Physics with neutrons (PH2053)

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Lecture 09

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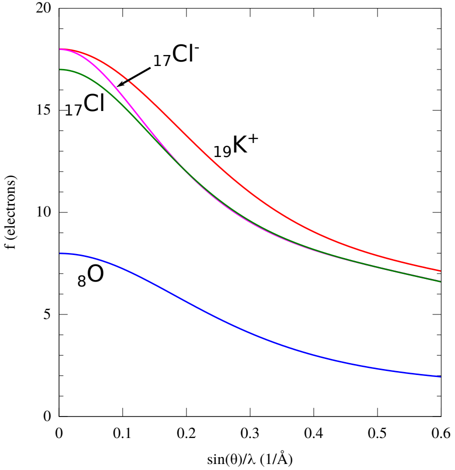
X-ray atomic form factor



— https://en.wikipedia.org/wiki/Atomic_form_factor

Coherent vs. incoherent scattering

- everything scatters x-rays *coherently*
- everything scatters neutrons *coherently* and *incoherently*
  - the coh/inc ratio is isotope-dependent
  - experimental separation is only with few instruments possible
- coherent: interference between different scatterers
- incoherent: interference of scatterer with itself

energy-resolved?		coherent	incoherent
no	diffraction	✓	✗
yes	spectroscopy	✓	✓

Two variables: momentum and energy

$\hbar Q$ momentum transfer between neutron/x-ray and sample
Q in Å^{-1} or nm^{-1} («reciprocal space»)

$\hbar\omega$ energy transfer between neutron/x-ray and sample
often in meV – the $\hbar$ is basically never written

$$\vec{Q} \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad \vec{r} \tag{1}$$

$$\omega \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad t \tag{2}$$

$$Q_{\text{elastic}} = \frac{4\pi}{\lambda} \cdot \sin\left(\frac{2\theta}{2}\right) \tag{3}$$

Coherent neutron/x-ray spectroscopy

$$G_{\mathrm{pair}}(\vec{r}, t) \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad I_{\mathrm{pair}}(\vec{Q}, t) \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad S_{\mathrm{pair}}(\vec{Q}, \omega) \qquad (4)$$

- G space–time paircorrelation function
- $\vec{r}$ displacement
- t time
- I intermediate scattering function
- $\vec{Q}$ momentum transfer
- S scattering function
- ω energy transfer

Coherent neutron/x-ray spectroscopy

$$I_{\text{pair}}(\vec{Q}, t) \sim \left\langle \sum_{j}^{N} \sum_{k>j}^{N} b_j^c b_k^c \exp\left[\mathrm{i}\vec{Q} \cdot \left(\vec{R}_j(t_0 + t) - \vec{R}_k(t_0)\right)\right] \right\rangle_{t_0} \quad (5)$$

b_a^c coherent scattering length of scatterer a
$\vec{R}_a(t)$ position of scatterer a at time t

Very rough translation into real space:
«If we call the position of scatterer k at a certain time the origin, how large is the probability that scatterer j is at the position $2\pi/\vec{Q}$ a time t later?»

Coherent neutron/x-ray diffraction: $t = 0$ / $\int_{-\infty}^{\infty} \mathrm{d}\omega$

$$G_{\text{pair}}(\vec{r}) \quad \stackrel{\mathcal{FT}}{\longleftrightarrow} \quad S_{\text{pair}}(\vec{Q}) \tag{6}$$

G spatial paircorrelation function

$\vec{r}$ displacement

S structure factor

$\vec{Q}$ momentum transfer

Coherent neutron/x-ray diffraction: $t = 0$ / $\int_{-\infty}^{\infty} \mathrm{d}\omega$

$$S_{\mathrm{pair}}(\vec{Q}) \sim \left\langle \sum_{j}^{N} \sum_{k>j}^{N} b_j^c b_k^c \exp\left[\mathrm{i}\vec{Q}\cdot\left(\vec{R}_j(t_0) - \vec{R}_k(t_0)\right)\right]\right\rangle_{t_0} \qquad (7)$$

b_a^c coherent scattering length of scatterer a
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Very rough translation into real space:
«If we call the position of scatterer k at a certain time the origin, how large is the probability that scatterer j is at the position $2\pi/\vec{Q}$ at the same time?»

