

Samples: Isotropic $S(q,\omega)$

E. Farhi, ILL

Isotropic density samples: liquids, gases, powders, amorphous

- Scattering law, a bit of theory
- How to get $S(q,w)$ data sets
- Exercise: a liquid TOF spectrometer
- Exercise: separate contributions



Disclaimer: in case of errors and uncertainties, please correct me...

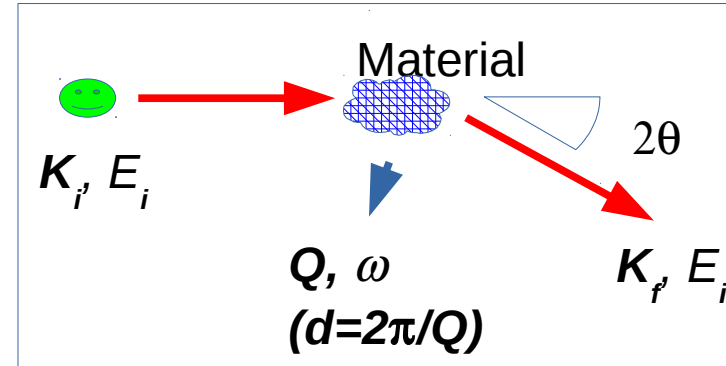


Neutron-matter interaction

Selections rules

$$K_f = K_i + Q$$

$$E_f = E_i + \omega$$



Bragg's law (diffraction on structure – atoms separated by distance d)

$$n\lambda = 2\pi / K_i = 2d \sin \theta$$

Scattering law (intensity per solid angle and energy, dynamics)

$$\frac{d^2 \sigma}{d\Omega dE_f} = \frac{\sigma}{4\pi} \frac{K_f}{K_i} S(Q, \omega)$$

Dynamical structure factor $S(Q, \omega)$ is characteristic of each material
 Reflects ordering of matter (atom/molecule positions – movements - domains)



Scattering law

The double differential scattering cross section gives the probability for a neutron to scatter for a given solid angle and energy

Neutronist's Mantra
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma}{4\pi} \frac{k_f}{k_i} NS(q, \omega)$$
 Holy Book (Squires)

The total intensity is the full integral over all scattering possibilities.

Effective total scattering cross section
$$\hat{\sigma} = \iint \frac{d^2\sigma}{d\Omega dE_f} d\Omega dE_f$$
 V.F. Sears. Adv. Phys., 24, 1, 1975.



Computing the total scattering probability

The total scattering cross section is given in (Ω, E_f) space, but S is given in (q, ω)
A variable change must be done for the integration (Jacobian).

We like to play games
in (q, ω) space

$$\frac{d\Omega}{d\theta} = -2\pi \sin\theta$$
$$\frac{dq}{d\theta} = -\frac{k_i k_f \sin\theta}{q}$$

