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New Scattering Kernels and Neutron Cross Sections for Superfluid He

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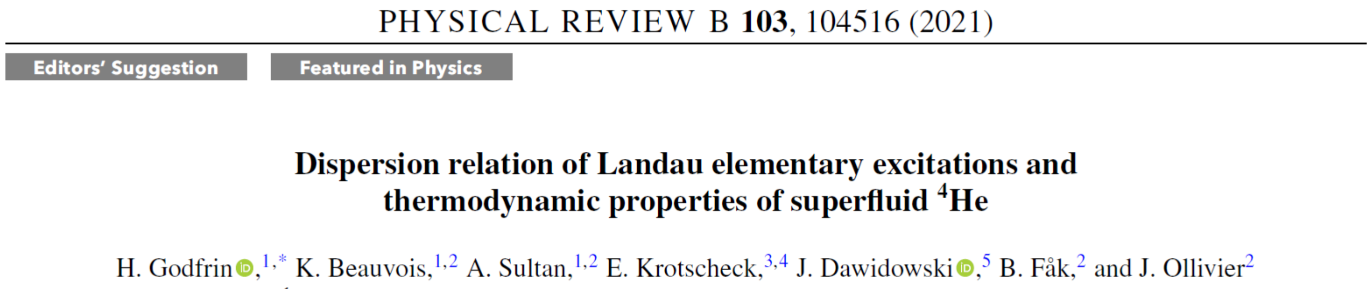
WORKSHOP ON UCN AND VCN SOURCES AND THEIR APPLICATIONS

8-11 April 2024, Almaty, Kazakhstan

Introduction

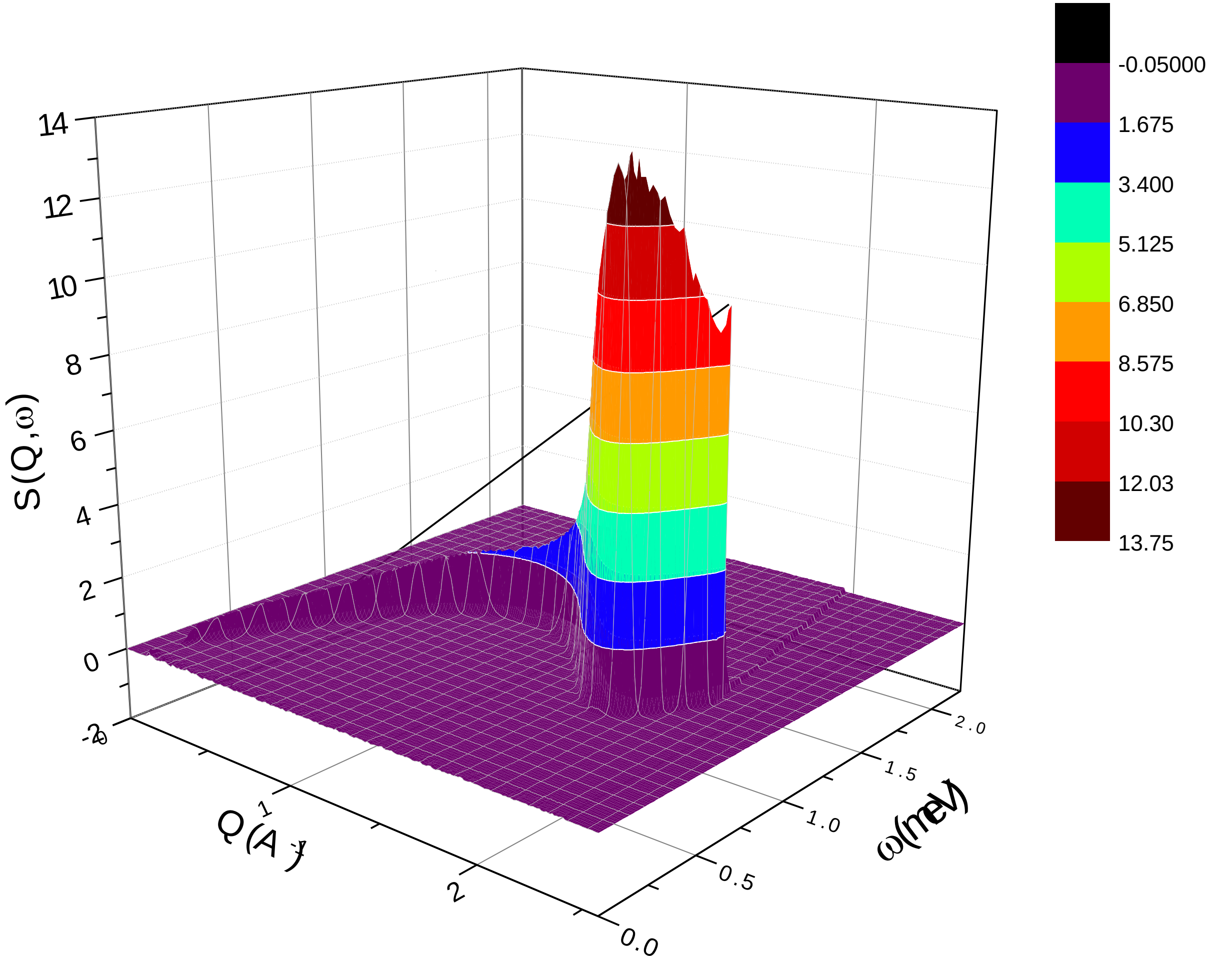


PHYSICAL REVIEW B **103**, 104516 (2021)

Editors' Suggestion **Featured in Physics**

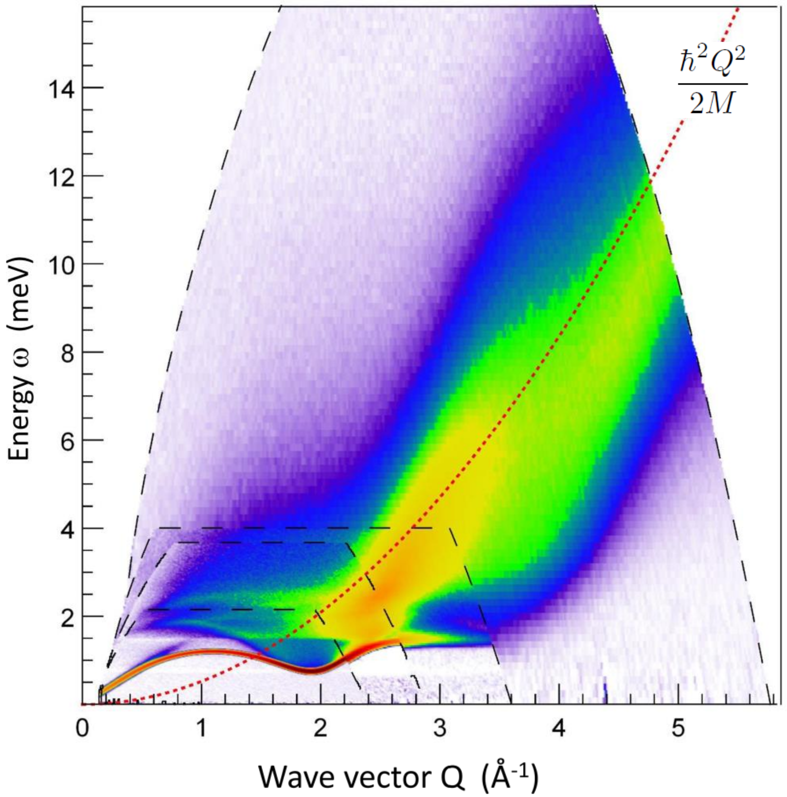
Dispersion relation of Landau elementary excitations and thermodynamic properties of superfluid ^{4}He

H. Godfrin,[1,*] K. Beauvois,[1,2] A. Sultan,[1,2] E. Krotscheck,[3,4] J. Dawidowski,[5] B. Fåk,[2] and J. Ollivier[2]



Introduction

Low-energy neutron scattering at small momentum transfer and temperatures ≲ 1 K from superfluid ^{4}He is dominated by the collective phonon-roton mode.