Incoherent neutron spectroscopy

$$G_{\text{self}}(r,t) \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad I_{\text{self}}(Q,t) \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad S_{\text{self}}(Q,\omega) \tag{8}$$

- G space–time autocorrelation function
- r displacement
- t time
- I intermediate scattering function
- Q momentum transfer
- S scattering function
- ω energy transfer

Incoherent neutron spectroscopy

$$I_{\text{self}}(Q,t) \sim \left\langle \sum_{j}^{N} b_j^i b_j^i \exp\left[\mathrm{i}\vec{Q}\cdot\left(\vec{R}_j(t_0+t)-\vec{R}_j(t_0)\right)\right]\right\rangle_{t_0,\Omega} \tag{9}$$

b_a^i incoherent scattering length of scatterer a
$\vec{R}_a(t)$ position of scatterer a at time t

Very rough translation into real space:
«If we call the position of scatterer j at a certain time the origin, how large is the probability that this scatterer is within a sphere of size $2\pi/Q$ a time t later?»

Incoherent neutron diffraction? $t = 0 \;/\; \int_{-\infty}^{\infty} \mathrm{d}\omega$

$$G_{\text{self}}(r) \quad \overset{\mathcal{FT}}{\longleftrightarrow} \quad S_{\text{self}}(Q) \tag{10}$$

G spatial autocorrelation function

r displacement

S scattering function

Q momentum transfer

Incoherent neutron diffraction? $t = 0$ / $\int_{-\infty}^{\infty} \mathrm{d}\omega$

$$S_{\mathrm{self}}(Q) \sim \left\langle \sum_{j}^{N} b_j^i b_j^i \exp\left[\mathrm{i}\vec{Q} \cdot \left(\vec{R}_j(t_0) - \vec{R}_j(t_0)\right)\right] \right\rangle_{t_0,\Omega} \tag{11}$$

b_a^i incoherent scattering length of scatterer a
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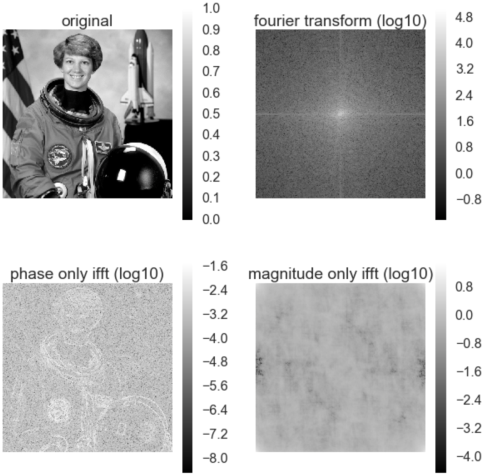
Very rough translation into real space:
«If we call the position of scatterer j at a certain time the origin, how large is the probability that this scatterer is within a sphere of size $2\pi/Q$ at the same time?»

So do we simply Fourier transform everything?



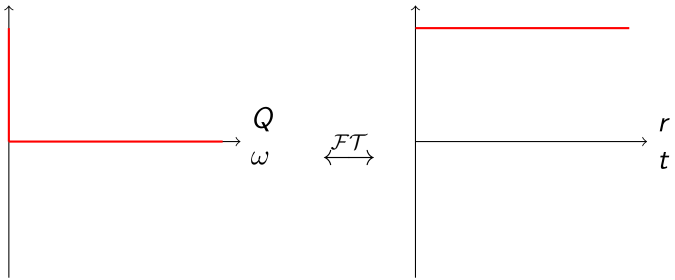
No. . .

