



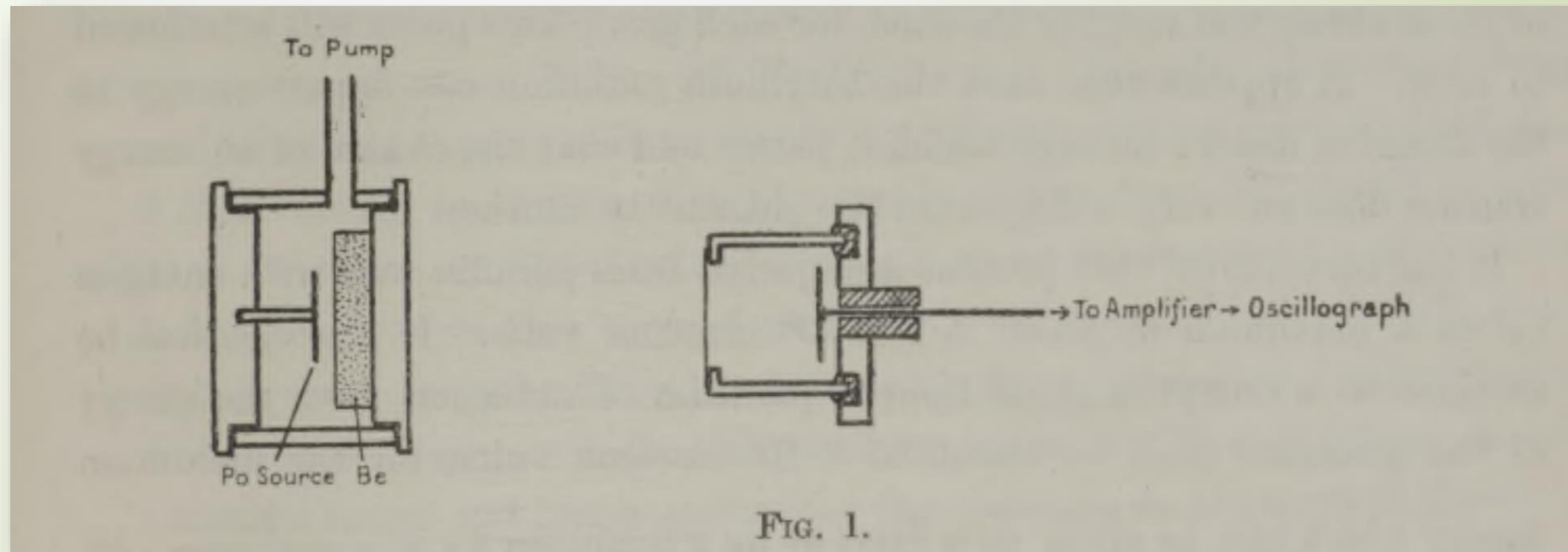
# Neutron Compton Scattering

**Giovanni Romanelli – Università degli Studi di Roma Tor Vergata**

12° of September 2022 - 17° Oxford School on Neutron Scattering

# Neutron scattering off hydrogen in the Chadwick experiment:

*Elastic? Quasi-elastic? Inelastic? Else?*

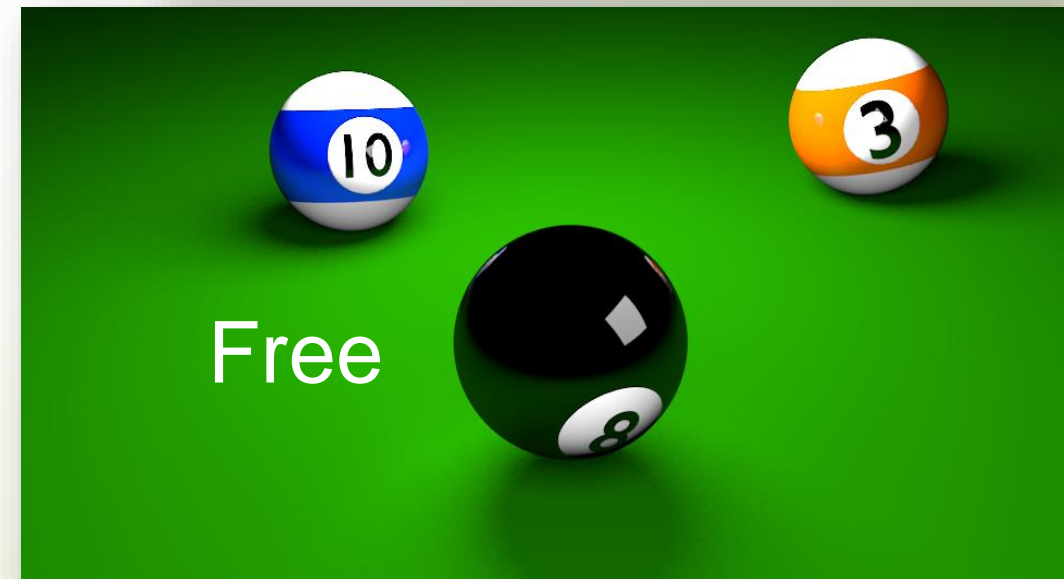
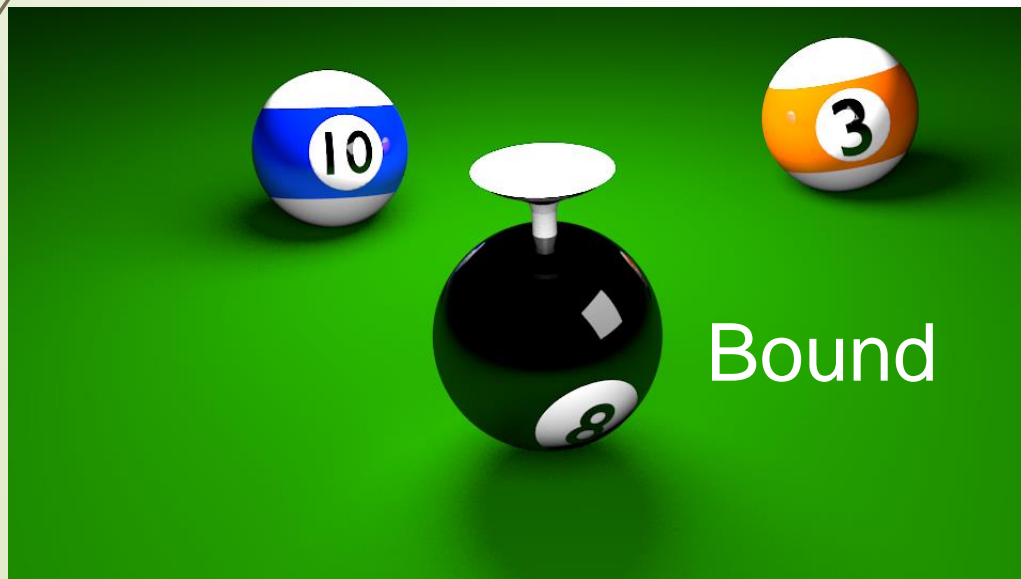
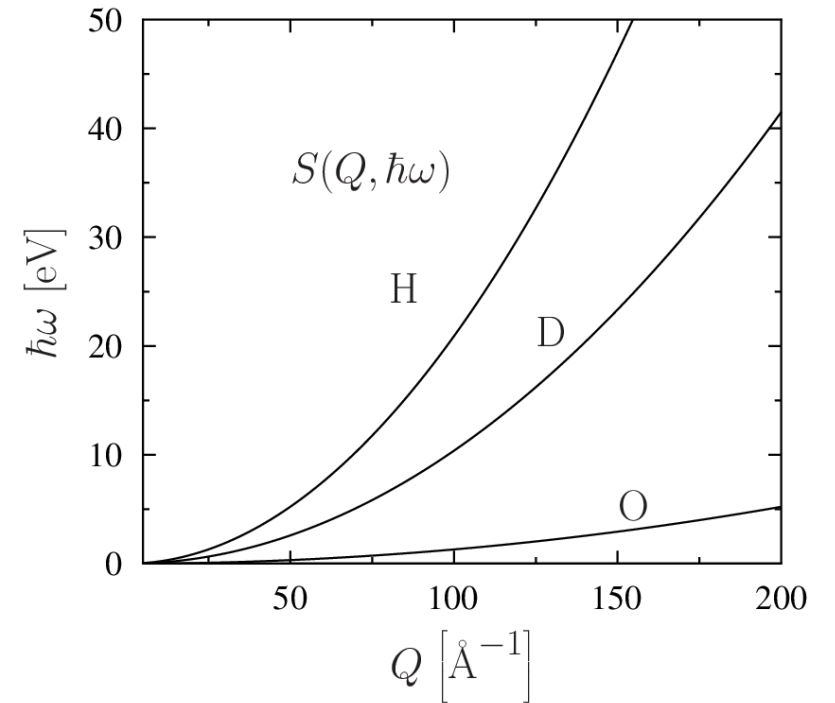