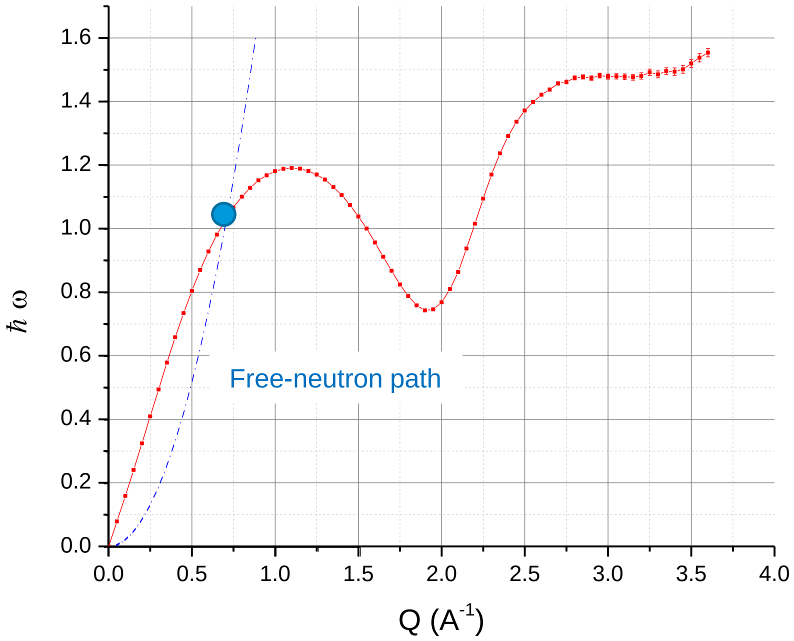
S(Q,ω) of superfluid ^{4}He as a function of wave vector and energy transfer, measured at T ≲100 mK

K. Beauvois *et al.*, *Phys.Rev.* B **97**, 184520 (2018)

Introduction

- The major mechanism for the production of ultra-cold neutrons (UCNs) is due to the downscattering of 1 meV neutrons. This happens at the crossing point between a free neutron and the phonon-roton dispersion curve.
- Multi-phonon excitations can play a role in UCN production.
- In addition, superfluid ^{4}He also exhibits zero absorption cross section and limited up-scattering at low temperatures.
- These properties make it an attractive option as a source of UCNs at neutron scattering facilities.

Dispersion relation $\mathcal{E}(Q)$ of the single excitations

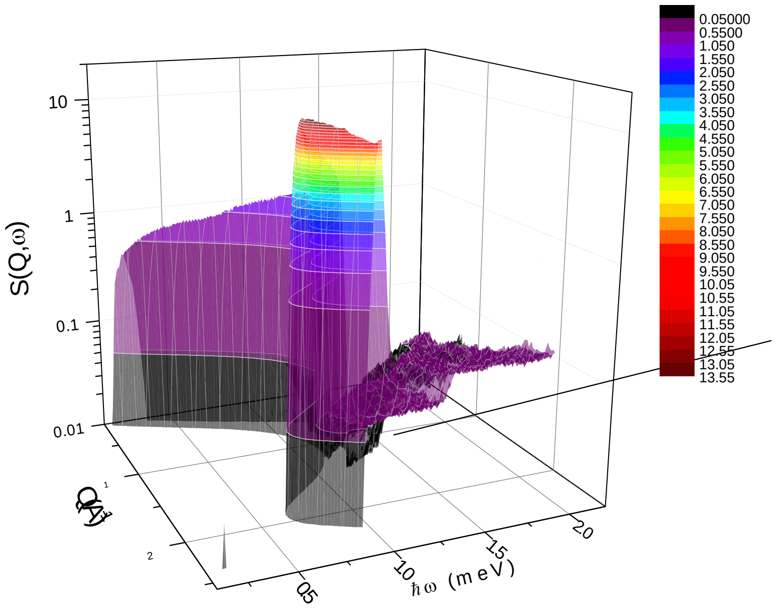


Introduction

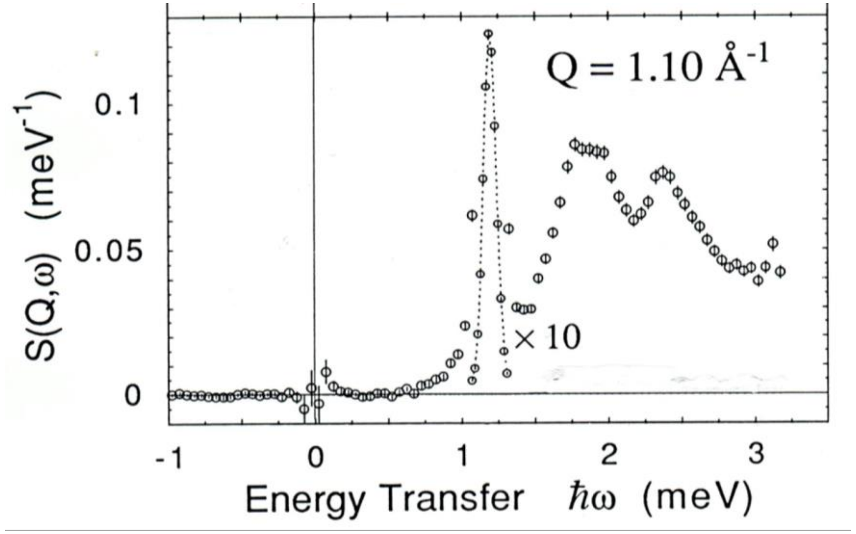
- Limited models exist for neutronics calculation using modern code such as Geant4, MCNP, OpenMC and PHITS.
- Bernnat et. al. (1997,2002) – Developed a simple model for liquid helium in ACE format. However, it was not suitable for UCN calculations.
- Abe and Morishima (1997-2001) – Developed a model for temperatures between 0.1 K and 4.0 K and multi-group libraries. The multi-phonon component was not included.
- With developments of new tools, such as NCrystal, we developed a new model including both single-phonon and multi-phonon components with the aim to be used with modern Monte-Carlo code.
- The model has been published in:

J.R. Granada, D.D. DiJulio, J.I. Marquez Damian, G. Muhrer,
Nucl. Instr. and Methods in Physics Research **A** 1053 (2023) 168284

