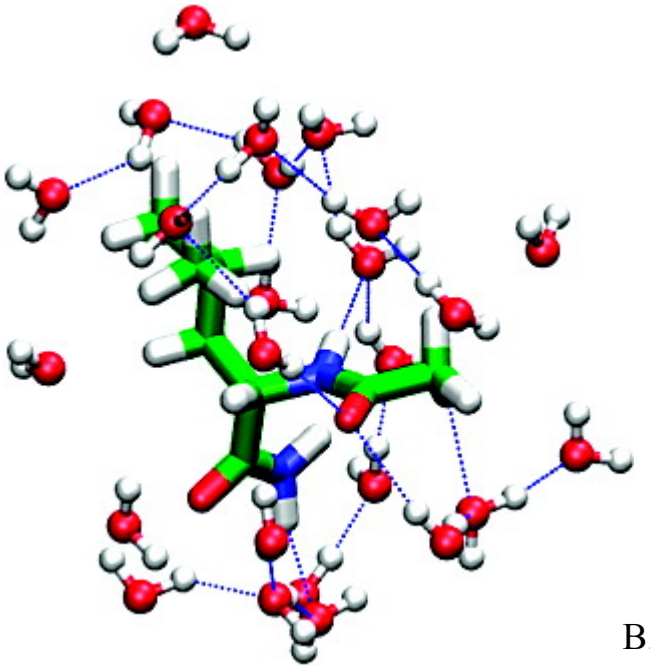
Hydration water dynamics near d-NAGMA studied by DCS

Group B
Summer School 2009
June 26, 2009



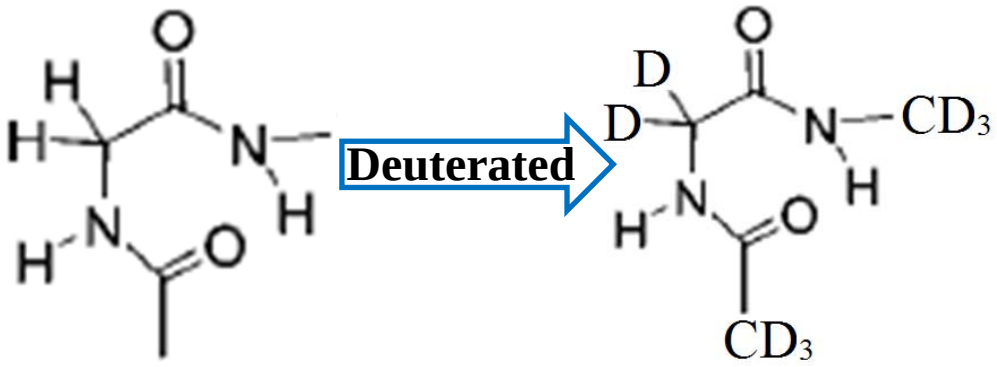
B. Born, H. Weingärtner, E. Bründermann, M. Havenith, *JACS* **131**, 3752(2009).

Outline

1. Motivation
2. Methods
3. Analysis of DCS data
4. Experimental results
5. Conclusion

Motivation

1. Protein hydration concerns:
   - the interaction between water and proteins
   - the structure and dynamics of water affected by proteins
2. Many techniques have been used to solve this problem:
   IR, NMR(MRD), X-ray, Neutron Scattering, Dielectric Resonance.
3. QENS could give more information regarding the dynamics of the hydration water near proteins.
4. Deuterated model peptides (NAGMA, 1.5M) are used to study water under various temperatures.