Effective cross section
in (q, ω) space

$$\hat{\sigma} = \sigma \iint \frac{S(q, \omega) q}{2k_i^2} dq d\omega$$

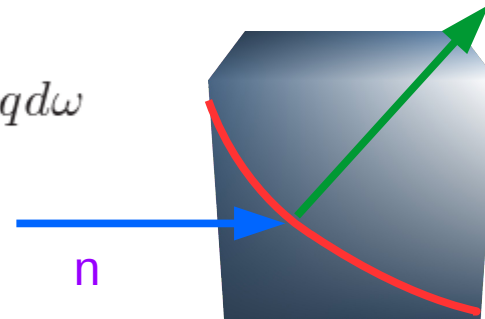
Probability to transmit

$$p = e^{-\rho \hat{\sigma} x}$$

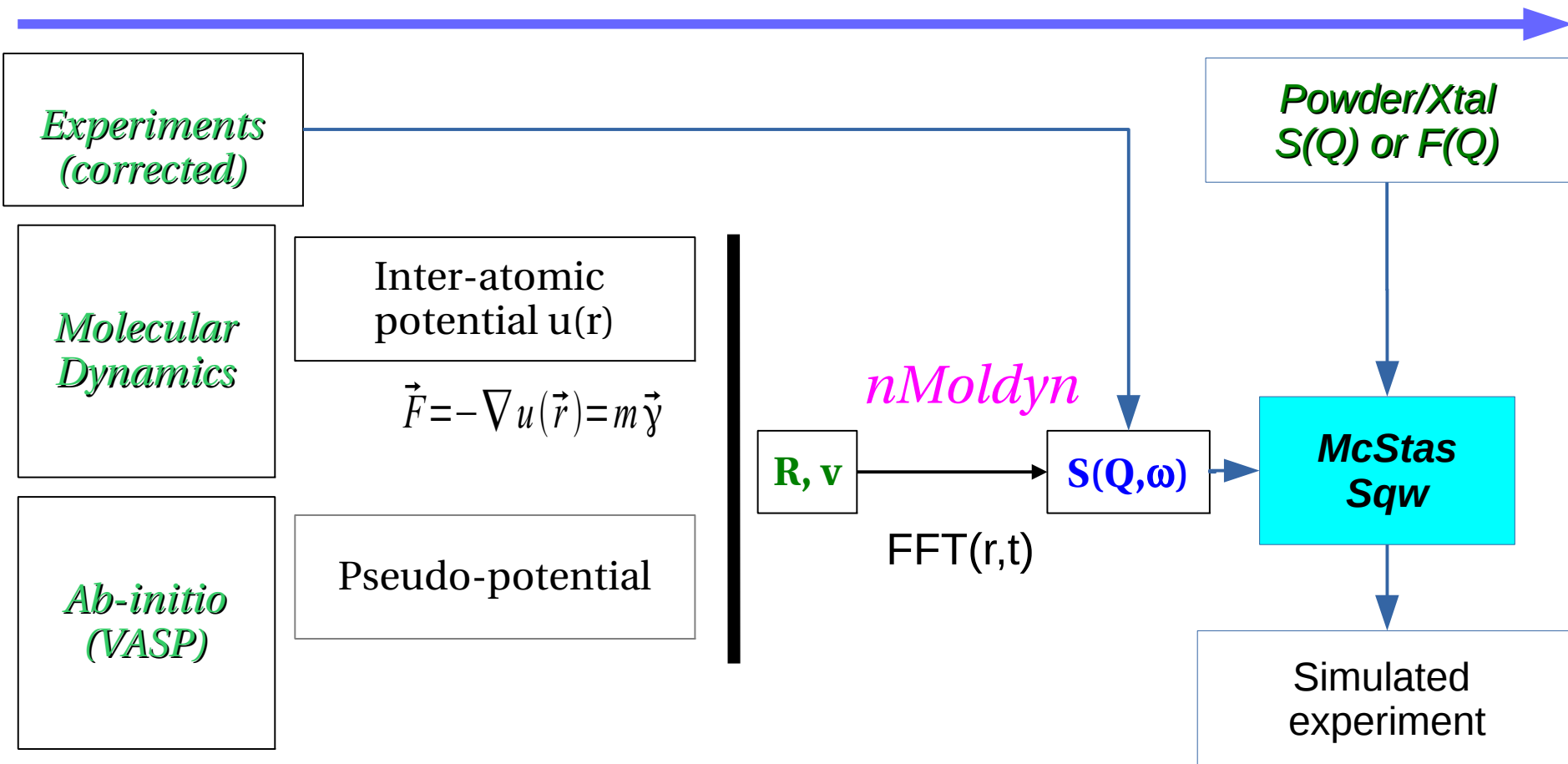
Scattering distribution

$$S(q, \omega)$$

with importance sampling to
scatter preferably where S is large



How to get $S(q,w)$ data sets



MD step is done prior to the virtual experiment (NAMD, VASP, GROMACS). Computationally intensive (e.g. use clusters). Then use FFT(r,t)

McStas provides a few sample $S(Q,w)$: Rb, Ge, H₂O, D₂O, D₂, ...

Isotropic_Sqw: Provides **elastic** and **inelastic** for both **coherent** and **incoherent** channels



Sqw: Exercise 1: a liquid TOF

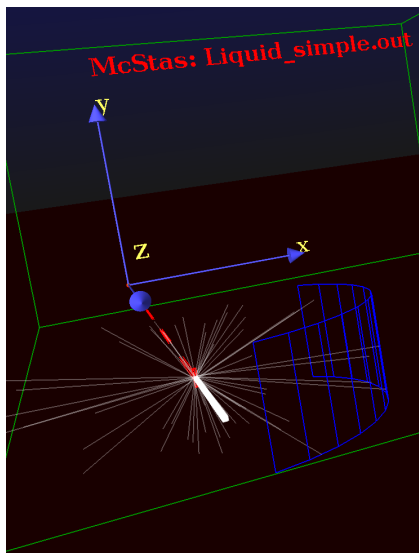
Aim: A simple spectrometer (diffractometer)