The Model



H. Godfrin (priv. comm.)



K. Andersen *et al.* (1994)

At temperatures below T ≈ 1.3 K, the neutron scattering from superfluid ^{4}He can be into distinct single-phonon and multi-phonon contributions, given by

$$\boxed{S(Q,\omega) = S_s(Q,\omega) + S_m(Q,\omega)}$$

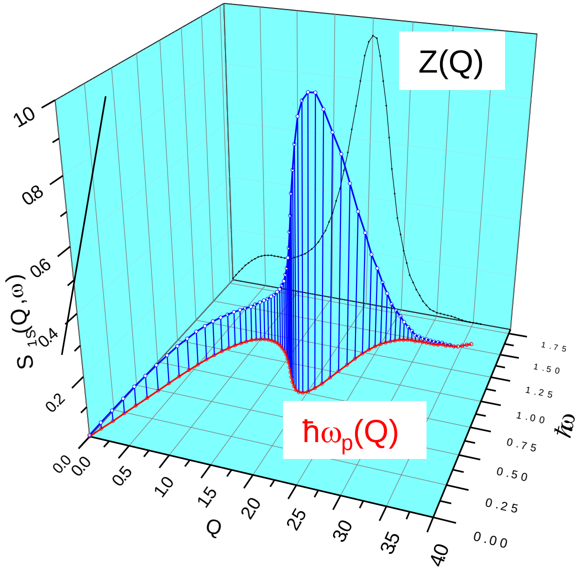
where $S_S(Q, \omega)$ is the single-phonon contribution and $S_M(Q, \omega)$ is the multi-phonon contribution

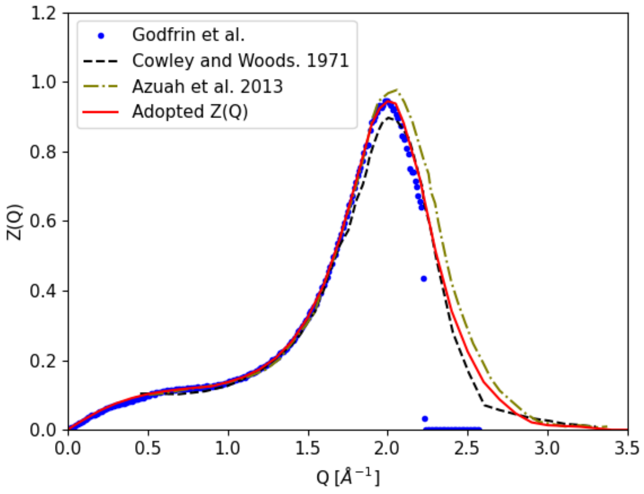
The Model

For the single-excitation term below 3.4 Å^{-1}, we have used a Lorentzian of the form

$$S_s(Q,\omega) = \frac{Z(Q)}{\pi}\,\frac{\Gamma(Q)}{(\hbar\omega - \hbar\omega_p(Q))^2 + \Gamma(Q)^2}$$

where $\hbar\omega_p(Q)$ is the energy of the single-phonon excitations and $\Gamma(Q)$ is the halfwidth at half maximum and depends on the temperature of the liquid. $Z(Q)$ is the single-phonon structure factor.





The Model

$S_M(Q, \omega)$ is the multi-phonon contribution and depends on the self-scattering function, $S_M^{self}(Q, \omega)$. The self-scattering function can be calculated using the standard phonon expansion approach, within the Gaussian Approximation, and starting at the n = 2 term, given by

$$S_M^{\mathrm{self}}(Q,\omega) = h(Q)e^{-W(Q)} \sum_{n=2}^{\infty} \frac{1}{n!}(W(Q))^n \tau_n(\omega)$$

where

$$\tau_1(\omega) = \frac{P(\omega)}{\lambda_s} e^{-\frac{\hbar\omega}{2k_B T}} \quad , \quad W(Q) = \frac{\hbar^2 Q^2}{2Mk_B T}\lambda_s \quad , \quad \lambda_s = \int_{-\infty}^{\infty} P(\omega) e^{\frac{\hbar\omega}{2k_B T}} d\omega$$

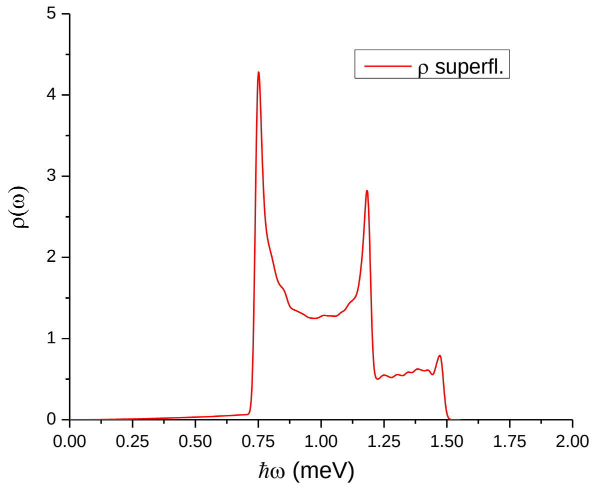
h(Q) is introduced as a normalizing function for $S_M^{self}(Q, \omega)$ as the expansión starts at n=2. The function *P(ω)* is related to the weighted frequency distribution *ρ(ω)* through

$$P(\omega) = \frac{\rho(\omega)}{\frac{2\hbar\omega}{k_B T} sinh(\frac{\hbar\omega}{2k_B T})}$$

The Model

The phonon weighted frequency distribution, $\rho(\omega)$, can be computed from experimental data. $S_s^{exp}(\omega)$ is denoted as the integral over Q of the experimental dispersion curve, $S_s^{exp}(Q,\omega)$, and thus

$$\rho(\omega) = \frac{\hbar\omega}{k_B T}[e^{\frac{\hbar\omega}{kT}} - 1]S_s^{\mathrm{exp}}(\omega)$$



The multiphonon term of the total scattering function, applying the Sköld approximation, is then

$$\boxed{S_M(Q,\omega) = H(Q)S_M^{\mathrm{self}}\left(\frac{Q}{\sqrt{u(Q)H(Q)}},\omega\right)}$$

With this definition, and the form of $S_1(Q,\omega)$, the total scattering function $S(Q,\omega)$ will satisfy the first Sum Rule

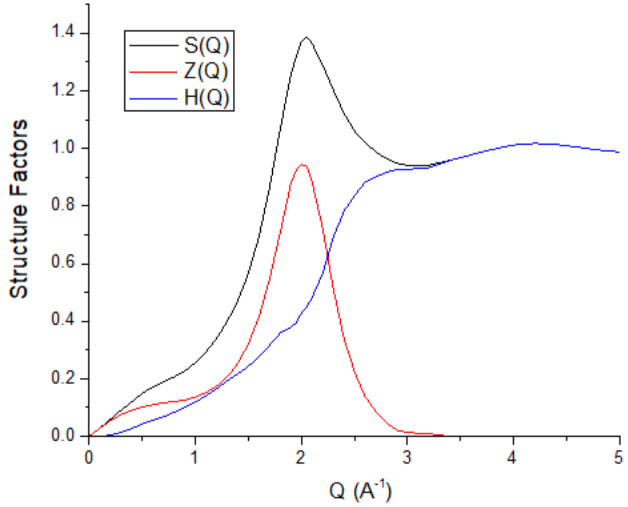
$$\boxed{S(Q) = \int_{-\infty}^{\infty} S(Q,\omega)d\omega \quad = Z(Q) + H(Q)}$$

