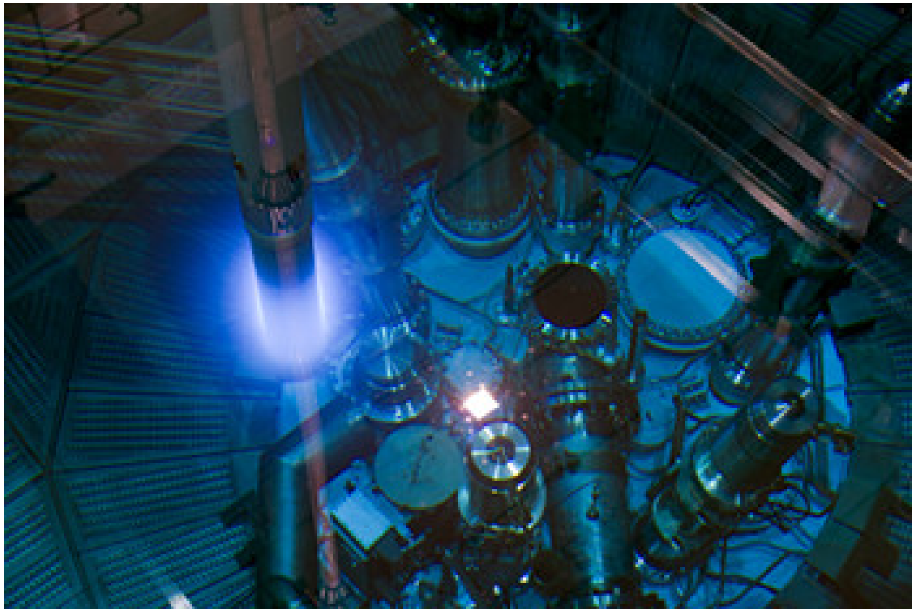
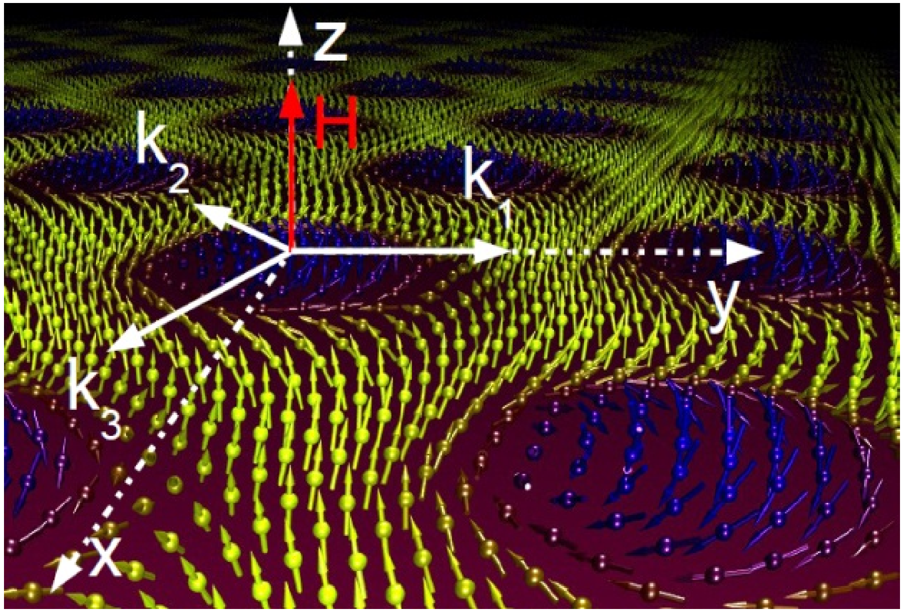
Physics with Neutrons I, WS 2015/2016





