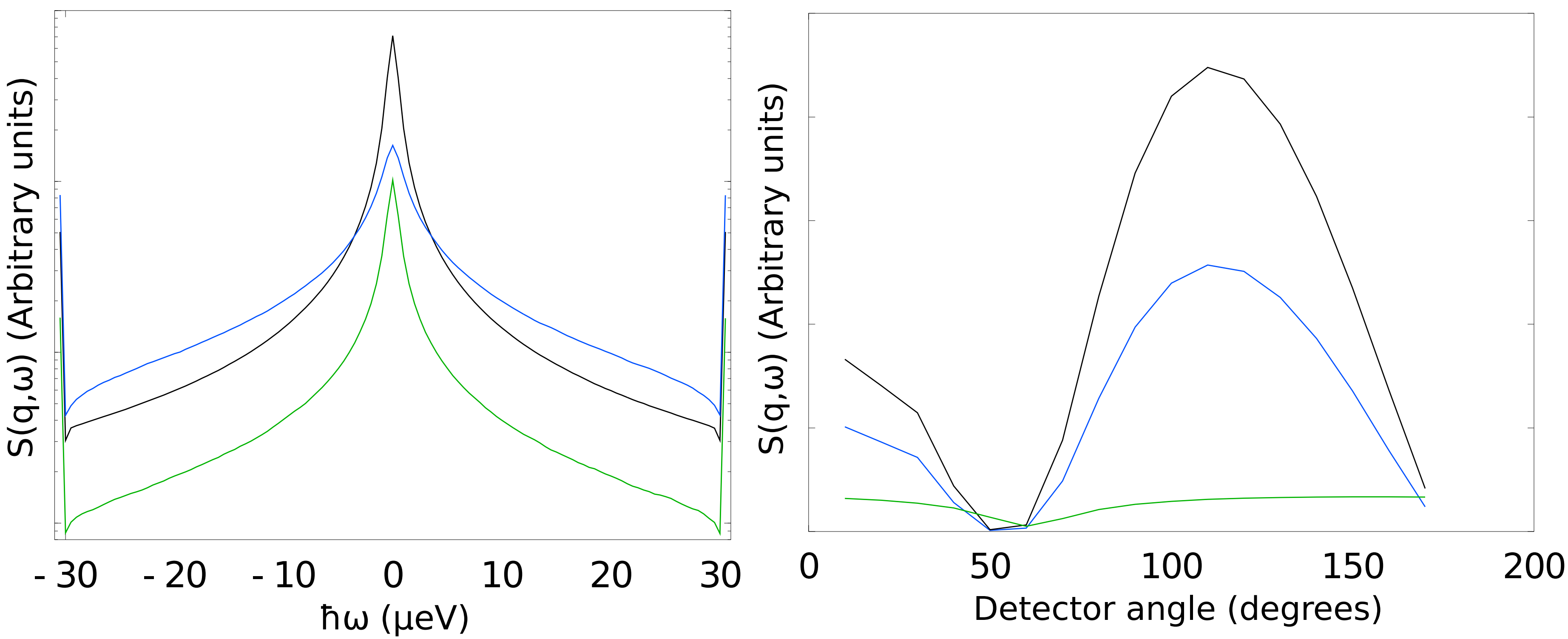




Example 2: Kohlrausch model



Kohlrausch simulation



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MSCA3 future development

- Finalize backscattering simulation
- Apply to real-world problems
- Publish
- Extend code for time-of-flight instruments

Conclusions

- MSCA3 – a multiple scattering simulation for backscattering instruments
- Work-in-progress
- Simulates both multiple scattering and second pass scattering