- Because the phase information is lost in the scattering process, we cannot «simply» take the signal we measured in reciprocal space and Fourier transform it back to real space

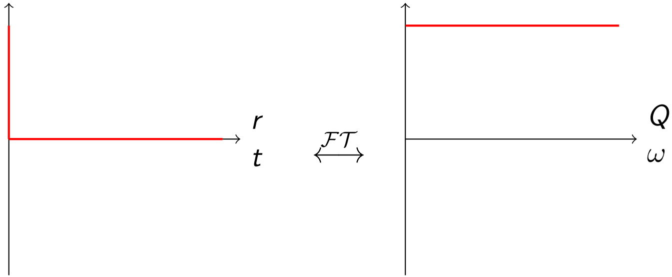
No... but yes!

- Because the phase information is lost in the scattering process, we cannot «simply» take the signal we measured in reciprocal space and Fourier transform it back to real space
- But we can generate structure & dynamics in real space, Fourier transform that to reciprocal space, and compare it to the data

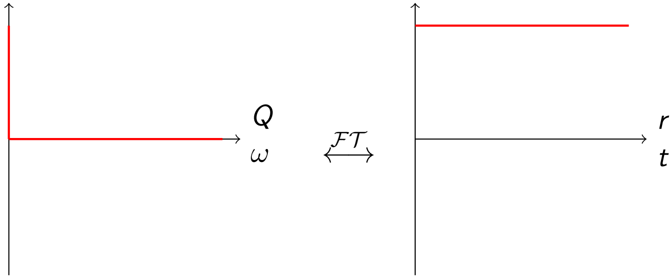
Fourier transform



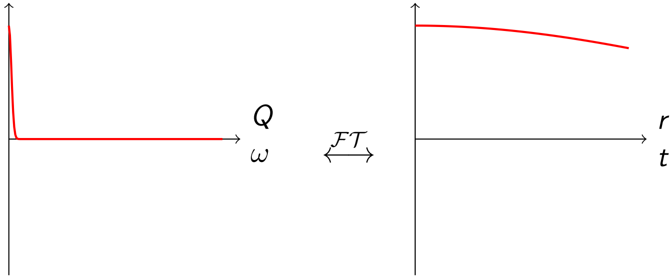
Fourier transform



Fourier transform



Fourier transform



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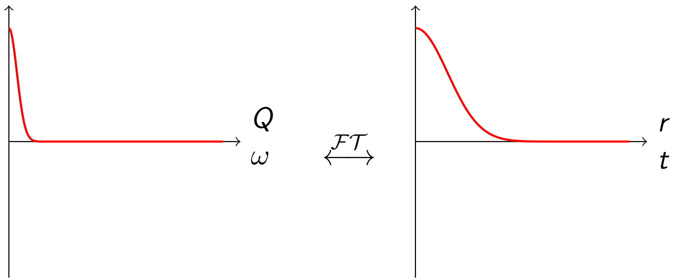

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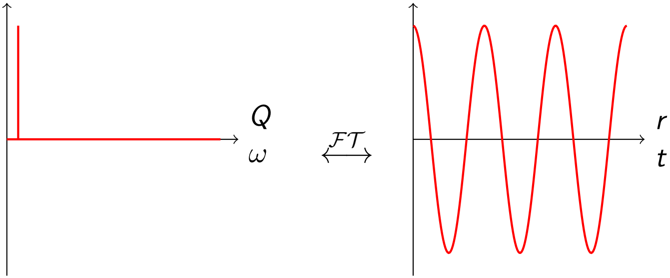
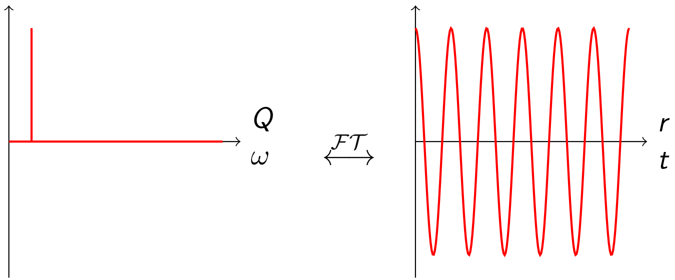
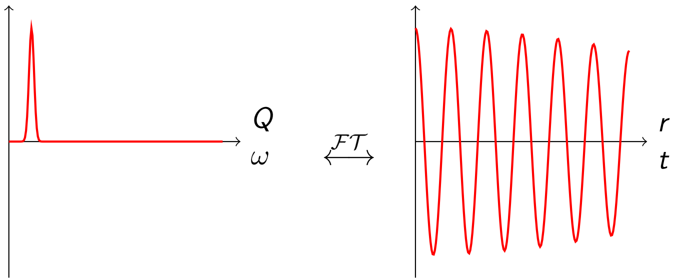