- Create a new instrument from 'template (test)'.
- Call it `Liquid_simple` and define input parameters (`lambda=2.36`, `string coh="Rb_liq_coh.sqw"`, `string inc="Rb_liq_inc.sqw"`)
- Insert a `Source_simple` $\phi 1\text{cm}$ sending $\lambda=\text{lambda}$ with $d\lambda/\lambda=1\%$. Focus onto a $1\times 1\text{cm}^2$ area.
- Insert an `Isotropic_Sqw` 3m away, using $\sigma_{\text{coh}}=\text{coh}$, $\sigma_{\text{inc}}=\text{inc}$ with $\phi 1\text{cm} \times 5\text{cm}$.



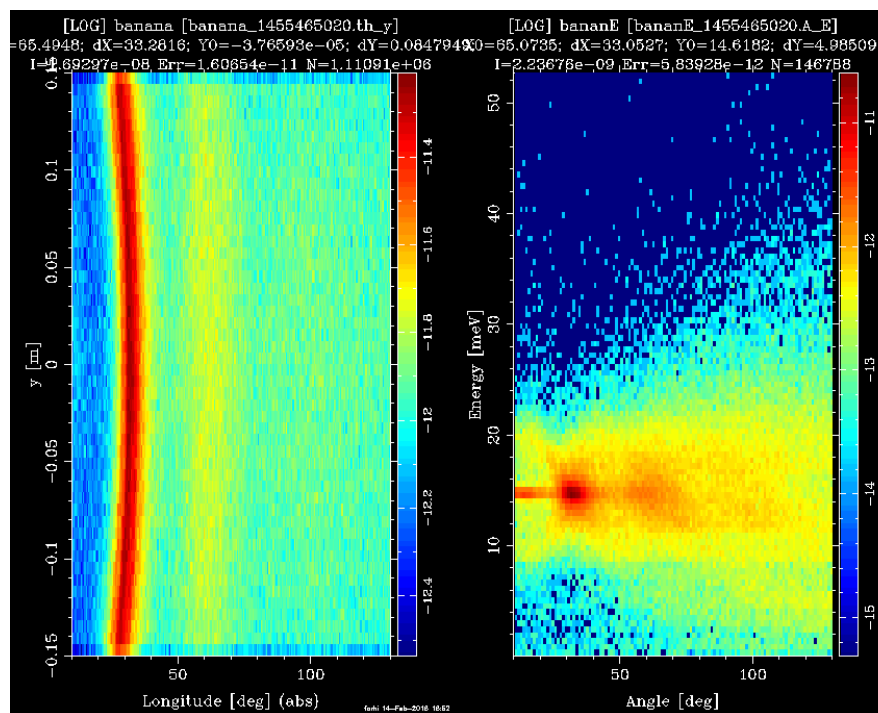
Sqw: Exercise 1: a liquid TOF

- Add a `Monitor_nD` cylindrical detector $\phi 1\text{m} \times 30\text{cm}$, sensitive to (θ, y) for diffraction, centred on the sample, with 100 bins.
- Add the same, but sensitive to **(angle,energy)** with automatic energy limits.
- Save, run in *Trace 3D* to check geometry.



Sqw: Exercise 1: a liquid TOF

- Run in Simulation/PGPLOT mode with $1e8$ neutron events.
- Plot results !
- Comment on the diffraction pattern and the inelastic one.



Sqw: Exercise 2: event better !

- Insert an instrument variable in the DECLARE block, as 'flag_scat'.

```
DECLARE %{\n    int flag_scat=0;\n}%}
```

- After the AT token of the 'sample', insert an EXTEND block that sets flag_scat to the number of SCATTERED events.

```
EXTEND %{\n    flag_scat=SCATTERED; // nb of scattered events\n}%}
```



Sqw: Exercise 2: event better !

- Duplicate the 2 monitors, and make them sensitive to **multiple-scattering** only. Add a WHEN(flag_scatt) between the COMPONENT and the AT keywords:

```
COMPONENT ...
```

```
WHEN(flag_scatt > 1)
```

```
AT ...
```

- Save and Run !

- How much multiple scattering ratio at $\lambda=2.36 \text{ \AA}$

- Make the sample $\phi 5\text{cm}$ and repeat.