The Model

The multi-phonon structure factor is computed as

$$H(Q) = S(Q) - Z(Q)$$

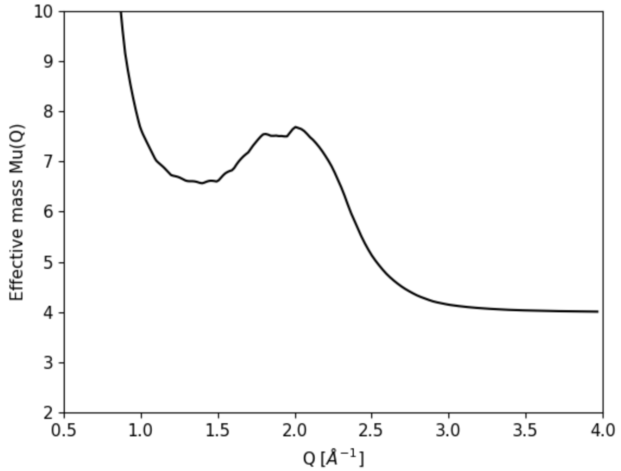
where the slope of $S(Q \rightarrow 0)$ at very low temperatures can be computed using the value v = 238.3m/s for the sound velocity



To satisfy the second Sum Rule

$$\boxed{\frac{\hbar^2 Q^2}{2M} = \hbar \int_{-\infty}^{\infty} \omega S(Q,\omega) d\omega}$$

an effective mass Mu(Q) has been introduced in the expression of $S_M(Q, \omega)$.

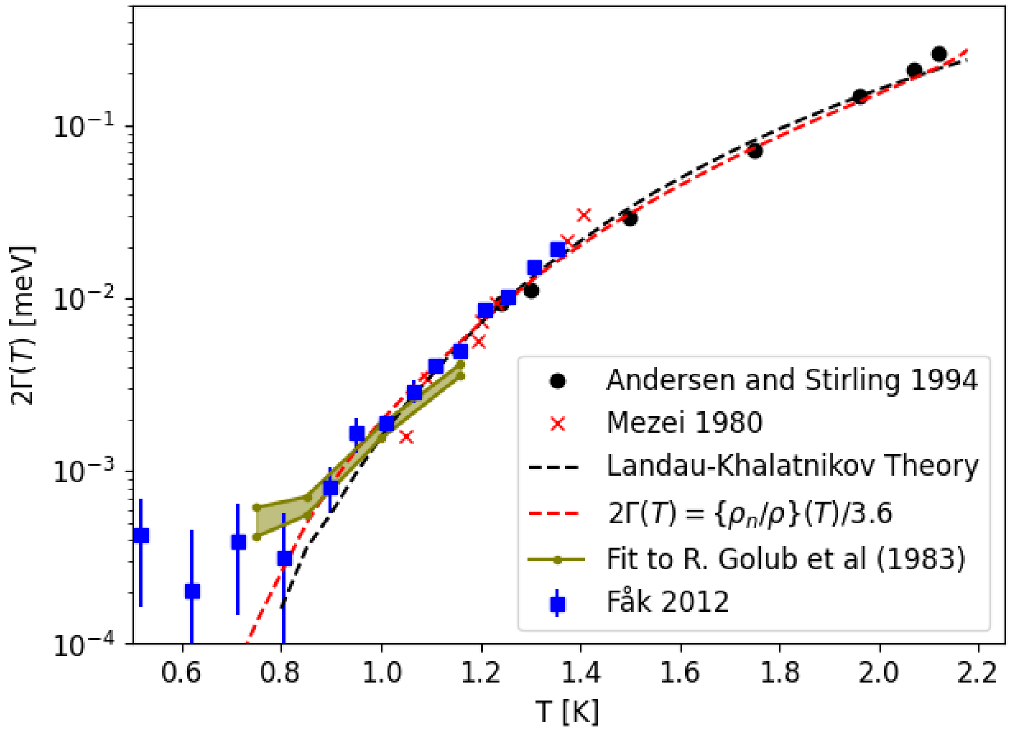


The Model

- The model is programmed into a modified version of the LEAPR module of NJOY2016.

- The main input to the model includes:
    - Phonon-roton dispersion curve
    - The single-phonon and multi-phonon structure factors, Z(Q) and H(Q), respectively
    - The weighted frequency distribution
    - The effective mass function
    - The normalizing function, h(Q), is calculated internally by the code

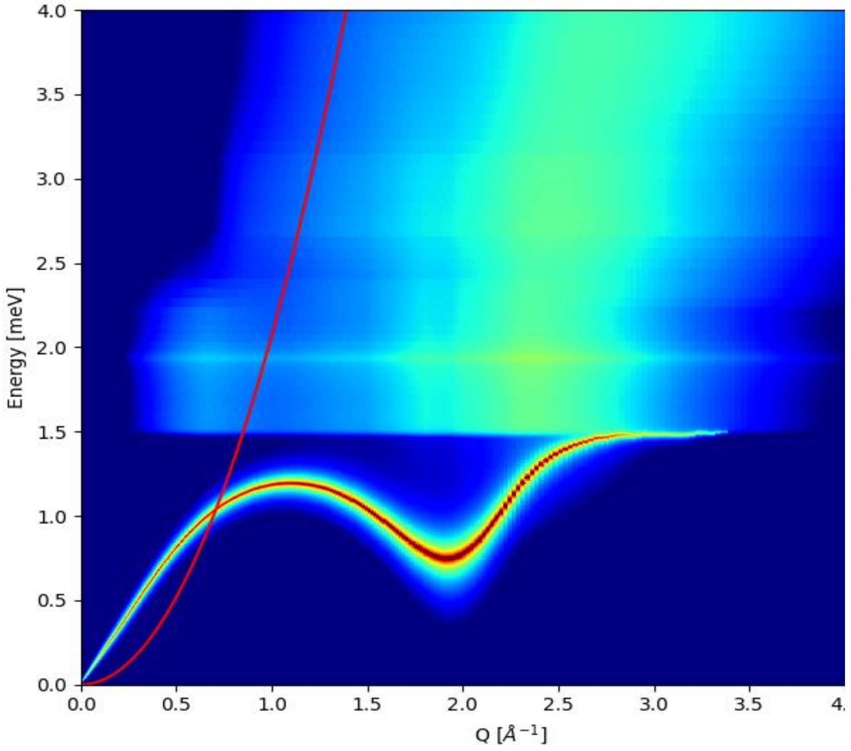
- An additional input is the width of the single phonon excitation Lorentzian
    - At 1.0 K and below, it was determined by fitting the cross-sections at low energies from R. Golub *et al* (1983).
    - At temperatures of 1.24 K and 1.3 K, the widths were adopted from K. Andersen *et al* (1994).