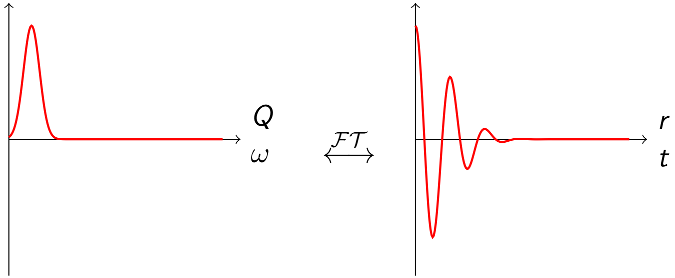
Fourier transform



Fourier transform



Fourier transform



Get $\vec{R}(t)$ from model or simulation

Structure:

- sphere
- cylinder
- layer of constant density
- Gaussian density profile

Dynamics:

- unhindered diffusion
- diffusion in harm. pot.
- oscillation in harm. pot.
- jumps

Get $\vec{R}(t)$ from model or simulation

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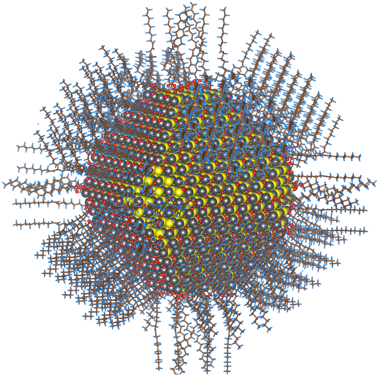
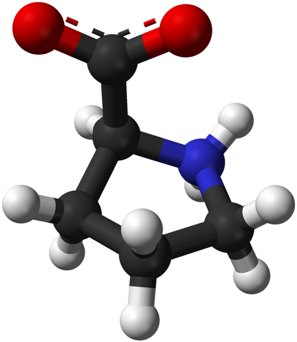
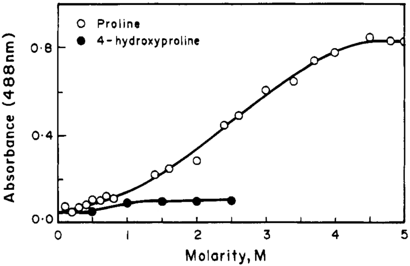
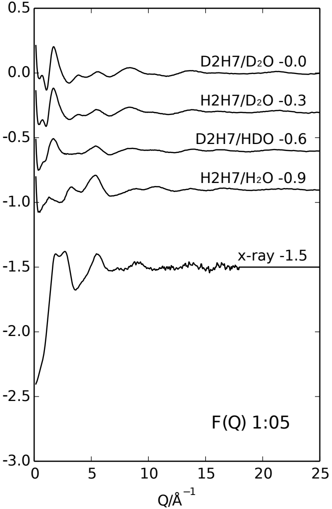


Proline: Amino Acid and Natural Hydrotrope





Wide-angle diffraction on a proline solution



— S. Busch *et al.* Journal of Physical Chemistry B, 118:14267, 2014

Coherent neutron/x-ray diffraction: $t = 0$ / $\int_{-\infty}^{\infty} \mathrm{d}\omega$