# The Impulse Approximation

$$k_0 + p = k_1 + p'$$

$$E_0 + \frac{p^2}{2M} = E_1 + \frac{p'^2}{2M}$$

$$\sigma_{free} = \frac{\sigma_{bound}}{\left(1 + \frac{m}{M}\right)^2}$$



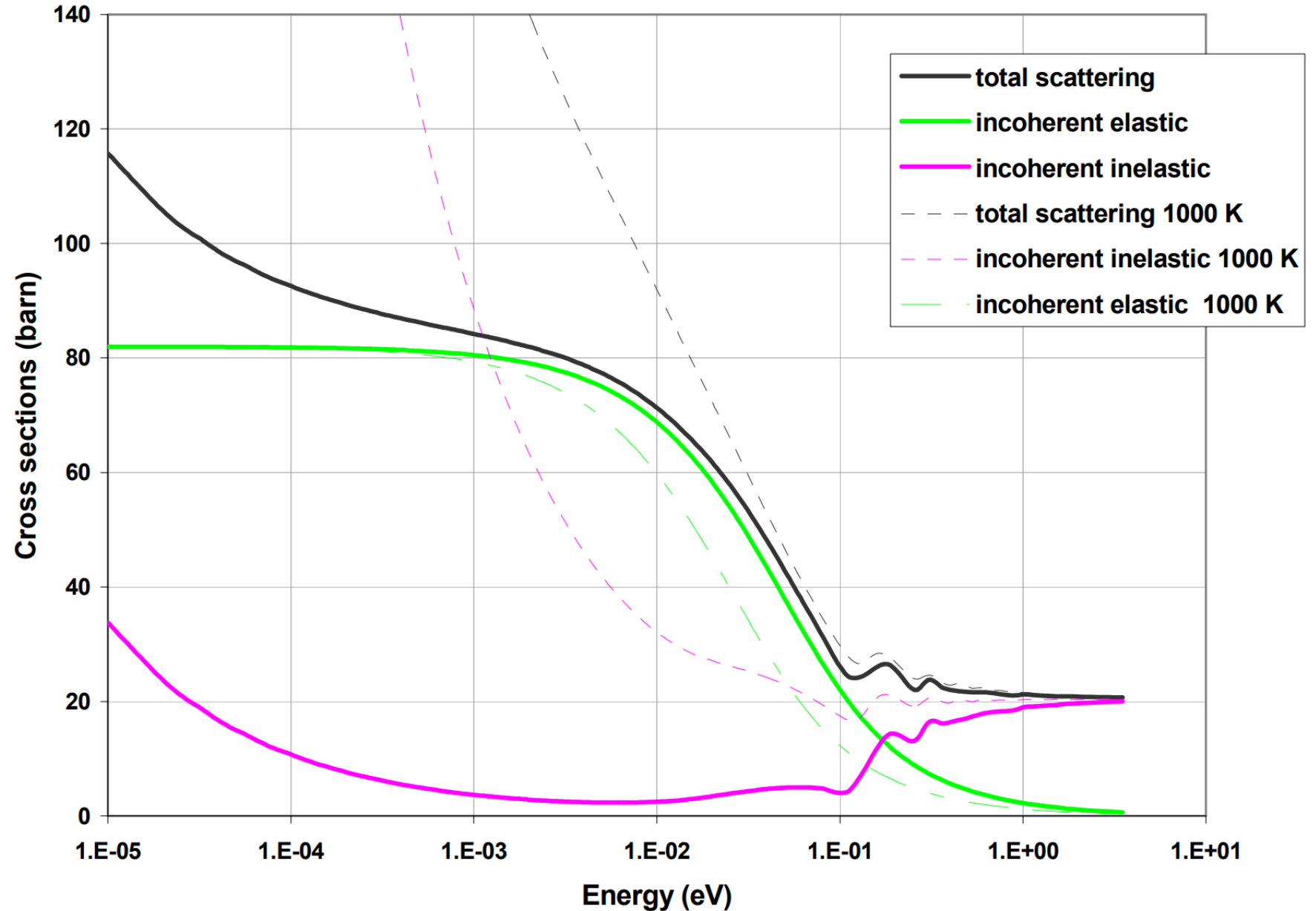
# The total scattering cross section for $ZrH_2$



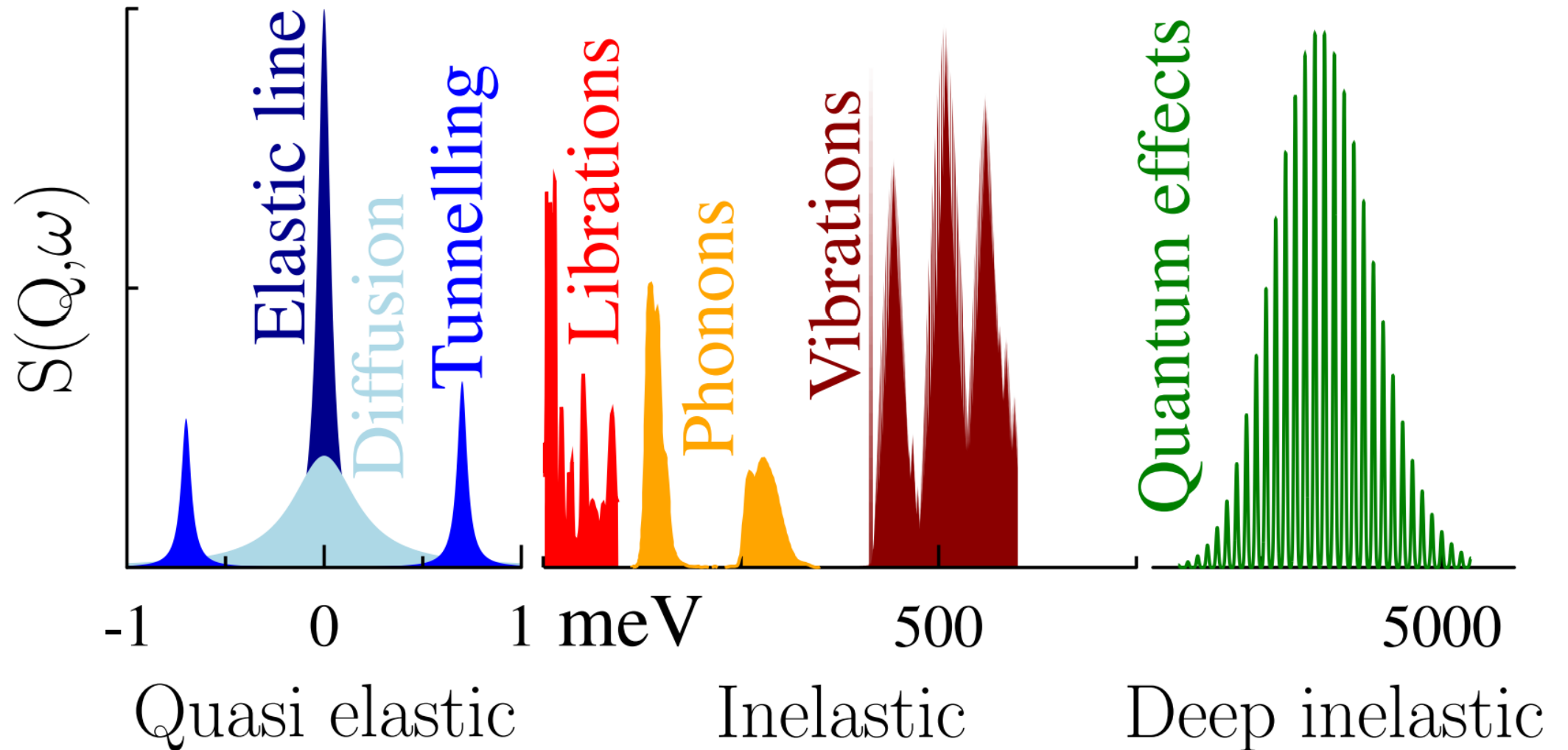
INTERNATIONAL ATOMIC ENERGY AGENCY  
INDC(NDS)-0470  
Distr. AC

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

Thermal Neutron Scattering Data  
for the Moderator Materials  
 $H_2O$ ,  $D_2O$  and  $ZrH_x$   
in ENDF-6 Format and as ACE Library  
for MCNP(X) Codes