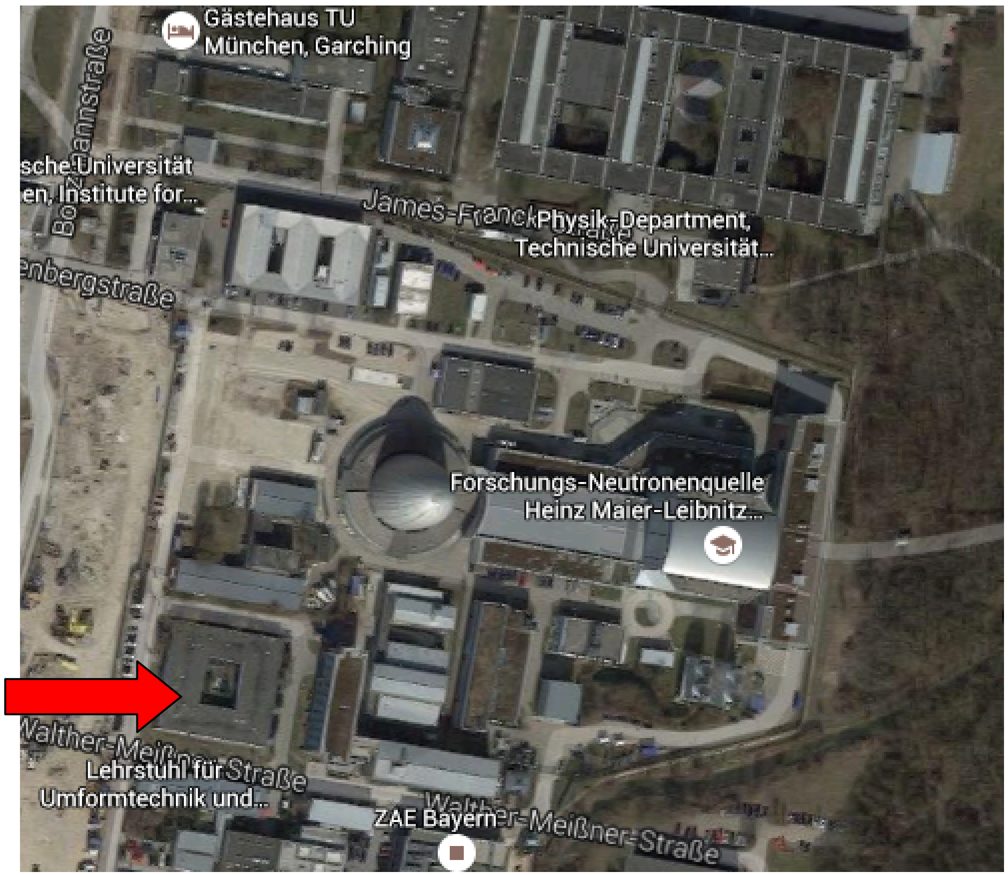
Lecture 13, 25.1.2016

MLZ is a cooperation between:

Exam (after winter term)

30min oral exam

Room
E40a



Correlation functions

Starting point: General cross-section

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \langle e^{-i\boldsymbol{Q}\hat{\boldsymbol{R}}_{j'}(0)} e^{-\boldsymbol{Q}\hat{\boldsymbol{R}}_{j'}(t)} \rangle e^{-i\omega t} \mathrm{dt}$$

$$I(\boldsymbol{Q},t) = \frac{1}{N}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \langle e^{-i\boldsymbol{Q}\hat{\boldsymbol{R}}_{j'}(0)} e^{-\boldsymbol{Q}\hat{\boldsymbol{R}}_{j'}(t)} \rangle$$

➡ Intermediate scattering function

Fourier transform (space) $$G(\boldsymbol{r},t) = \frac{1}{(2\pi)^3}\int I(\boldsymbol{Q},t) e^{-i\boldsymbol{Q}\boldsymbol{r}} \mathrm{dQ}$$

➡ Pair correlation function

Fourier transform (time) $$S(\boldsymbol{Q},\omega) = \frac{1}{(2\pi\hbar)}\int I(\boldsymbol{Q},t) e^{-i\omega t} \mathrm{dt}$$