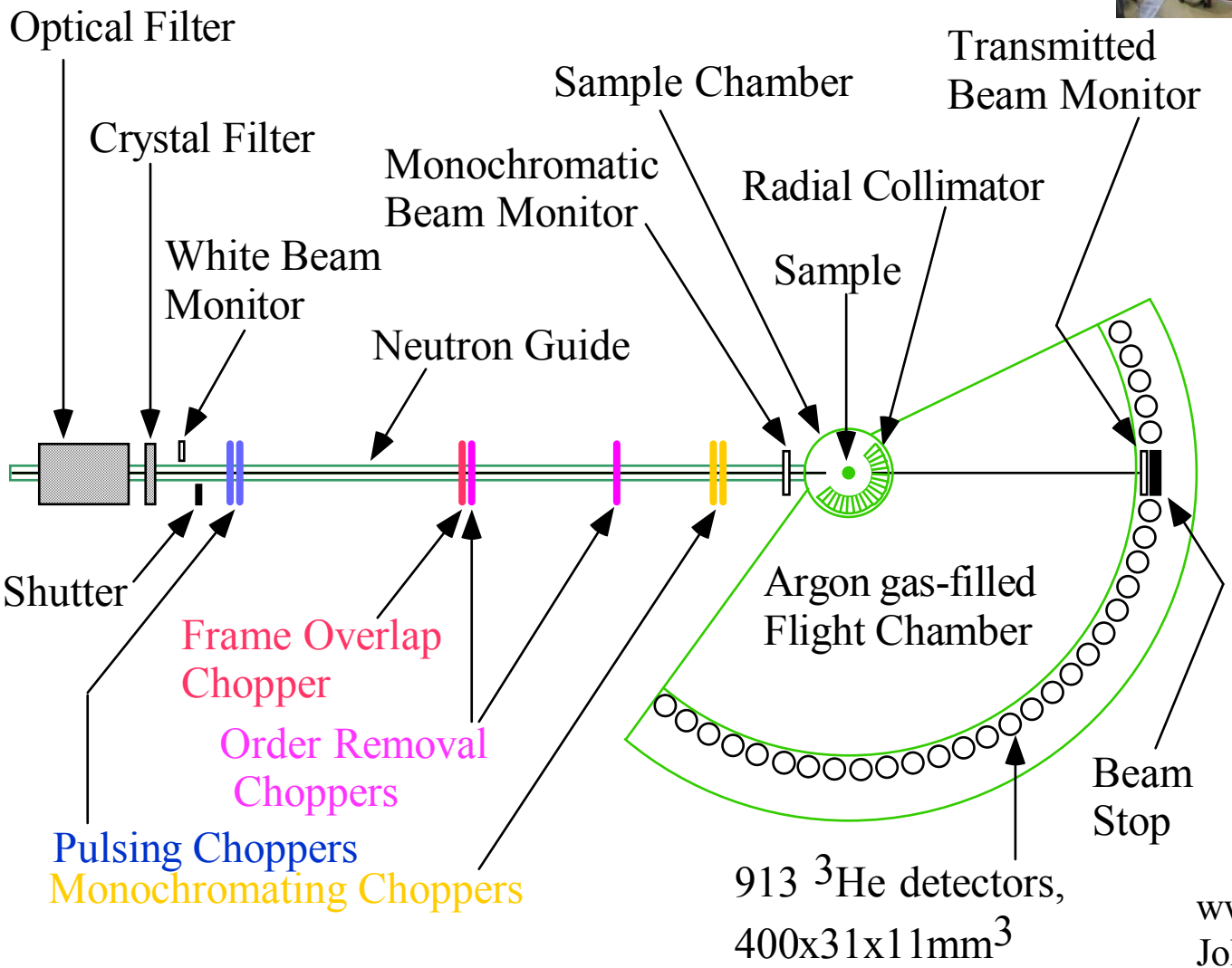


ID Kuntz, W Kauzmann, *Adv Protein Chem* **28**, 239 (1974)
JA Rupley, G Careri, *Adv Protein Chem* **41**, 37 (1991)
B Halle, *Phil. Trans. R. Soc. Lond. B* **359**, 1207 (2004)

Methods

Disk Chopper Spectrometer (DCS)

Wavelength $\lambda = 7.5$ Å, 0.3 Å^{-1} <Q<1.5 Å^{-1}



www.nist.gov
John Copley, SS09 talk

Analysis of DCS data

Double differential cross section is proportional to the incoherent scattering:

$$\frac{d^2\sigma}{dEd\Omega} = \frac{\sigma_{in}}{4\pi}\frac{k_s}{k_i} NS_{inc}\left(Q,\omega\right)$$