# From «elastic» to «deep inelastic»



# Recoil lines and West scaling variable

Experimental definition

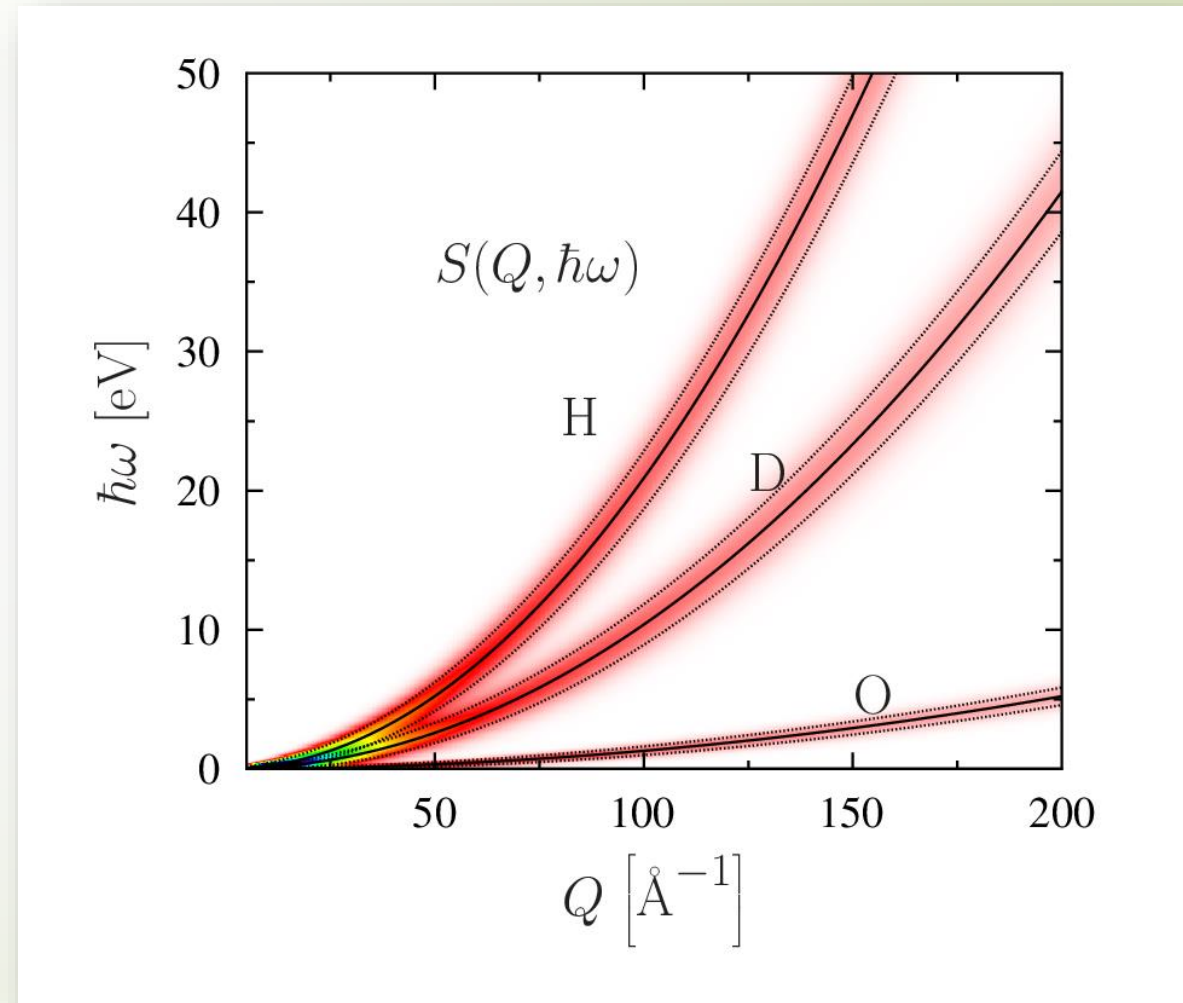
$$y = \frac{M}{\hbar Q} \left( \hbar\omega - \frac{\hbar^2 Q^2}{2M} \right)$$

Physical interpretation

$$\hbar y = \mathbf{p} \cdot \hat{\mathbf{Q}}$$

Momentum distribution

$$\langle p^2 \rangle = \sigma^2 = \int p^2 n(\mathbf{p}) d\mathbf{p}$$





## Some useful formulas for the Compton profile

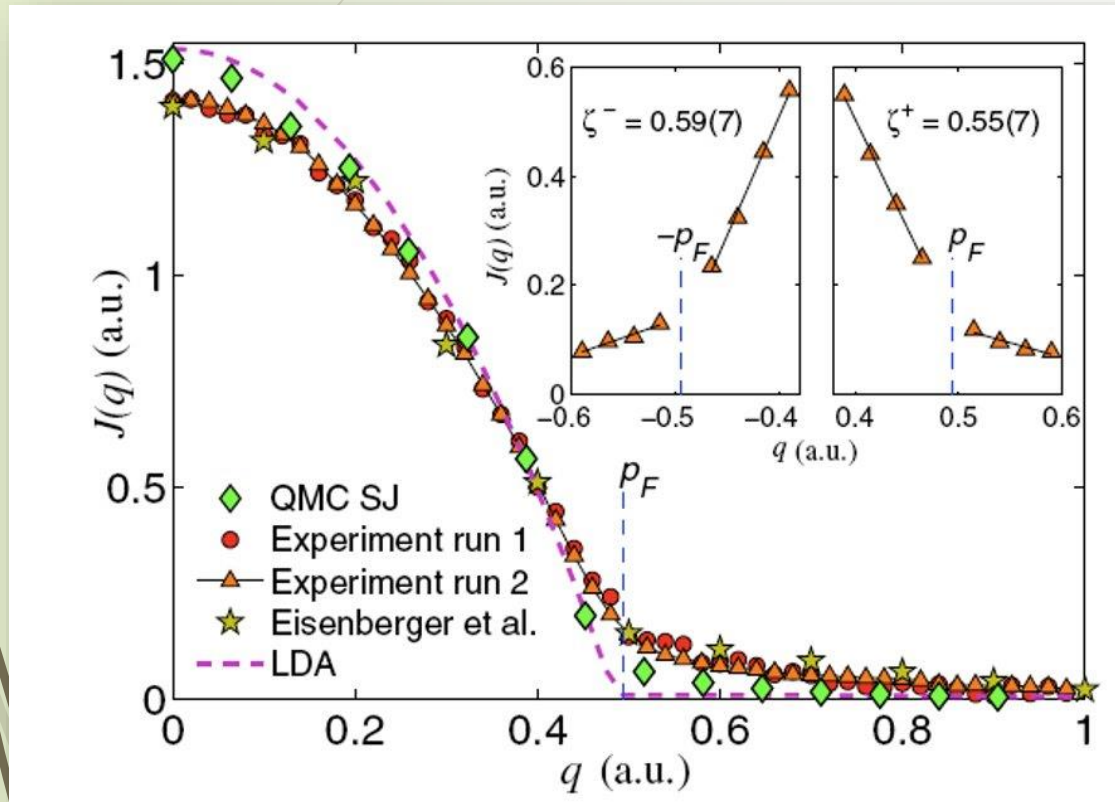
$$S_{IA}(\mathbf{q}, \omega) = \frac{M}{\hbar q} J(y, \hat{q})$$

$$J(y, \hat{q}) = \hbar \int n(\mathbf{p}') \delta(\hbar y - \mathbf{p}' \cdot \hat{q}) d\mathbf{p}'$$

$$J(y) = 2\pi\hbar \int_{|\hbar y|}^{\infty} p n(p) dp$$

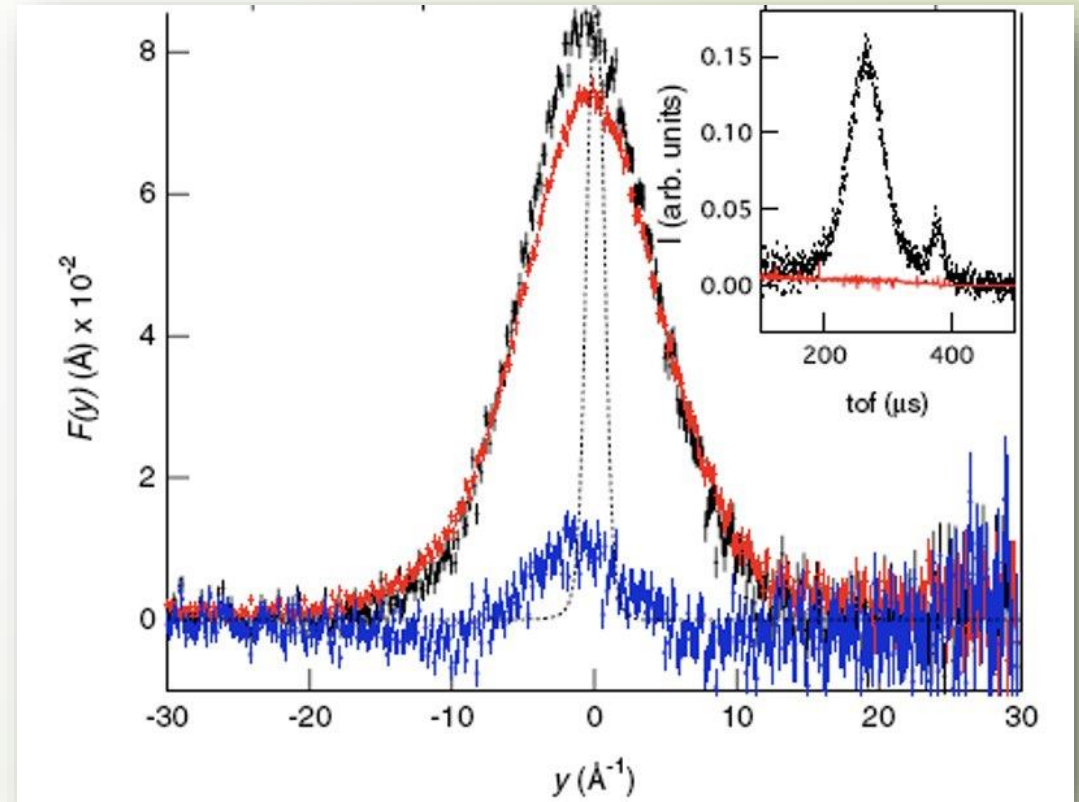
# Different types of Compton scattering

Electrons (ID16, ESRF)