➡ Scattering function, directly connected to cross-section

Physical meaning of pair correlation function G(r,t)

$$G(\boldsymbol{r},t) = \frac{1}{N}\sum_{j,j'}\int \langle \delta(\boldsymbol{r}' - \hat{\boldsymbol{R}}_{j'}(0))\delta(\boldsymbol{r}' + \boldsymbol{r} - \hat{\boldsymbol{R}}_j(t))\rangle \mathrm{d}r'$$

Correlation between atom j' at time t=0 at position r' and atom j at time t=t and position r'+r

Splits up in

$$G_s(\boldsymbol{r},t) = \frac{1}{N}\sum_{j}\int \langle \delta(\boldsymbol{r}' - \hat{\boldsymbol{R}}_{j}(0))\delta(\boldsymbol{r}' + \boldsymbol{r} - \hat{\boldsymbol{R}}_j(t))\rangle \mathrm{d}r'$$

Self correlation function

$$G_d(\boldsymbol{r},t) = \frac{1}{N}\sum_{j\neq j'}\int \langle \delta(\boldsymbol{r}' - \hat{\boldsymbol{R}}_{j'}(0))\delta(\boldsymbol{r}' + \boldsymbol{r} - \hat{\boldsymbol{R}}_j(t))\rangle \mathrm{d}r'$$

Correlation function

Coherent and incoherent part

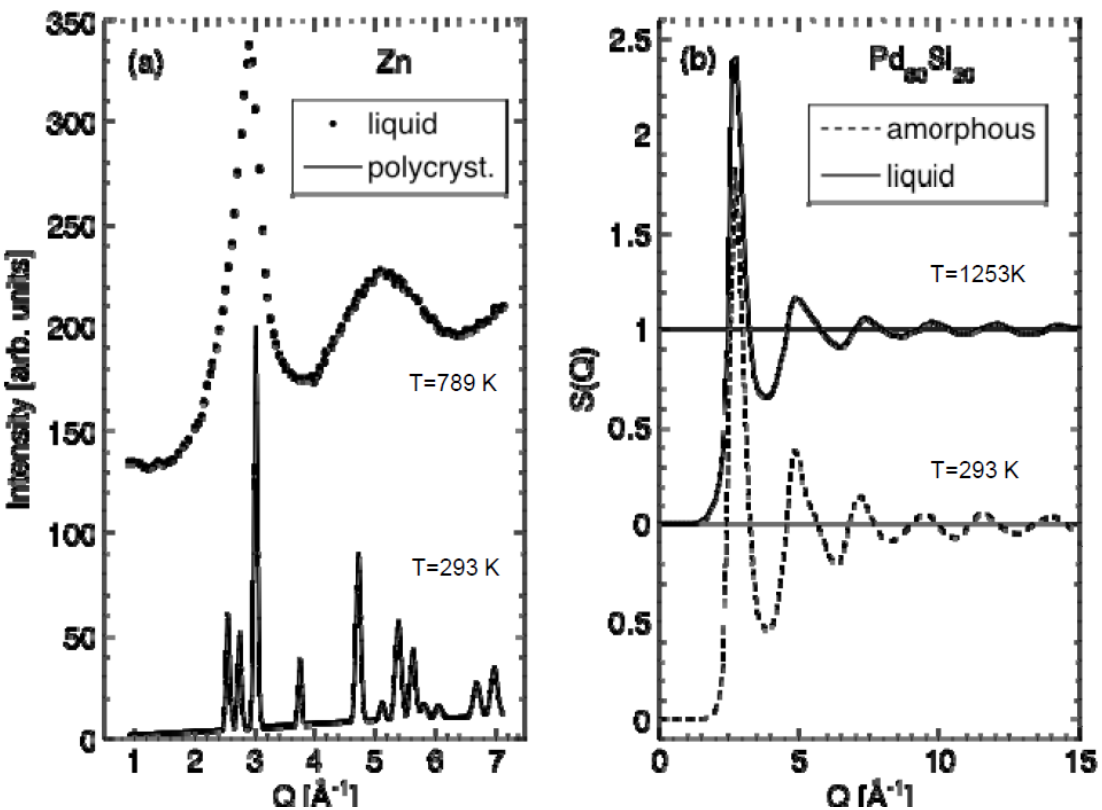
$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega}\right)_{coh} = N\frac{k'}{k}\langle b\rangle^2 S_{coh}(\boldsymbol{Q},\omega)$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega}\right)_{inc} = N\frac{k'}{k}(\langle b^2\rangle - \langle b\rangle^2) S_{inc}(\boldsymbol{Q},\omega)$$