S_{inc} is a convolution of vibrational, translational and rotational motions:

$$S_{inc}\left(Q,\omega\right) = e^{-\left\langle u^2\right\rangle Q^2/3} S_{inc}^{trans}\left(Q,\omega\right) \otimes S_{inc}^{rot}\left(Q,\omega\right)$$

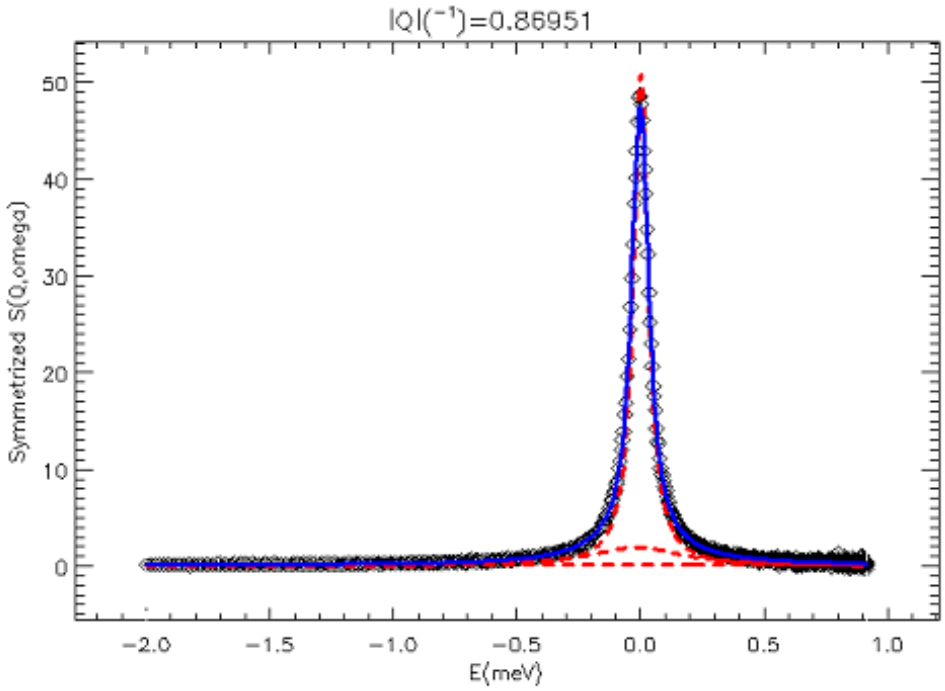
Fitting with 2 Lorentzian functions.

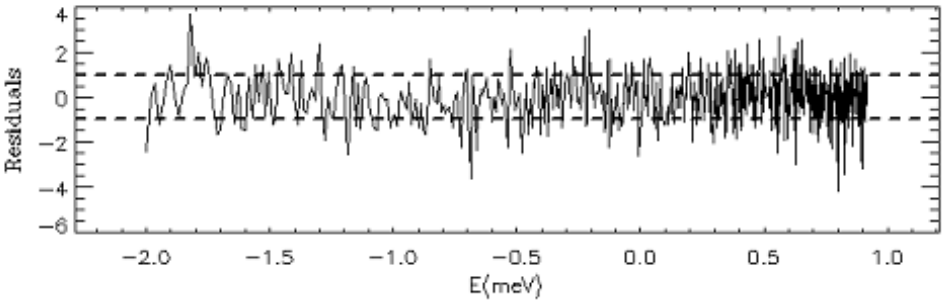
$$\Gamma_{trans}(Q) = \frac{D_{trans}Q^2}{1 + D_{trans}Q^2\tau_0}$$

M Bee, *Quasielastic Neutron Scattering*, Adam Hilger, 1988
D Russo, R Murarka, J Copley, T Head-Gordon, *JPCB* **109**, 12966 (2005).
C Malardier-Jugroot, M Johnson, R Murarka, T Head-Gordon, *PCCP* **10**, 4903 (2008).