Compton profile of Na; p- resolution  $\approx 13\%$  FWHM  
S. Huotari et al, PRL 105, 086403 (2010)

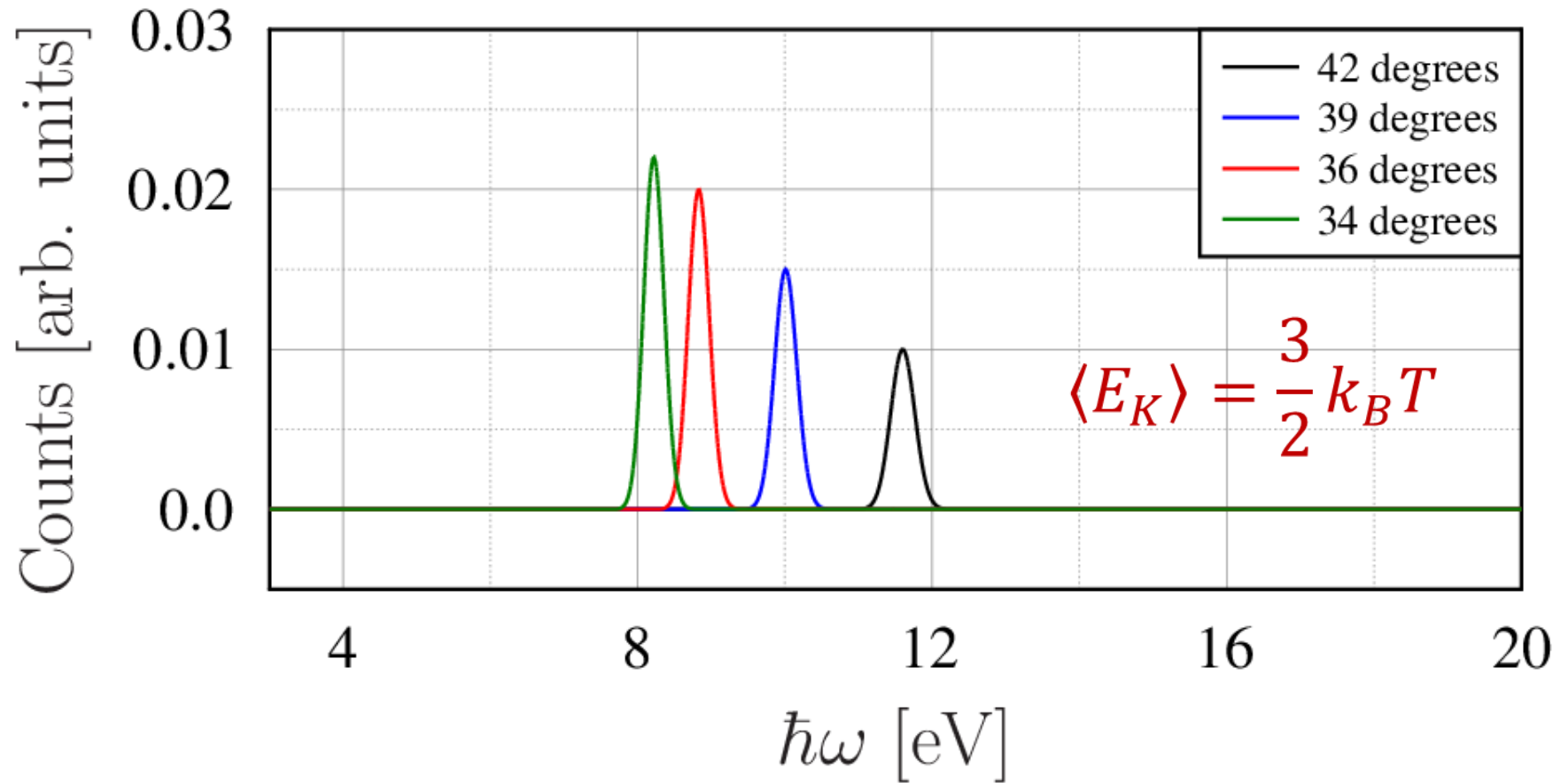
Protons (VESUVIO, ISIS)



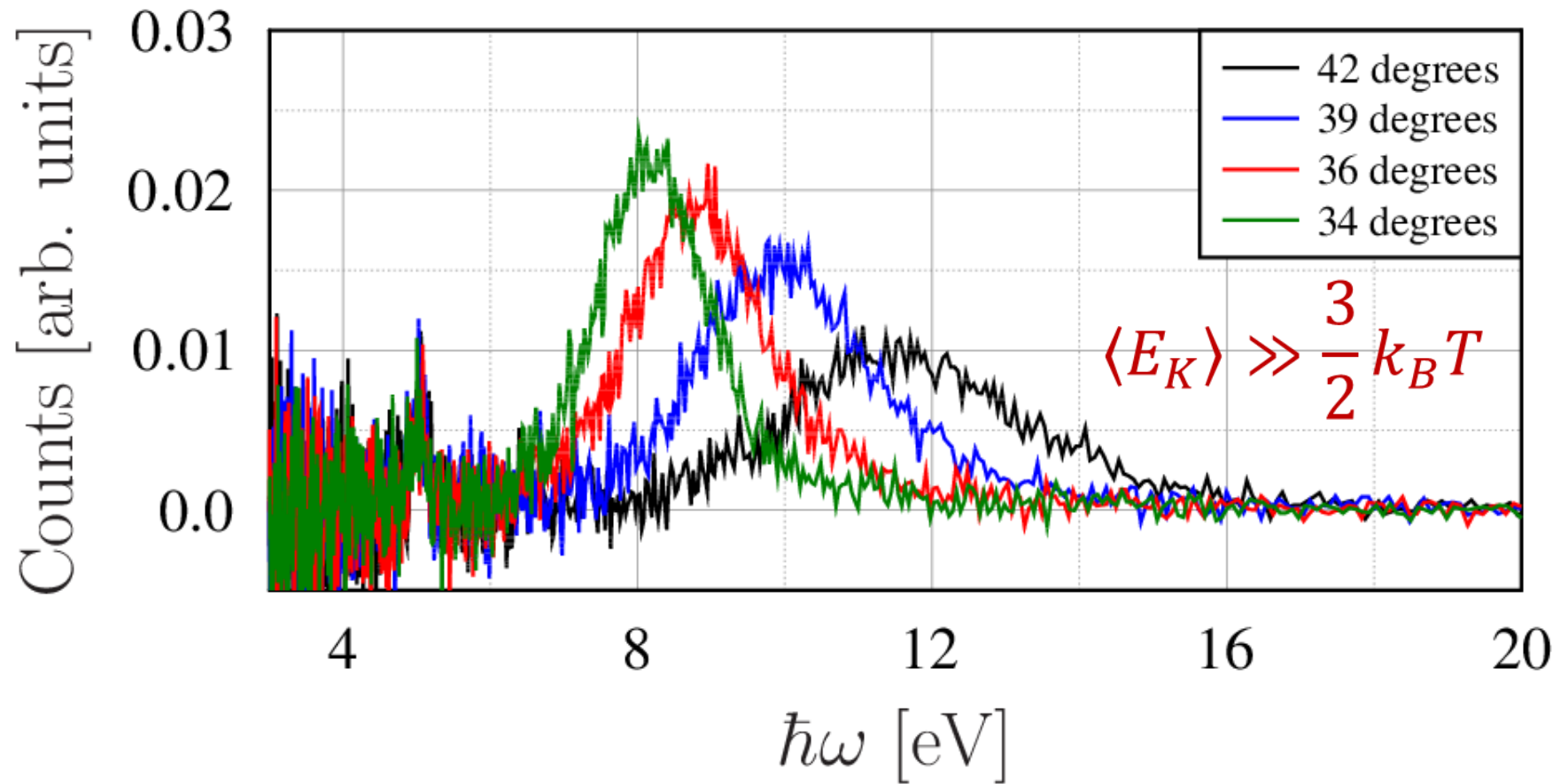
Neutron Compton profile of water; p-resolution  $\approx 14\%$   
A. Pietropaolo et al, PRL 100, 127802 (2008)