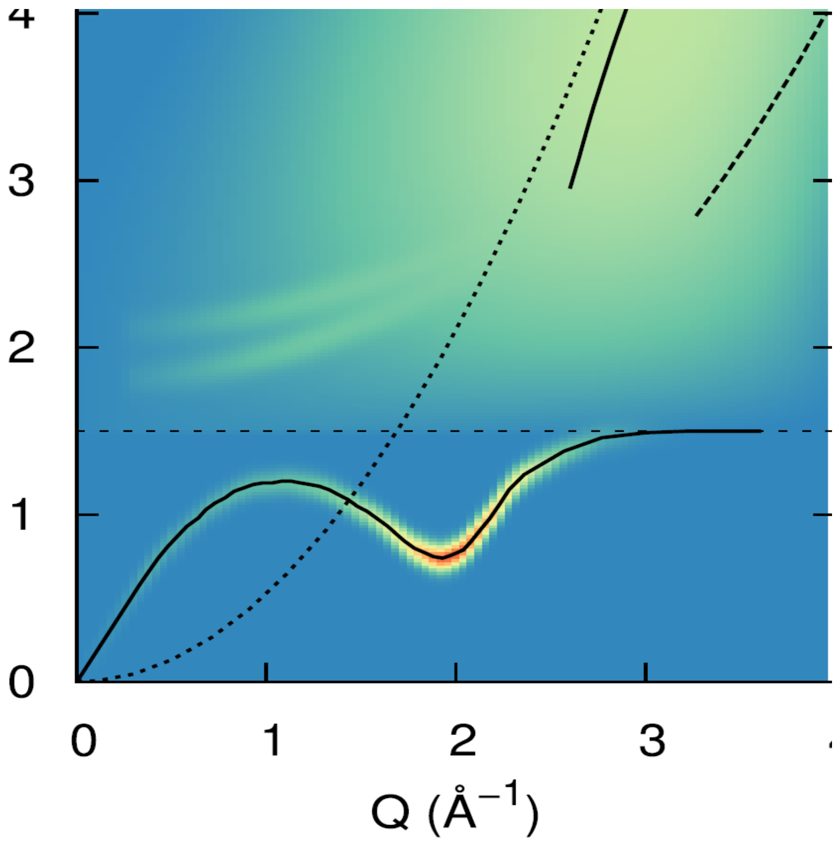


Results

THE SCATTERING FUNCTION S(Q, ω)

Calculated scattering kernel at 1.3 K. The red line is the dispersion curve of a free neutron.

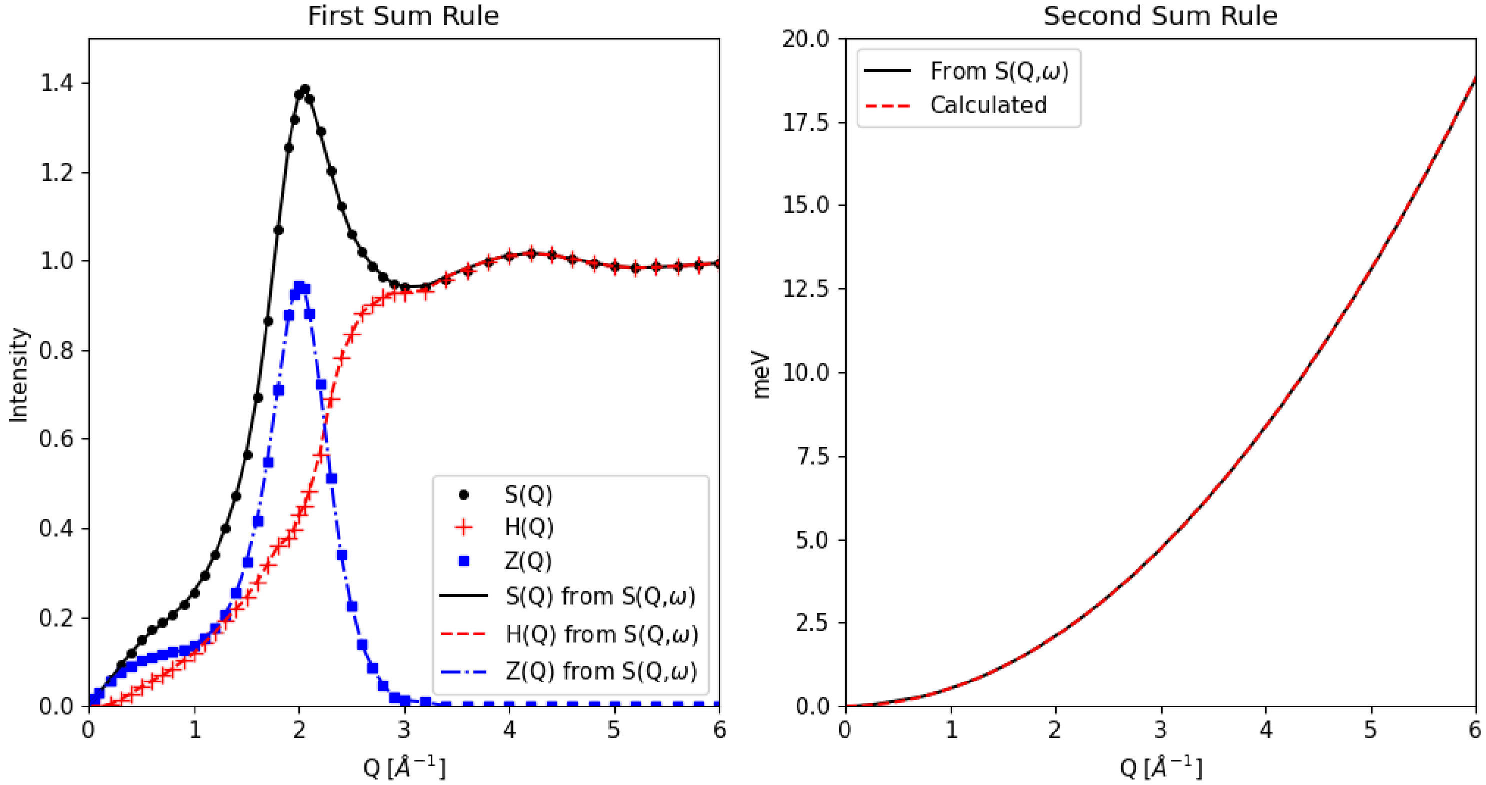




Adapted from Glyde (2018)