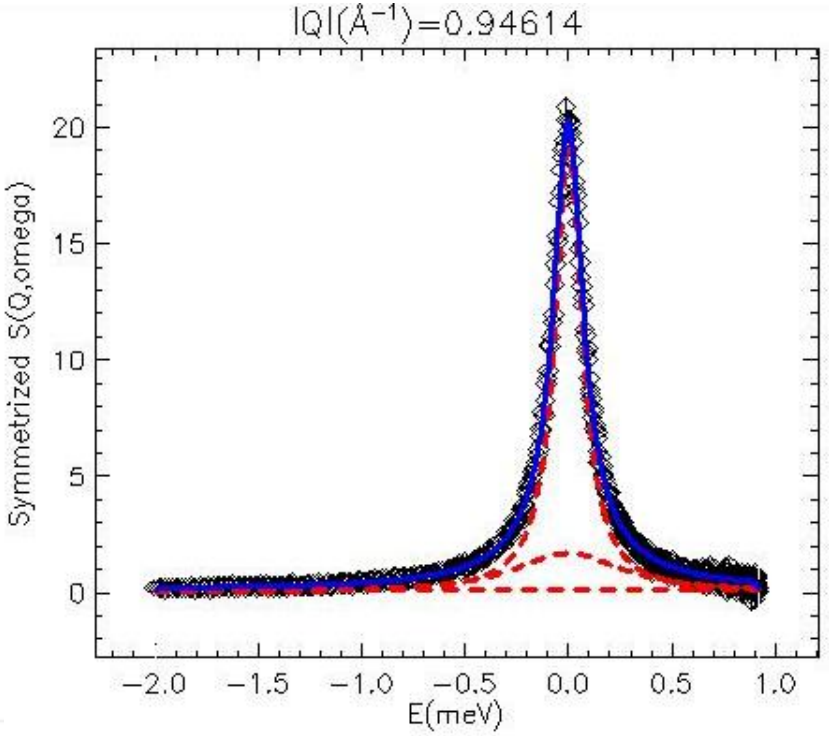
Two Lorentzian fitting

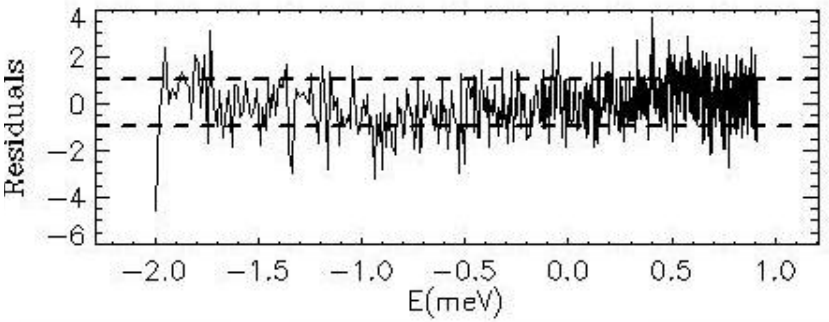
273K, $|Q|^{-1}$=0.86951 Å





310K, $|Q|^{-1}$=0.94614 Å

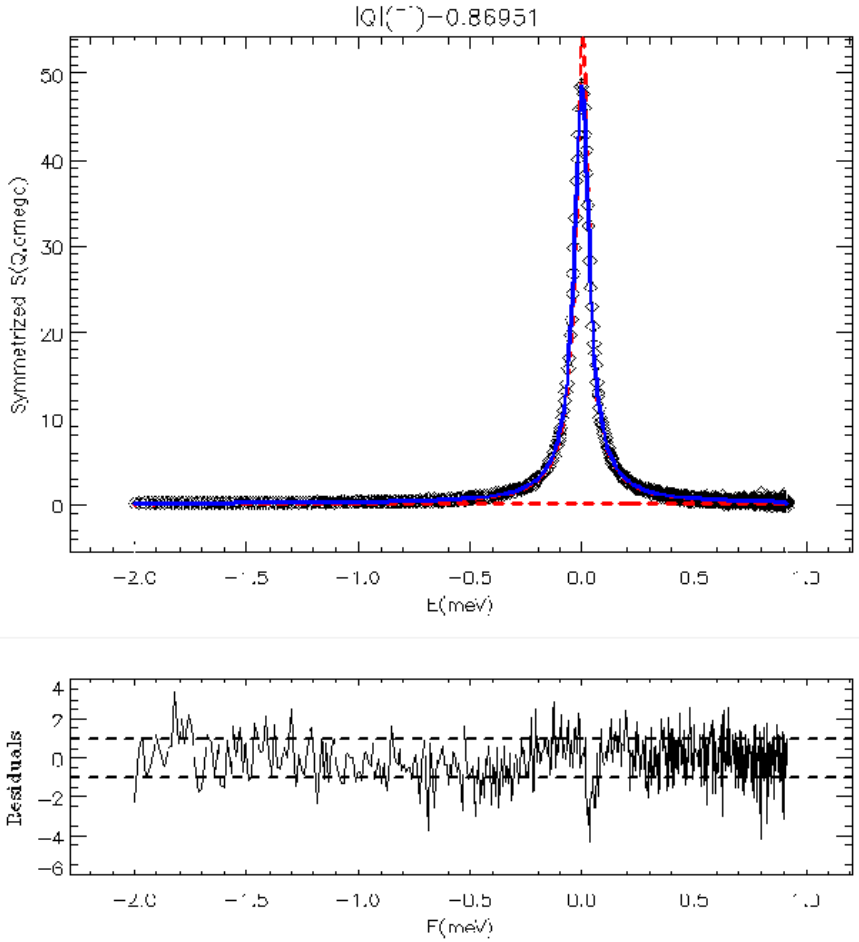