Pair correlation function G(r,t) useful for description of liquids

Liquid (amorphhous) sample ⟺ Crystalline sample

⇒ Similar density, no LRO, only short range correlations

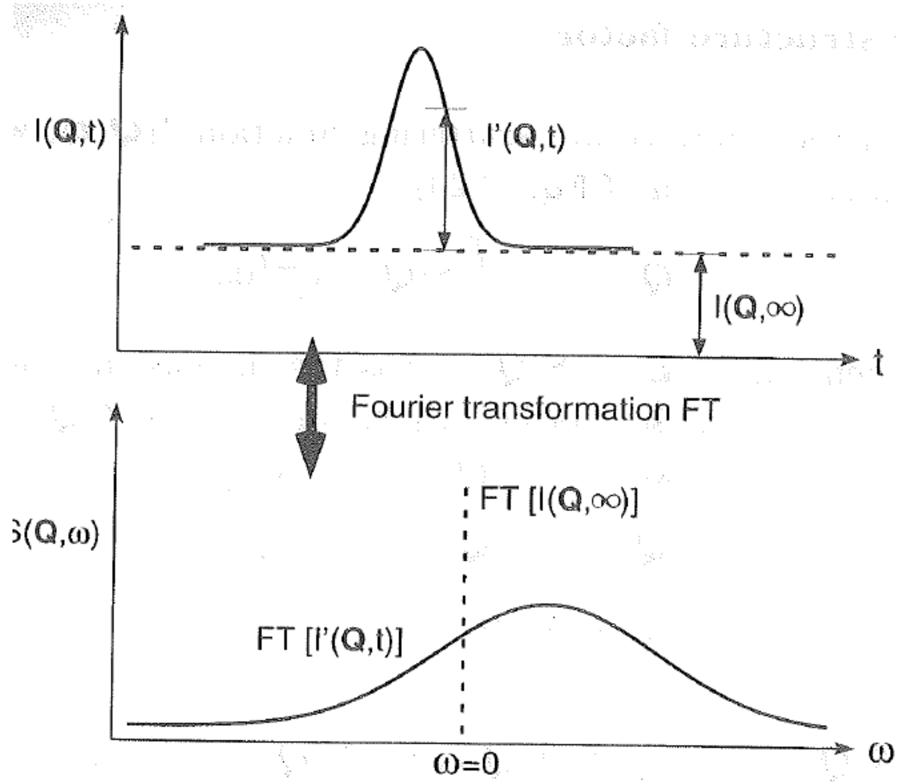


Static structure factor

Start with I(Q,t) and split into into two parts:

$$I(\boldsymbol{Q},t) = \hbar \int S(\boldsymbol{Q},\omega) e^{\omega t} \mathrm{d}\omega$$

$$I(\boldsymbol{Q},t) = I(\boldsymbol{Q},\infty) + I'(\boldsymbol{Q},t)$$



$$S(\boldsymbol{Q},\omega) = \frac{1}{\hbar}\delta(\omega) I(\boldsymbol{Q},\infty) + \frac{1}{2\pi\hbar}\int I'(\boldsymbol{Q},t) e^{-i\omega t} \mathrm{d}t$$

Elastic part — Inelastic part

➡ Infinite time correlations

Static structure factor: Looking at deviations of the mean density n(r)

$$G'(\boldsymbol{r}) = \frac{1}{N}\int \langle n(\boldsymbol{r}' - \boldsymbol{r}) - \langle n(\boldsymbol{r}' - \boldsymbol{r})\rangle)(n(\boldsymbol{r}') - \langle n(\boldsymbol{r}')\rangle)\rangle \mathrm{dr}'$$