Results

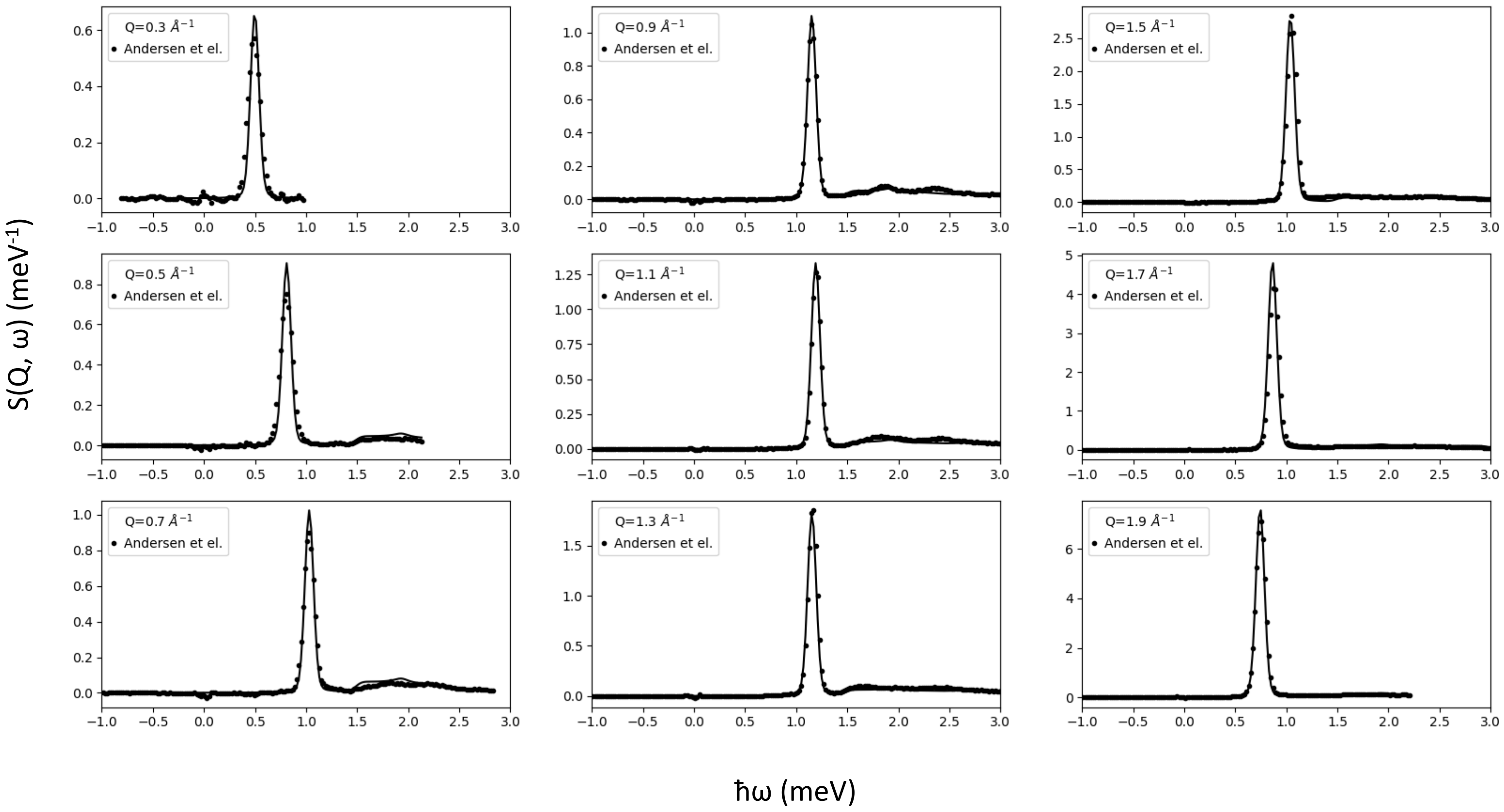
SUM RULES



Projected structure factors at 1.3 K from the scattering kernels compared to the input data.

Results

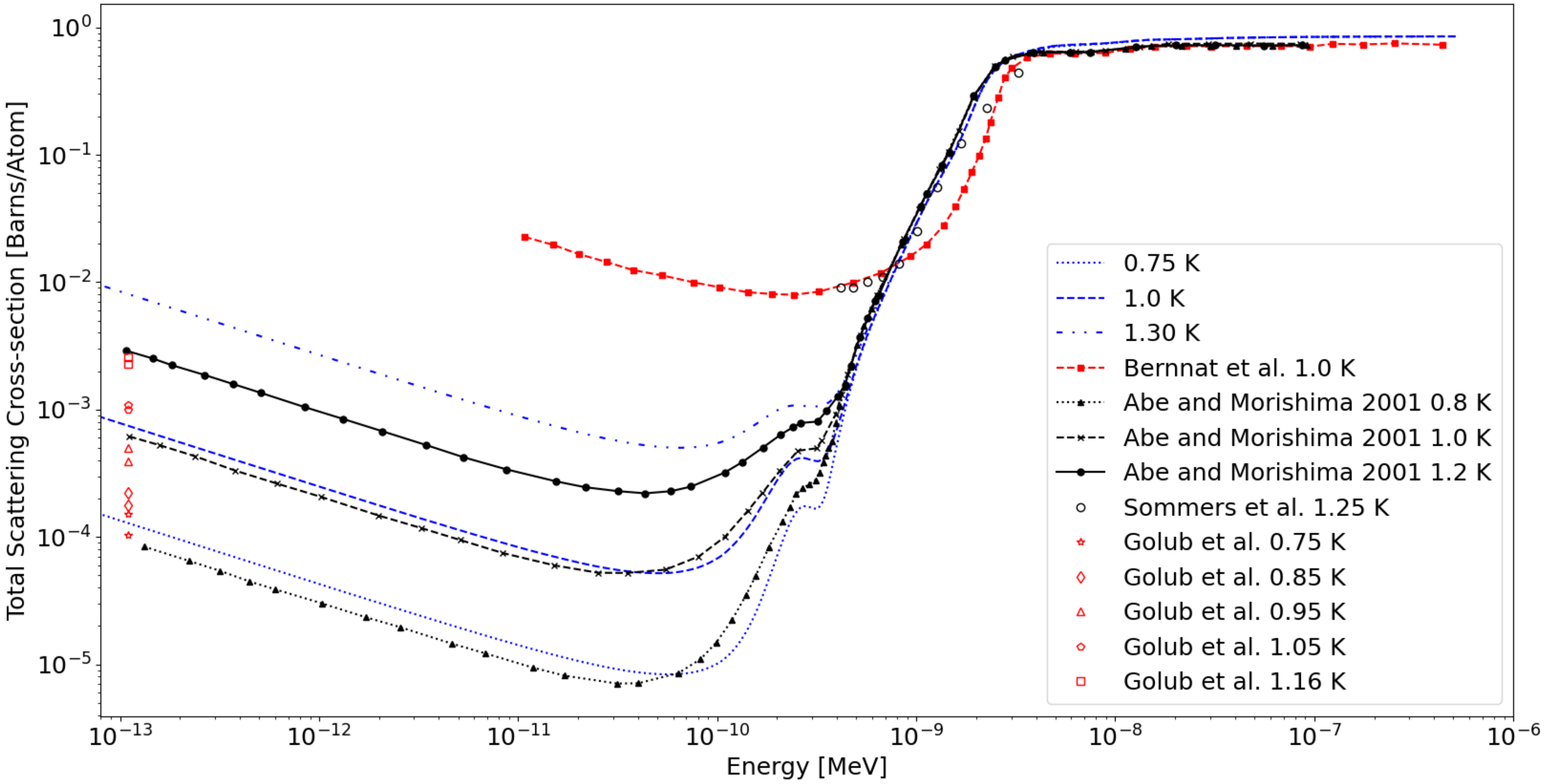
Dynamic structure factor at 1.24K convoluted with an instrument resolution function



Data from K. Andersen Thesis (priv. Comm.)