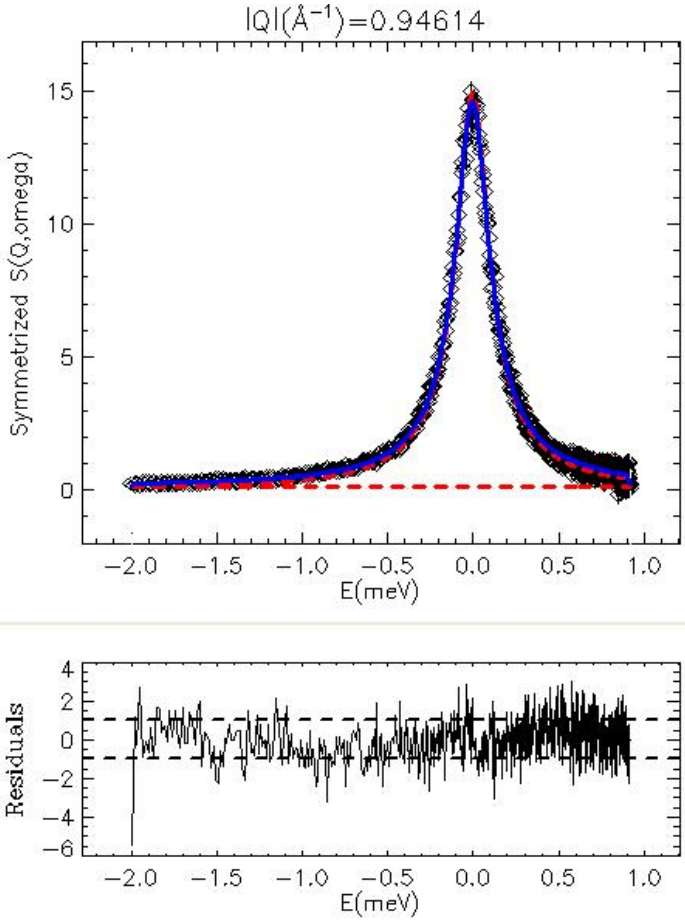
KWW stretched exponential(SE)

$$S_{inc}(Q,t) = e^{-\langle u^2 \rangle Q^2/3} \exp\left[-\left(\frac{1}{\tau_\alpha(Q,T)} \right)^{\beta(Q,T)} \right]$$