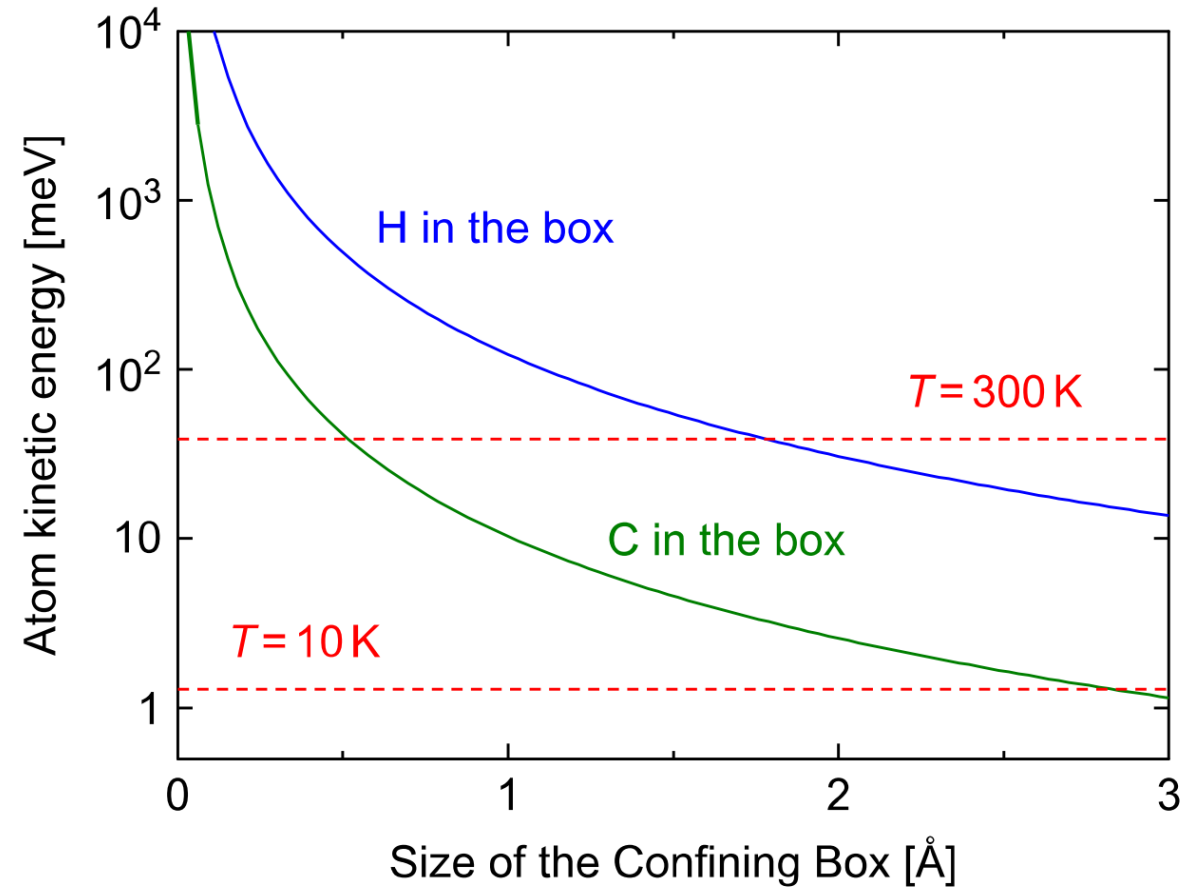
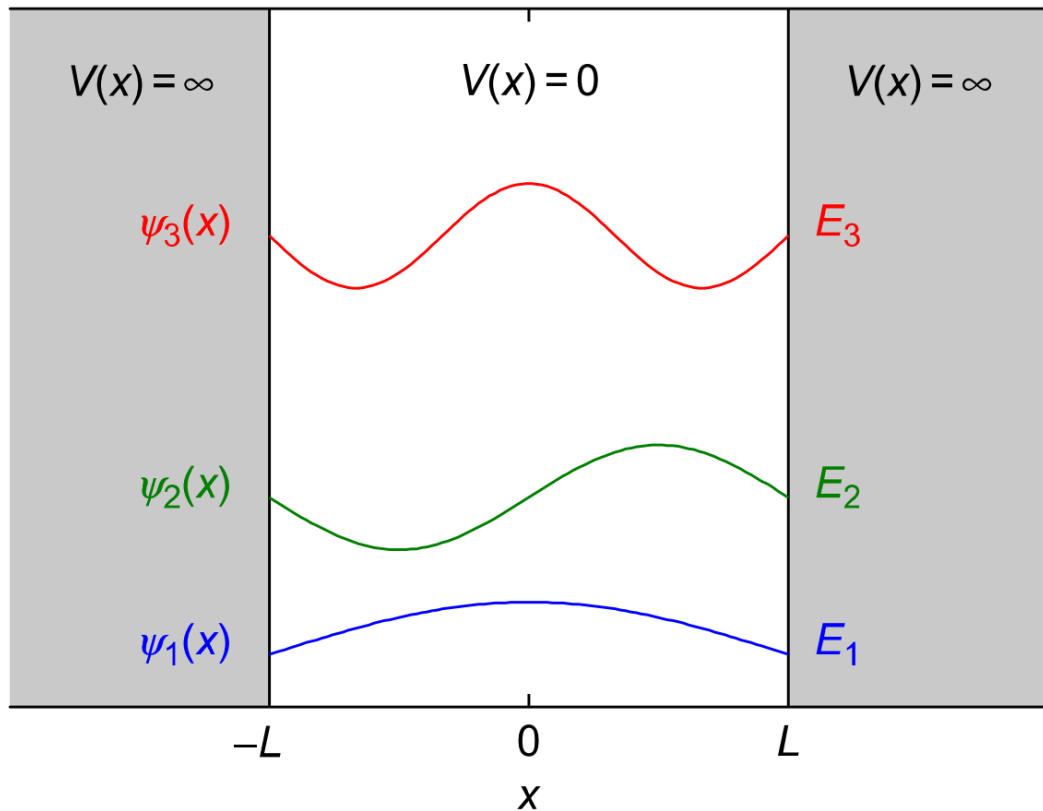
# Scattering from classical particles



# Scattering from quantum particles



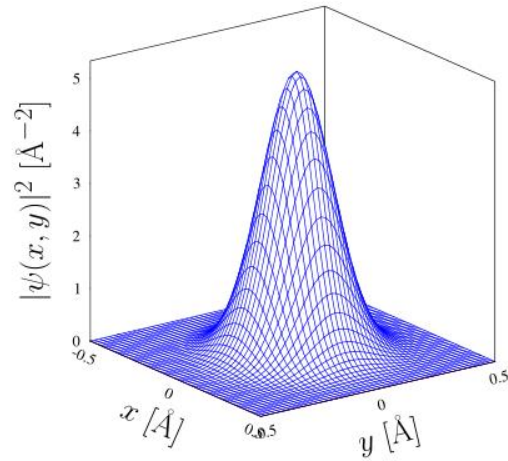
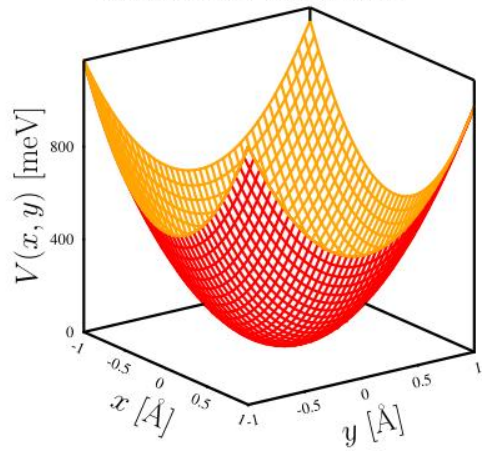
# Zero-point energy and local potential