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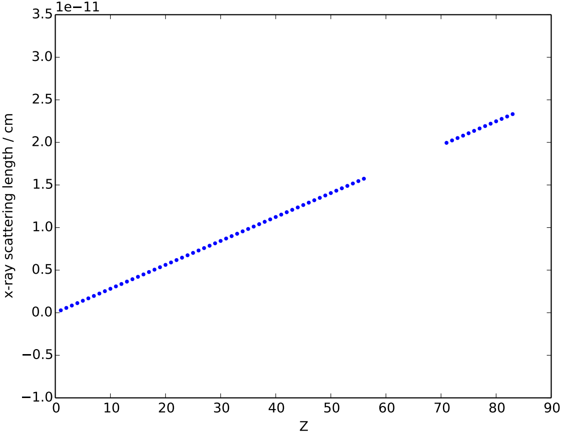
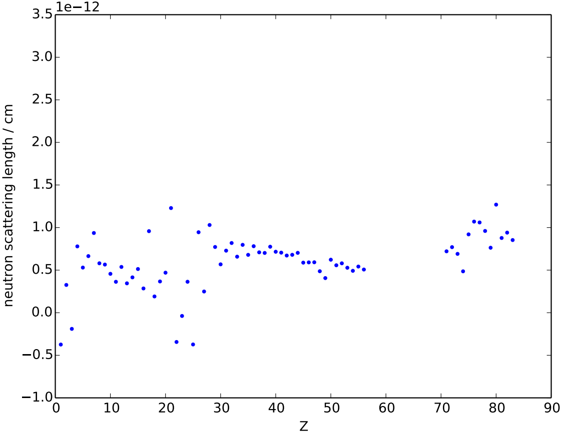
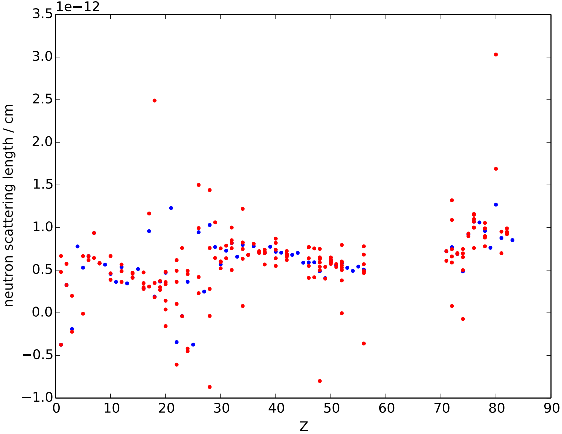
X-ray coherent scattering lengths



Neutron coherent scattering lengths, natural abundance



Neutron coherent scattering lengths, isotope effect



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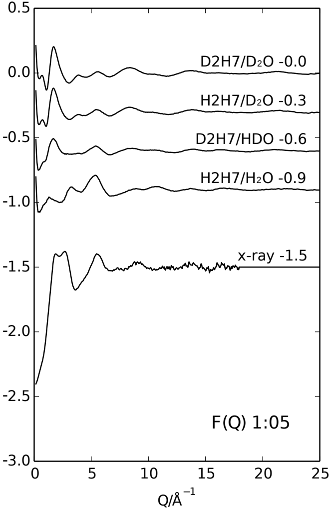
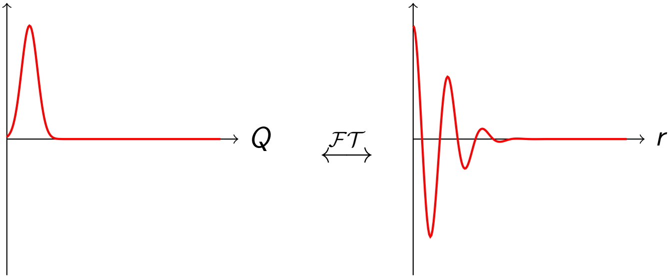


Fourier transform



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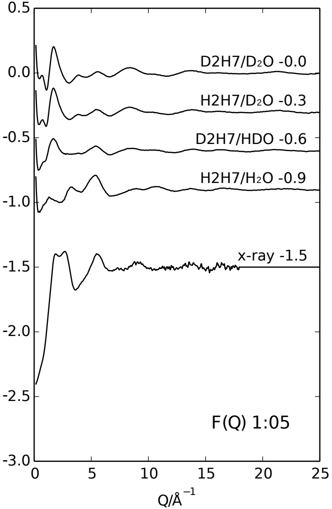

