Group Meeting Update

UTK n → n' Group Meeting
Feb. 17, 2023
Cary Rock

Number Density: H_2O

- The number of particles in a given volume or amount of material
- Calculated as: $n = N_A \frac{\rho}{\rho_M}$
- Example: H_2O

$\rho_{H_2O} = 1 g/cm^3,\ m_H = 1.008\ \mathrm{g/mol},\ m_O = 15.999\ \mathrm{g/mol}$

$M = 2m_H + m_O = 18.015\ \mathrm{g/mol}$

$$n = N_A * \frac{1}{18.015} = 3.343 \times 10^{22}$$

$$n_H = 2n = 6.686 \times 10^{22}$$

$$n_O = n = 3.343 \times 10^{22}$$

Calculating V_{opt}: H_2O

- The energy potential felt by the incoming particle
  - Nuclear, Coulomb, magic, whatever
    - b_{coh} is the coherent scattering length
    - n is the number density
    - m_n is the neutron's mass
      - $\mathrm{Re}(b_{coh})$ because can be complex

$$V_{opt} = \frac{2\pi\hbar^2}{m_n}\mathrm{Re}(b_{coh})n$$

$$V_{opt} = \frac{2\pi\hbar^2}{m_n}(\mathrm{Re}(b^H_{coh})n_H + \mathrm{Re}(b^O_{coh})n_O$$

$$b^H_{coh} = -3.7406 \text{ fm}$$
$$b^O_{coh} = \quad 5.803 \text{ fm}$$

$$V_{opt} = -14.6 \text{ neV}$$

Scattering Length

- The mean free path between scattering events
- $\lambda = 1/\Sigma$
- $\Sigma = \sum_i n_i \sigma_{sc}$
- Assumes other potentials/etc. can be safely ignored
  - Not always the case – water!

“Evaluation of the neutron scattering cross-section for light water by molecular dynamics”

Y. Abe, T. Tsuboi, S. Tasaki

- https://www.sciencedirect.com/science/article/pii/S0168900213013703

$$\frac{\mathrm{d}^2\sigma_s}{\mathrm{d}\Omega\mathrm{d}\varepsilon} = \frac{2}{\hbar}\frac{\sigma_b^{\mathrm{H}}}{4\pi}\sqrt{\frac{E}{E_0}}S_s^{\mathrm{H}}(\kappa,\omega) + \frac{1}{\hbar}\frac{\sigma_b^{\mathrm{O}}}{4\pi}\sqrt{\frac{E}{E_0}}S_s^{\mathrm{O}}(\kappa,\omega)$$

$$S_s^{\mathrm{X}}(\kappa,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}t e^{-\mathrm{i}\omega t}F_s^{\mathrm{X}}(\kappa,t)$$

$$F_s^{\mathrm{X}}(\kappa,t) = \exp\left[-\frac{\kappa^2}{2}\Gamma^{\mathrm{X}}(t)\right]. \quad (3)$$

The width function $\Gamma^{\mathrm{X}}(t)$ is given by [9]

$$\Gamma^{\mathrm{X}}(t) = \frac{\hbar}{m_{\mathrm{X}}}\int_0^{\infty}\mathrm{d}\omega\,\frac{g^{\mathrm{X}}(\omega)}{\omega}\left\{\coth\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right)(1-\cos\,\omega t) - \mathrm{i}\,\sin\,\omega t\right\}$$

Elastic Scattering Cross-Section

- E(thermal) =25 meV
- => σ_{sc} ~ O(110) barns at T = 293 K
- => λ_{sc} ~ .249 cm,
  Σ_{sc} ~ 4.011 cm
  - σ_{sc} = 49 b =>
    λ_{sc} ~ .61 cm
- Measured: 0.27 cm according to NIST (111 b)