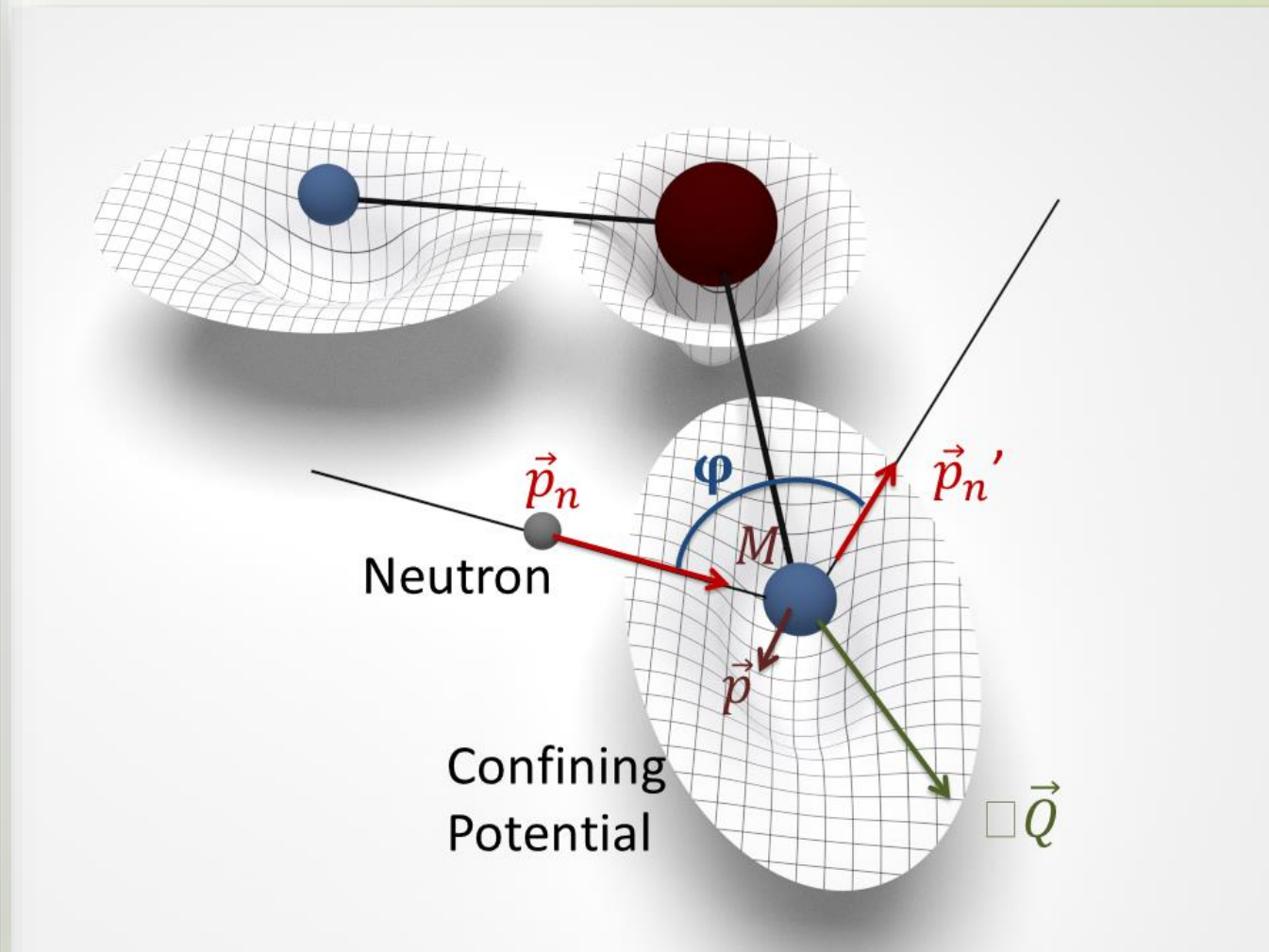
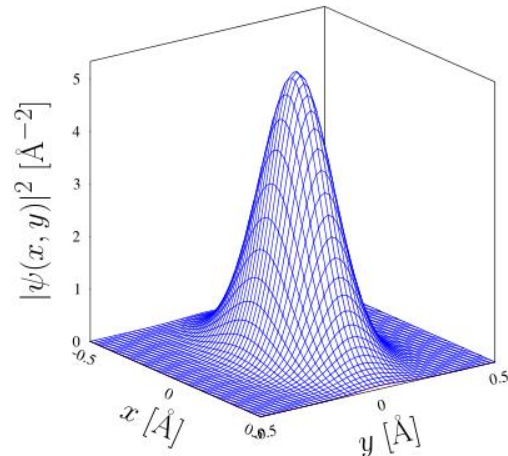
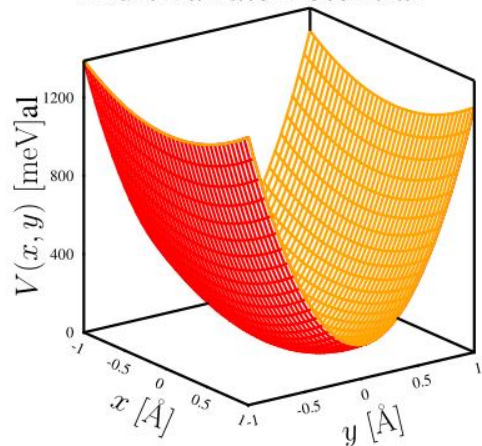
$$\mathcal{E}_n = \hbar\omega_n = \frac{n^2 \pi^2 \hbar^2}{2ML^2}.$$