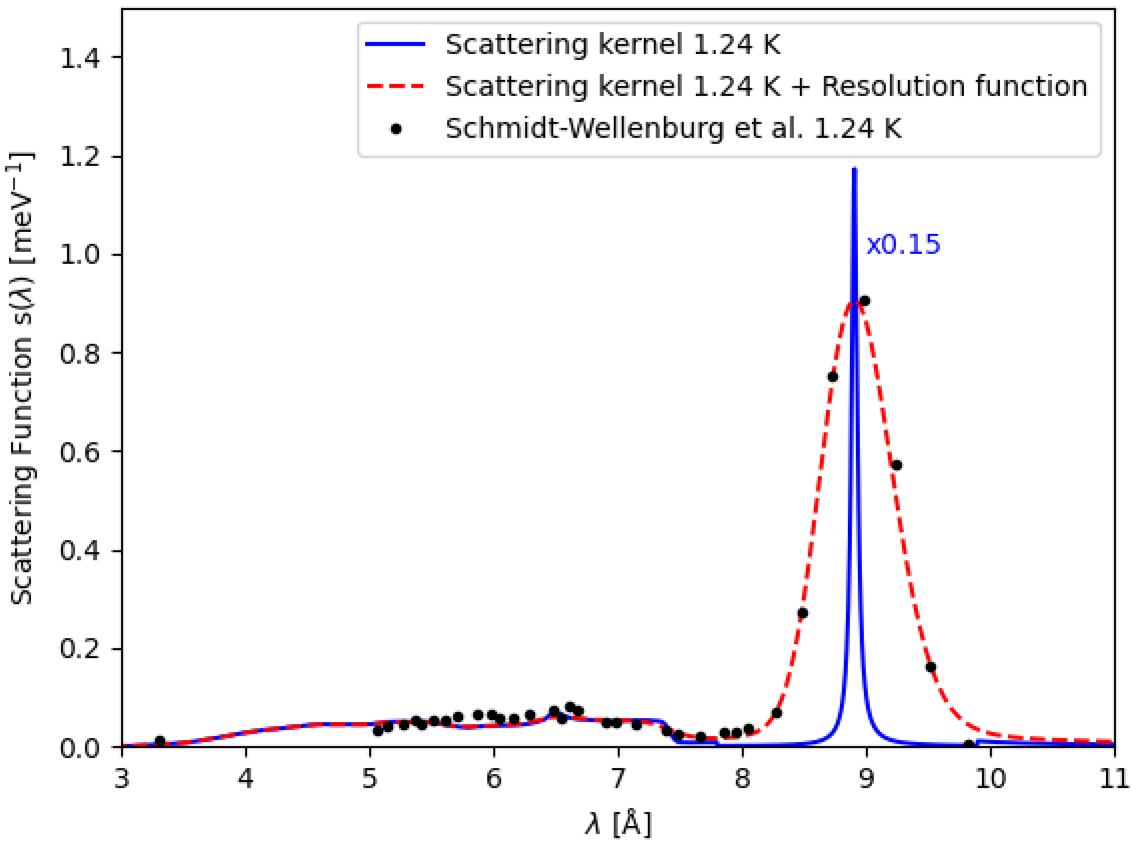
Results

TOTAL SCATTERING CROSS SECTION



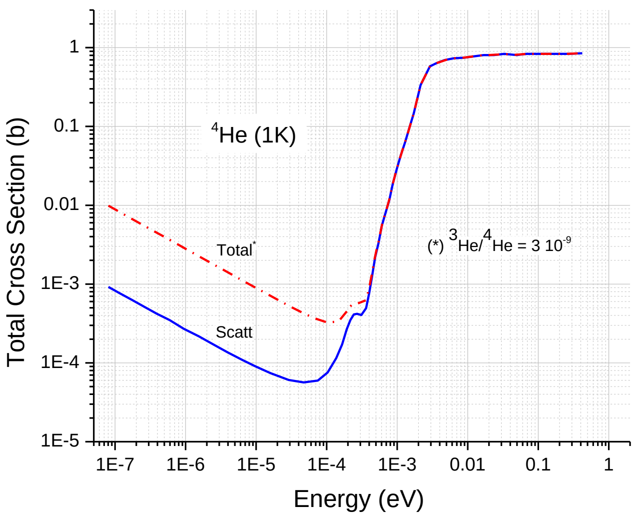
Results

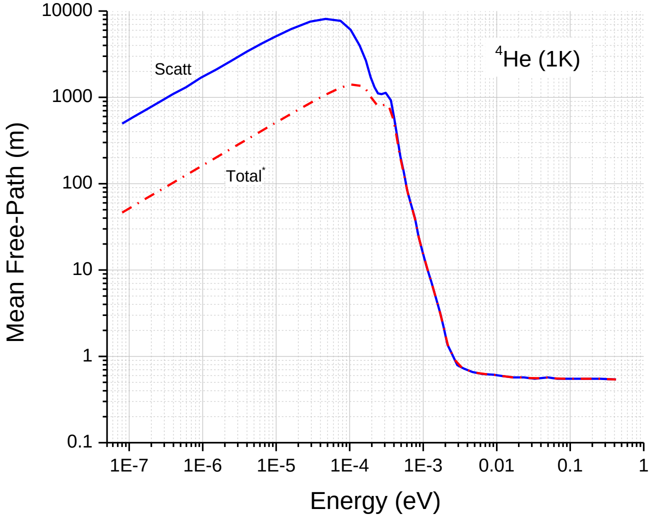
ULTRA COLD NEUTRONS PRODUCTION

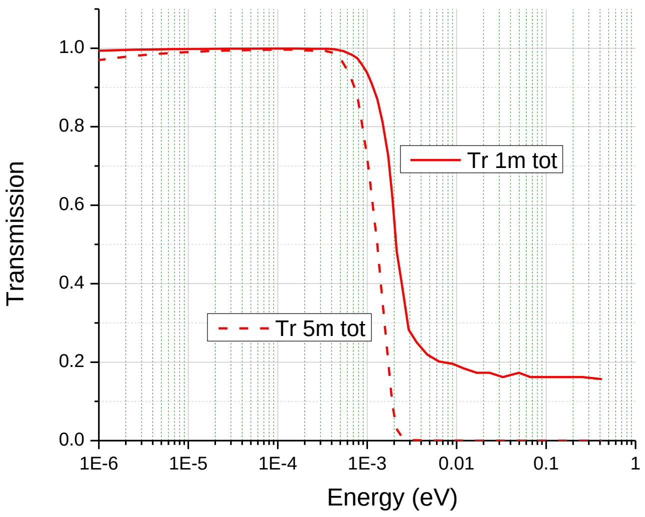


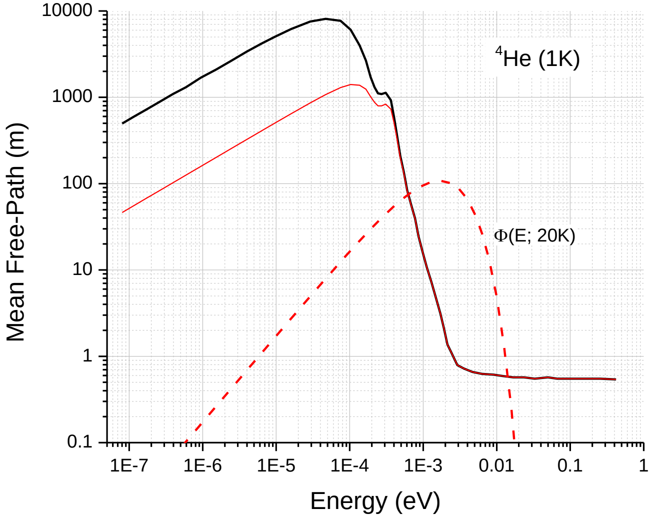
$$s(\lambda) = \hbar \int S(q, \hbar\omega)\delta(\hbar\omega - \hbar^2 k^2/2m_{\mathrm{n}})\,\mathrm{d}\omega$$