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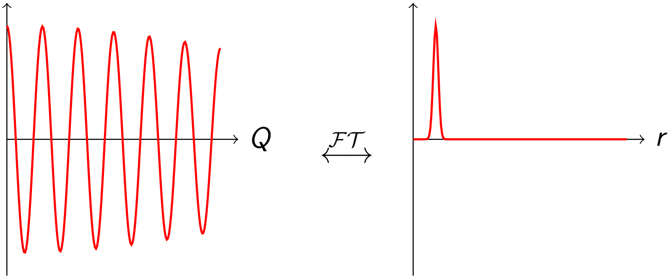

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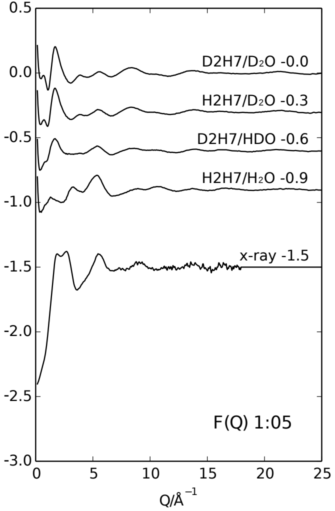
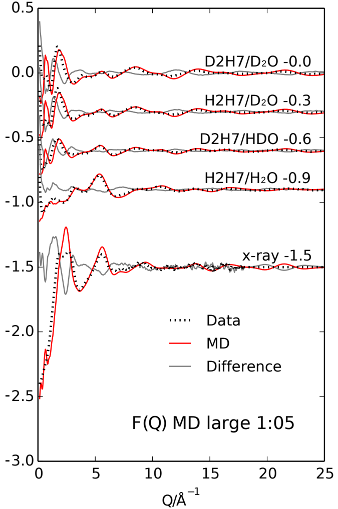
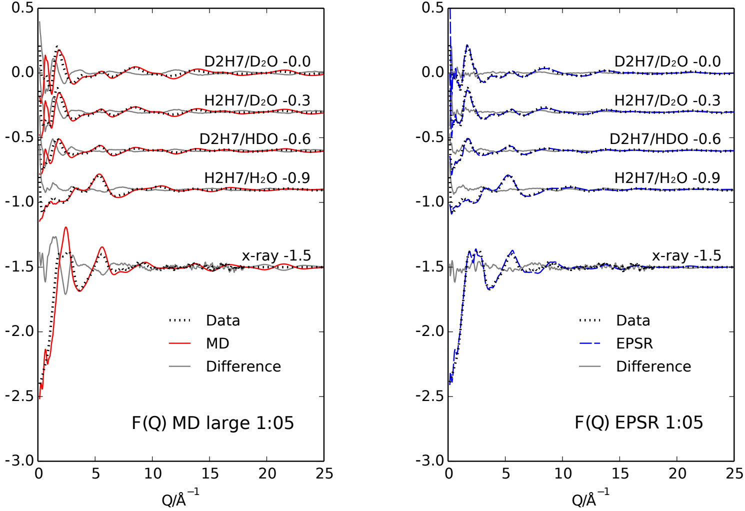


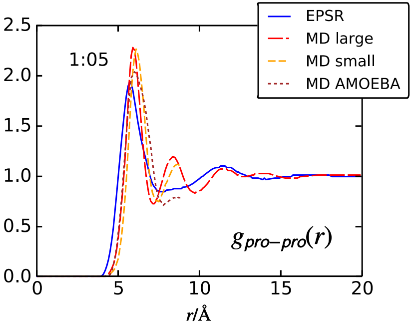
Wide-angle diffraction on a proline solution



Wide-angle diffraction on a proline solution



Structure of Proline Solutions



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