# Probing the anisotropy of the local potential

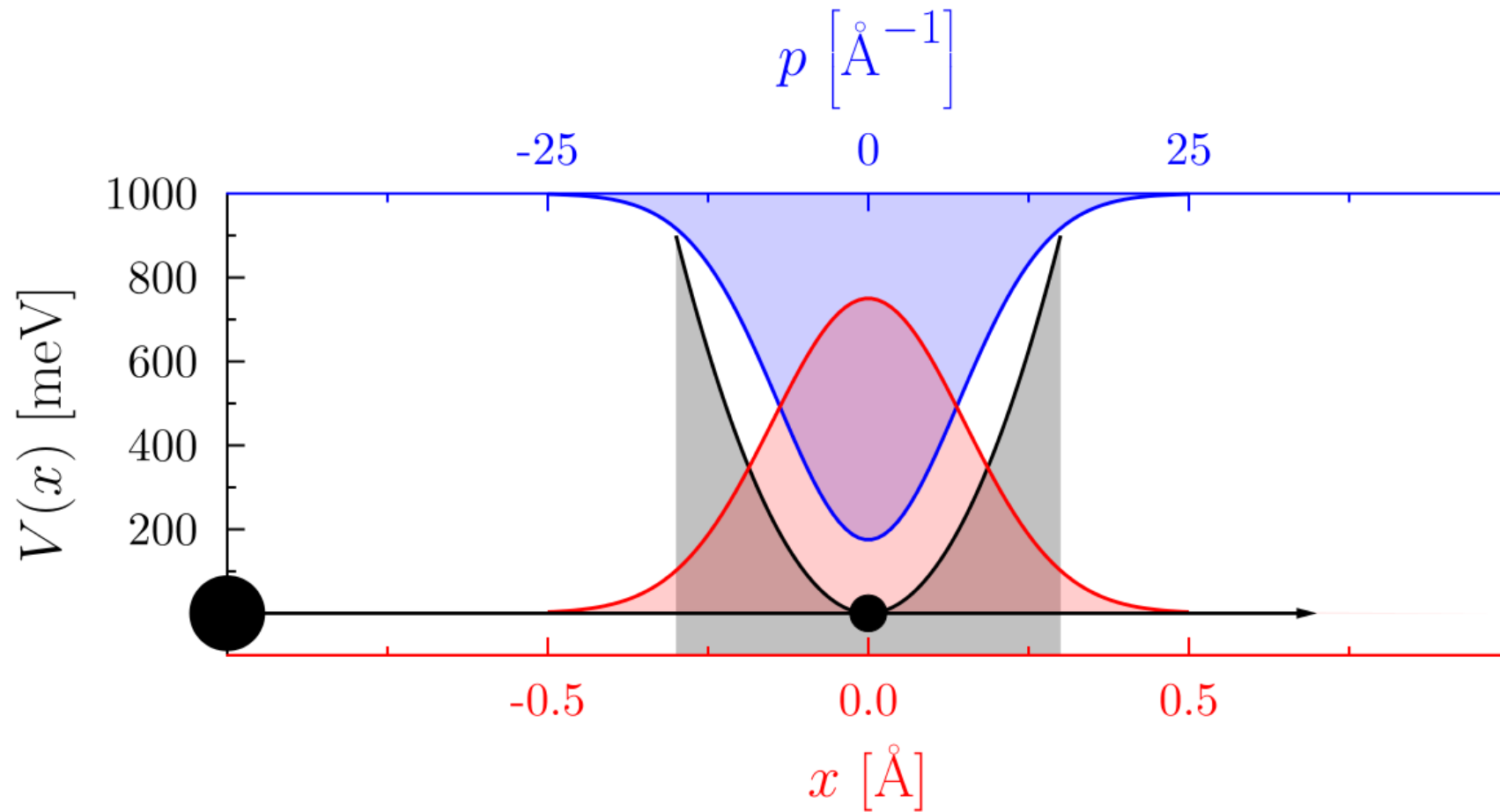
### Harmonic Potential



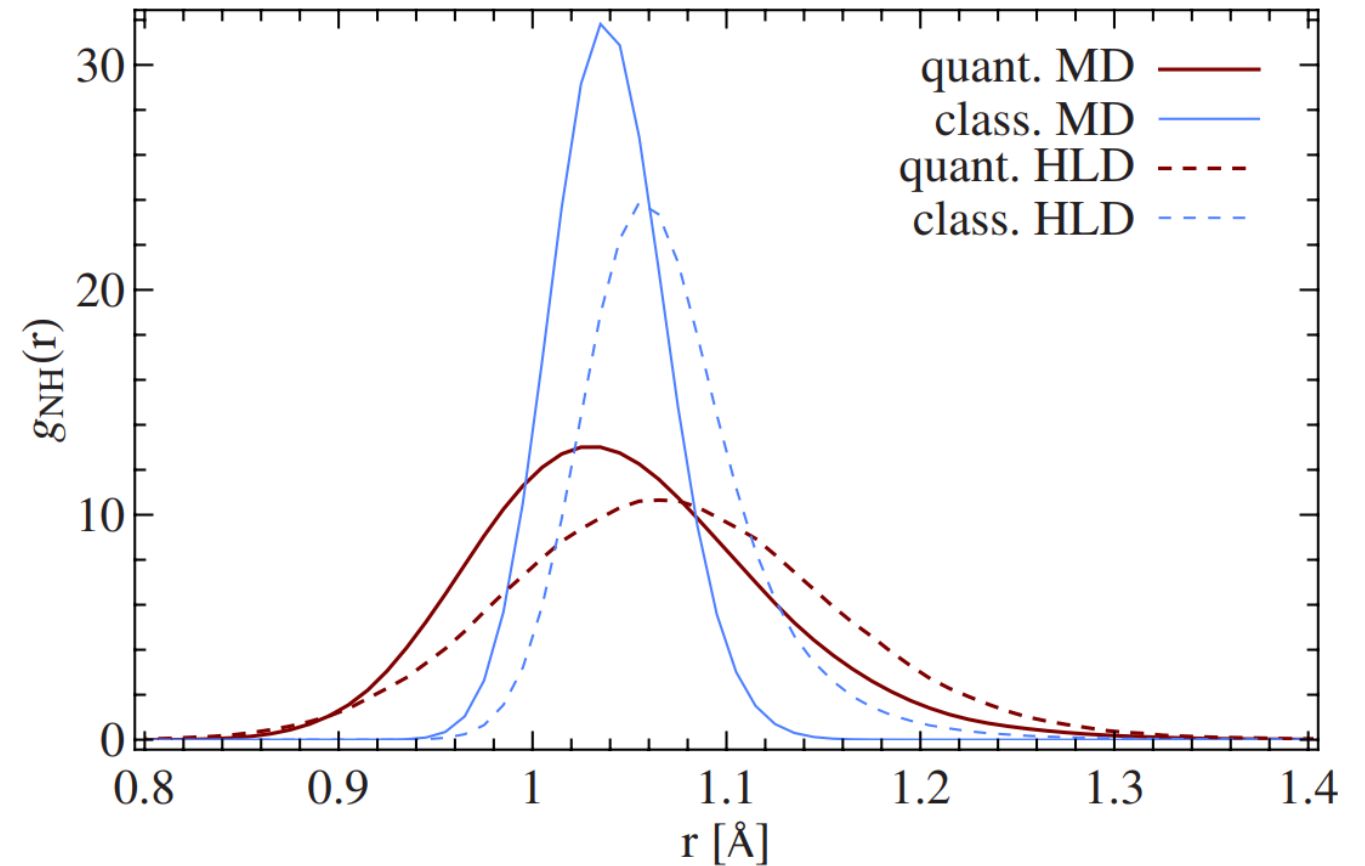
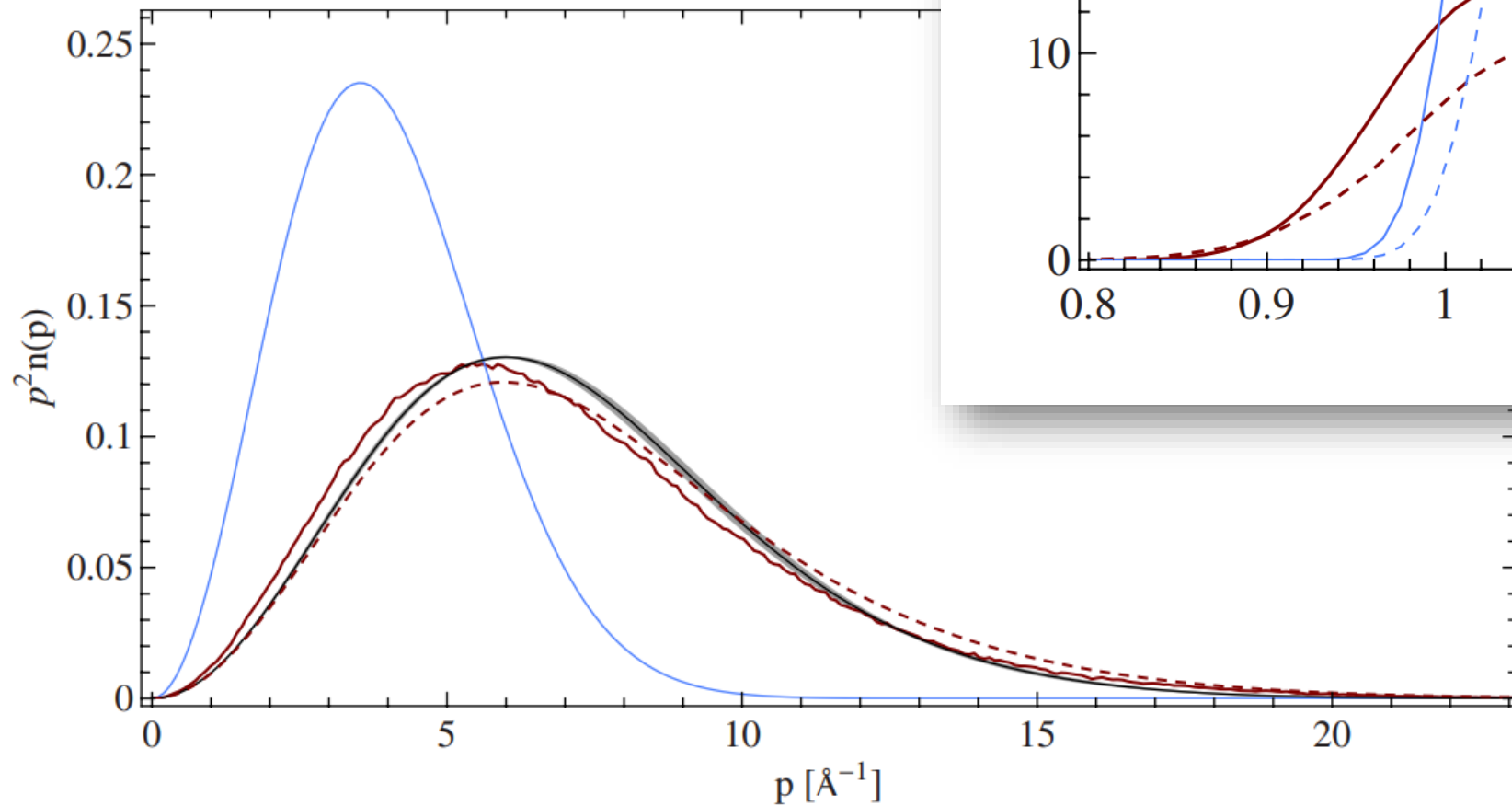
### Multivariate Potential



# Delocalisation in real and momentum spaces



# Delocalisation in real and momentum spaces

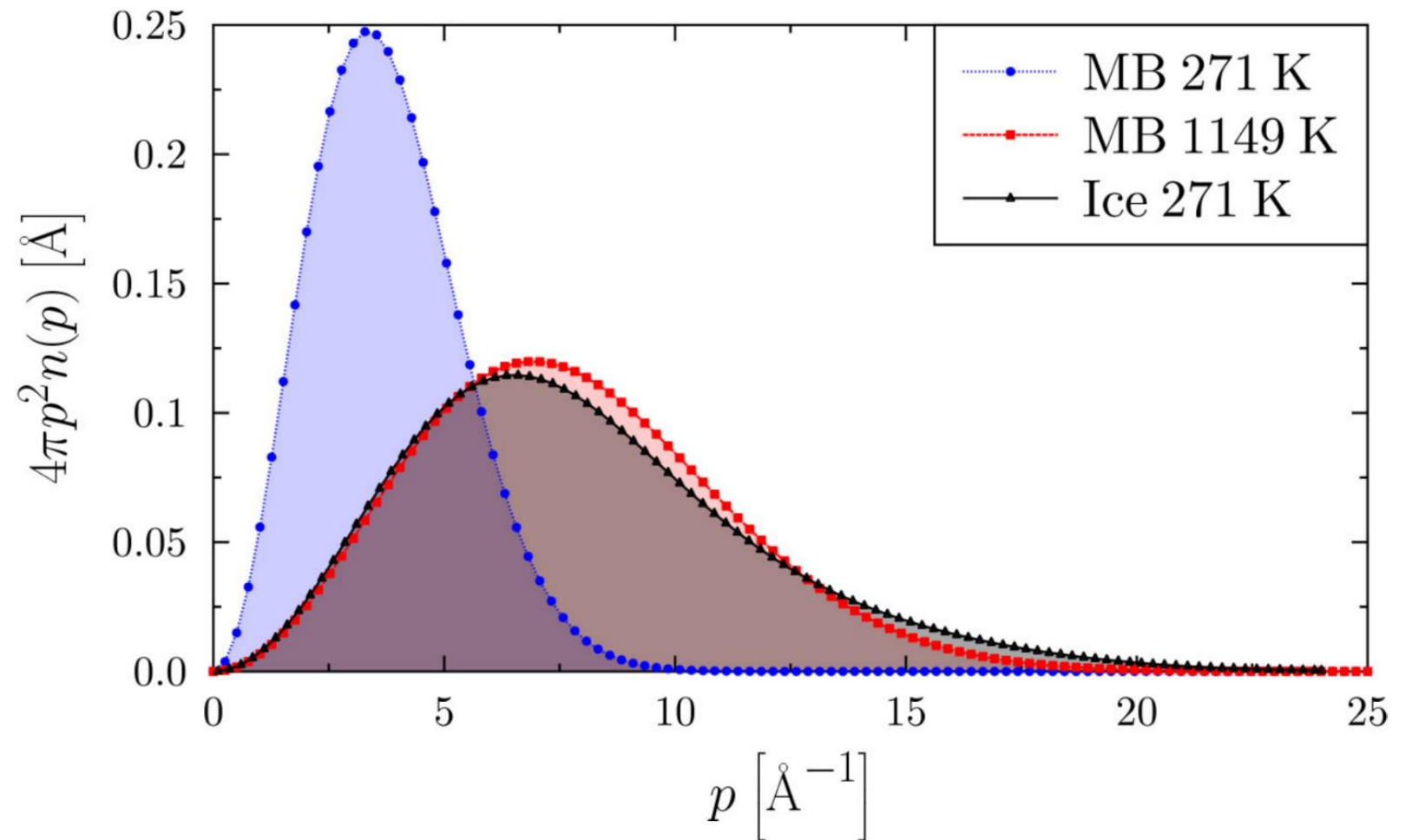


[M Ceriotti, G Miceli, A Pietropaolo, D Colognesi, A Nale, M Catti, M Bernasconi, and M Parrinello; \*Phys Rev B\*, 83, 174306 \(2010\)](#)