Results







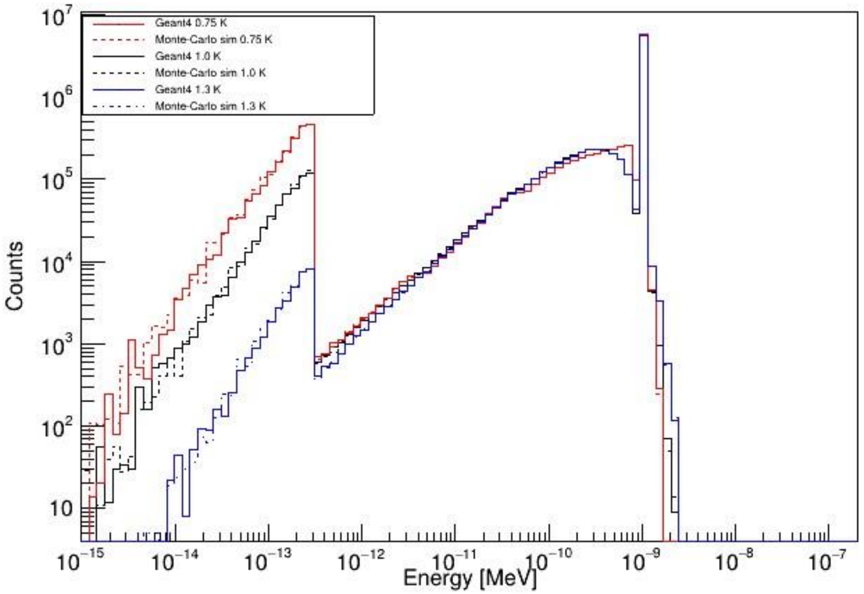


Upper limit He-3/He-4 taken from Yoshiki *et al.* (*Cryogenics* **45** (2005) 399–403)

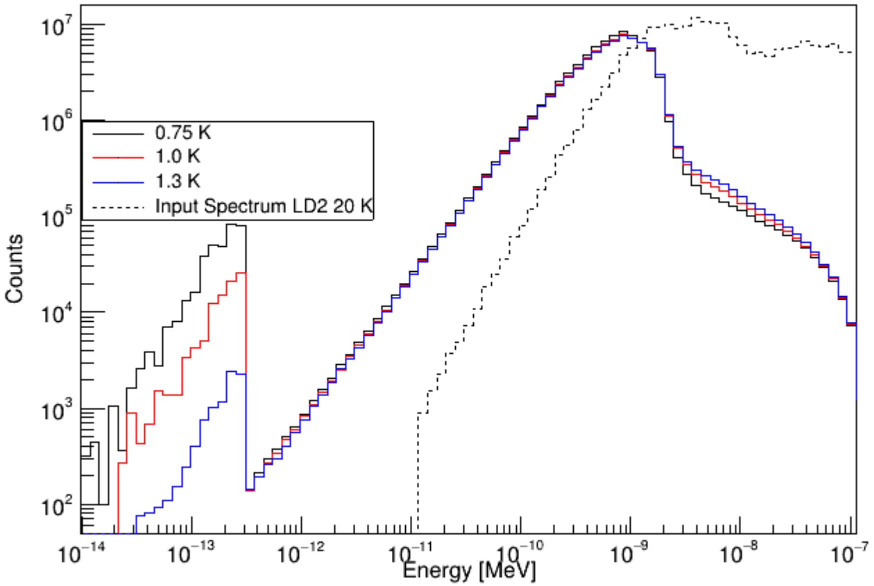
Monte-Carlo simulations

300 cm thick infinite slab, perfect reflecting walls for UCNs. Neutron beta-decay included.

Source = 1 meV neutrons



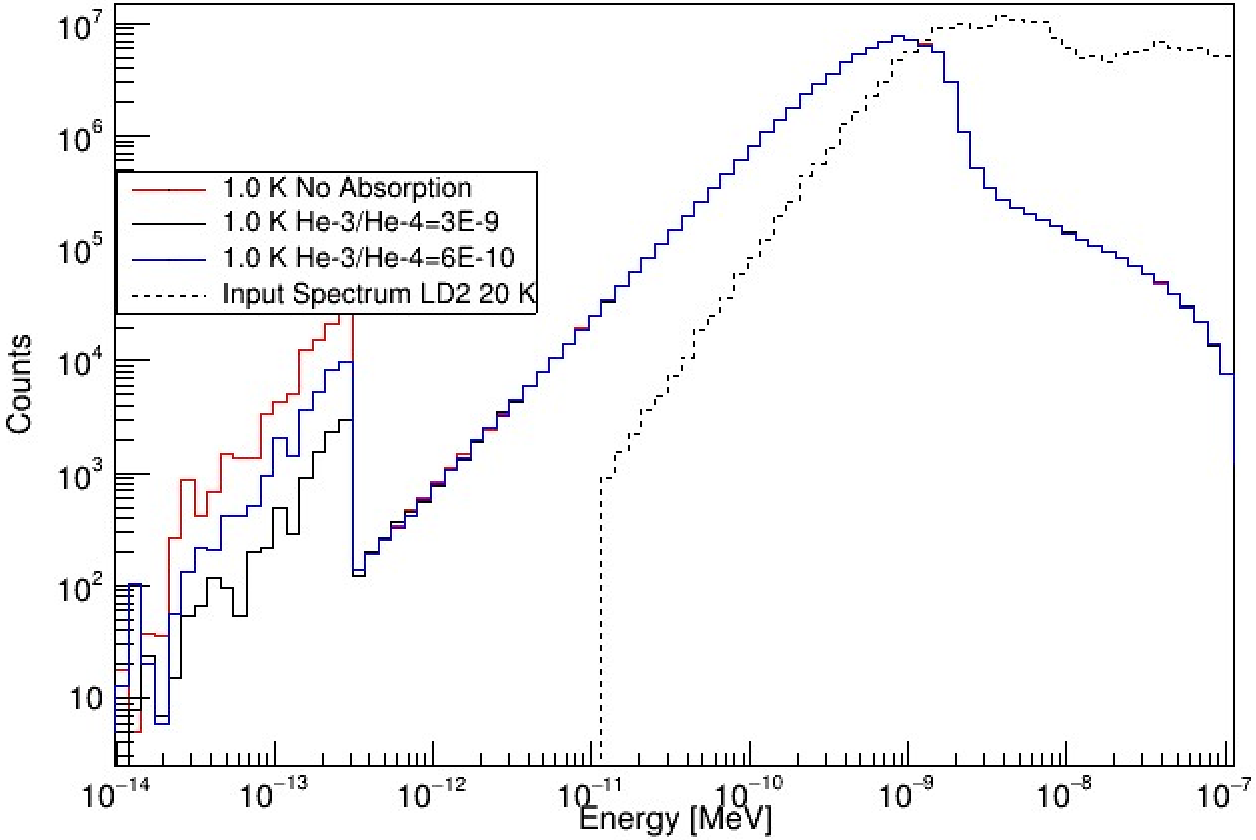
Source = 20 K LD2



Inspired by the work carred out in:
Abe and Morishima, *Nucl. Instr. and Methods in Physics Research* **A** (2002) 414-421

Monte-Carlo simulations

Impact of contamination of He-3



Conclusions

- We have developed a new model for the description of superfluid ^{4}He at low temperatures and programmed it into a custom version of NJOY2016 to produce thermal-scattering data.
- The model includes an exact description of the phonon-roton dispersion curve and a multi-phonon component, and we have shown that it reproduces well available measured cross-section and UCN production data.
- The current model can be used to create input that can be used together with NCrystal, either stand-alone or coupled together with a Monte-Carlo code, for calculations of UCN production from ^{4}He sources at low temperatures.

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Thank you for your attention!