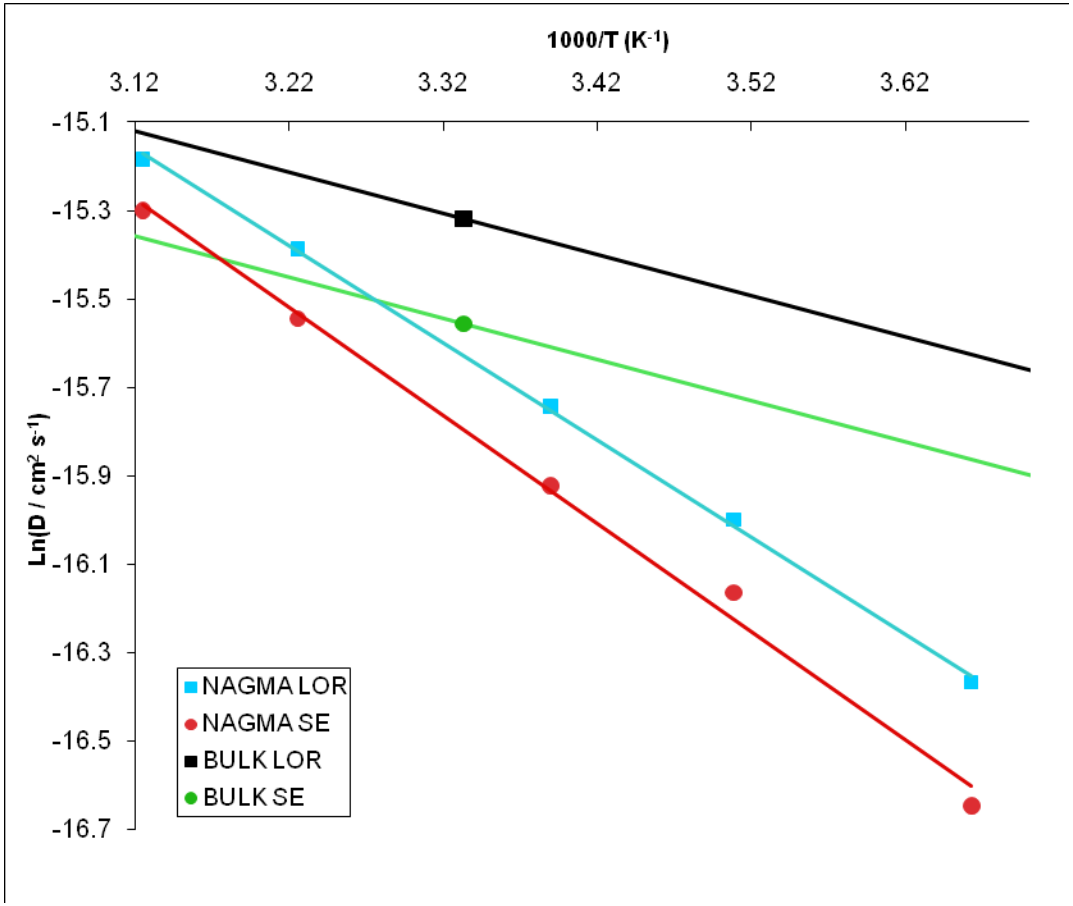
273K, $|Q|^{-1}$=0.86951 Å, β=0.7784



310K, $|Q|^{-1}$=0.94614 Å, β=0.8468



Translation diffusion vs. Temperature



$$\Gamma_{trans}(Q) = \frac{D_{trans} Q^2}{1 + D_{trans} Q^2 \tau_0}$$

$$\bar{\tau} = \frac{\tau_\alpha}{\beta} GammaFunc\left(\frac{1}{\beta}\right)$$

	Ea (kJ/mol)	
	WATER	NAGMA
Lorentzian	7.7404	18.4(1)
SE	7.7404	19.4(1)

J Teixeira, *et. al. PRA* **31**, 3 (1985)

Conclusions

Study of the water dynamic around proteins:

- Two models:
  - Fitting with 2 Lorentzian: take into consideration translational and rotational motions;
  - Stretched exponential (KWW): just translational part

    rotation?

    solution: increase resolution through lower q or intensity decrease.

- Diffusion is slower than bulk water in the temperature range of our study.

Acknowledgement

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