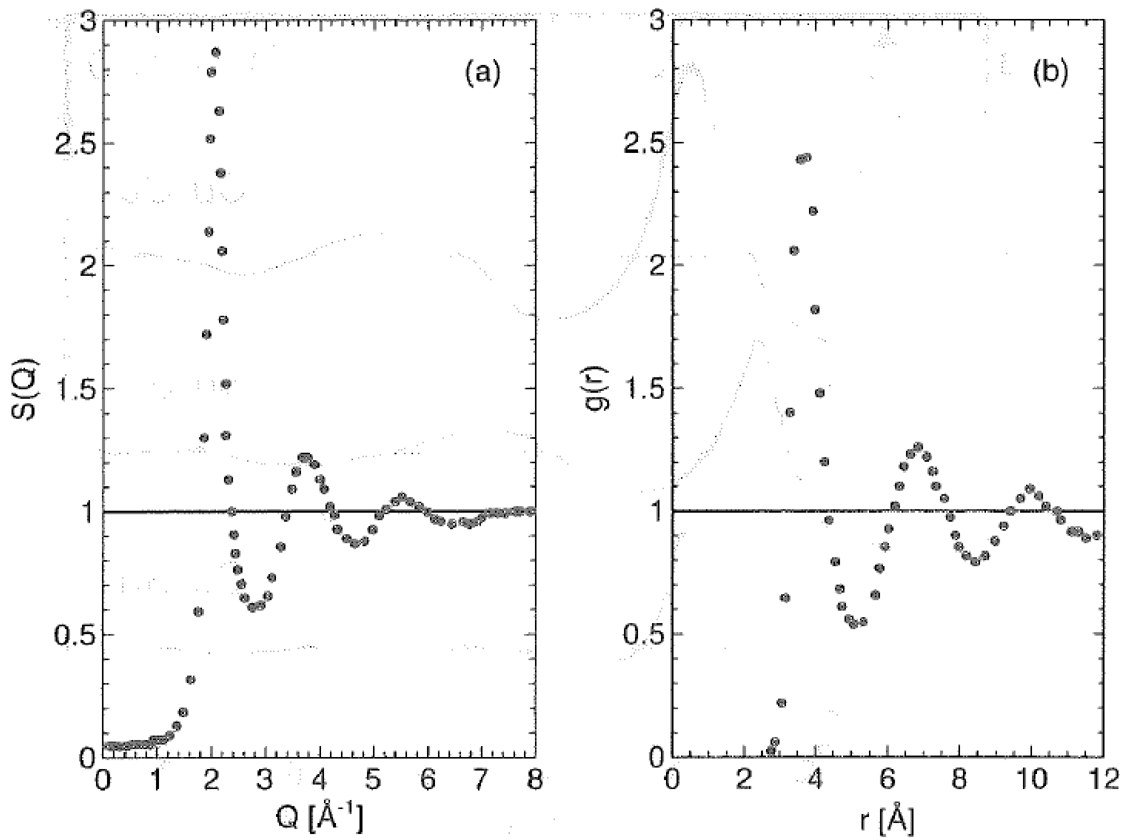
Elastic scattering from liquids

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = N\langle b\rangle^2(1 + \int (g(\boldsymbol{r}) - n_0)e^{i\boldsymbol{Q}\boldsymbol{r}}\mathrm{dr}$$

g(r): pair correlation function

$$S(Q) = 1 + 4\pi\int_0^\infty (g(r) - n_0)\frac{\sin Qr}{Qr}r^2\mathrm{dr}$$

Static structure factor: Looking at deviations of the mean density n(r)



Static structure factor: Scattering function

g(r) pair correlation function: Deviations from mean density n(r).

Limit Q->0 $S(Q=0)=1$

Limit Q->∞ $S(Q\to\infty)=n_0\kappa_T k_B T$ Isothemal compressibility