## Anisotropy of the local potential

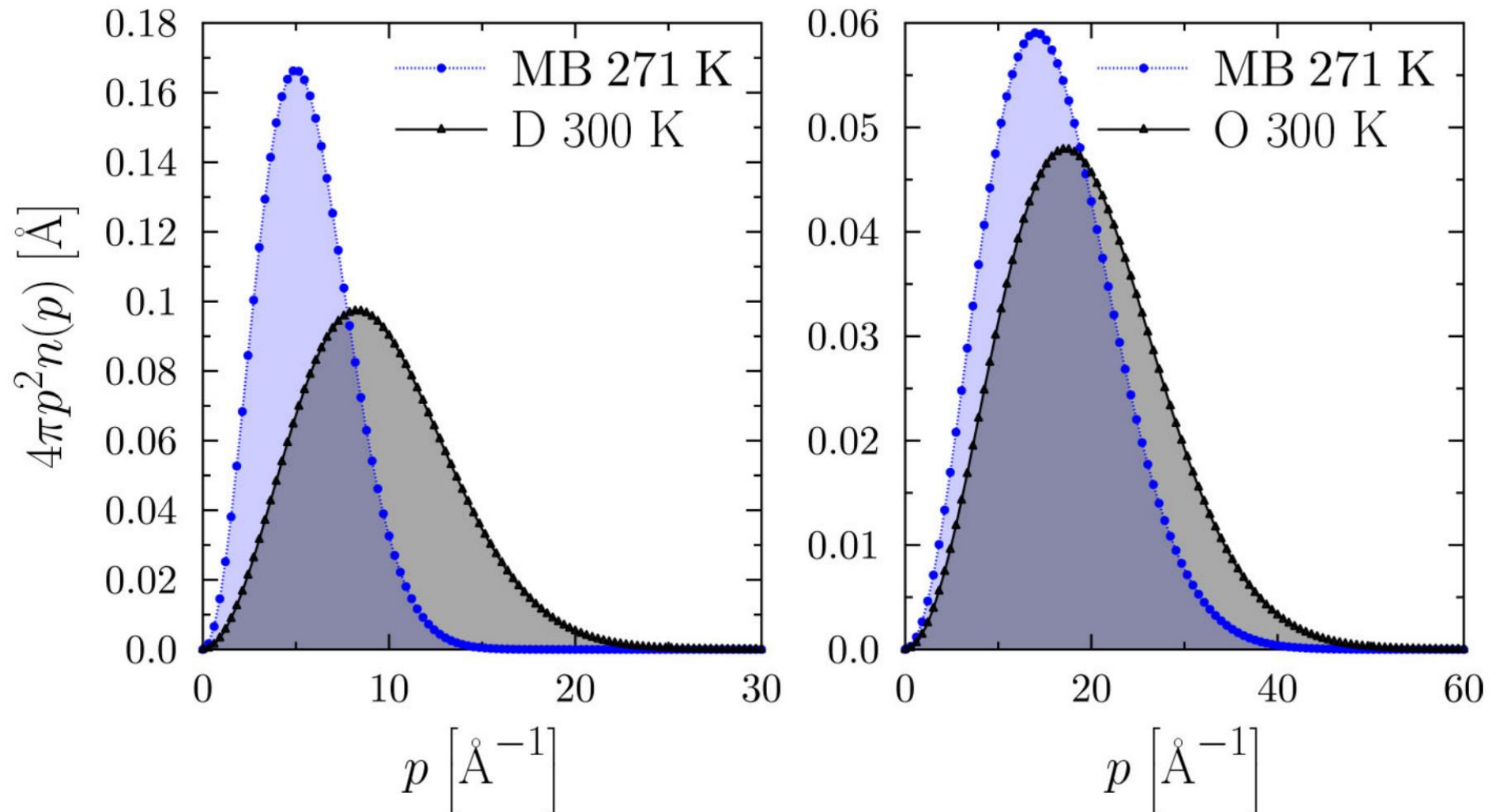
$$n(\mathbf{p}) = \exp\left(-\frac{p_x^2}{2\sigma_x^2} - \frac{p_y^2}{2\sigma_y^2} - \frac{p_z^2}{2\sigma_z^2}\right)$$



*C Andreani, R Senesi, M Krzystyniak, G Romanelli, F Fernandez-Alonso; Rivista del Nuovo Cimento, 291-340 (2018)*

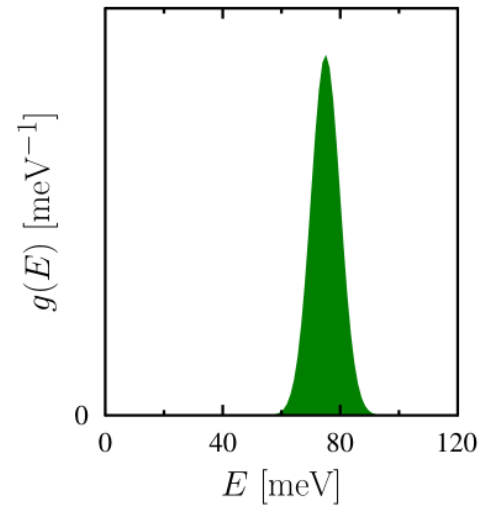
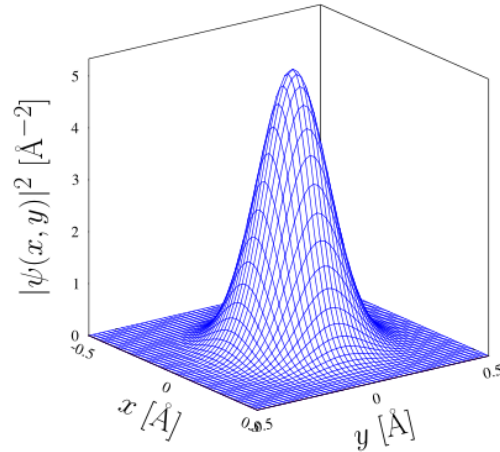
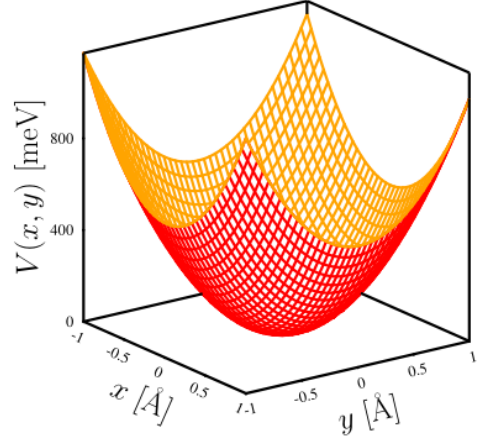
# Nuclear kinetic energy for heavier masses

*C Andreani, R Senesi, M Krzystyniak, G Romanelli, F Fernandez-Alonso; Rivista del Nuovo Cimento, 291-340 (2018)*

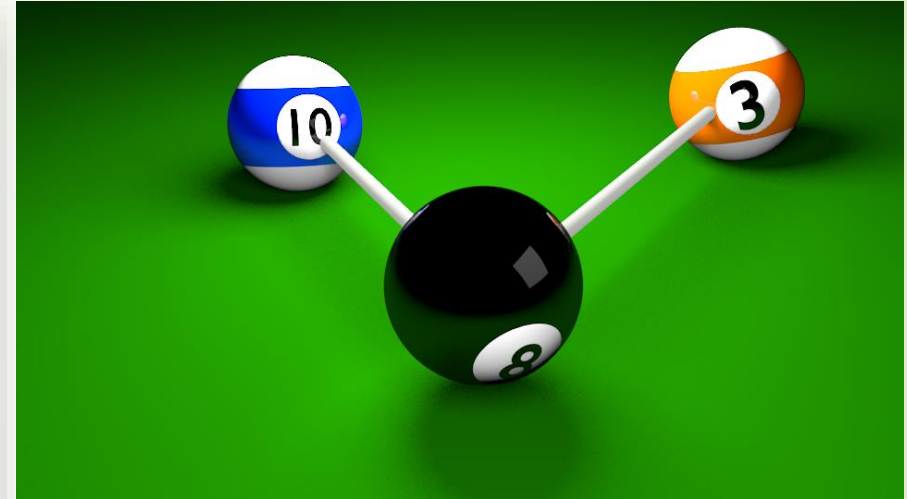
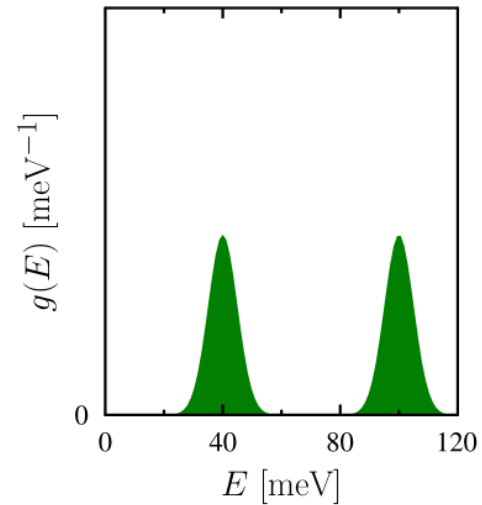
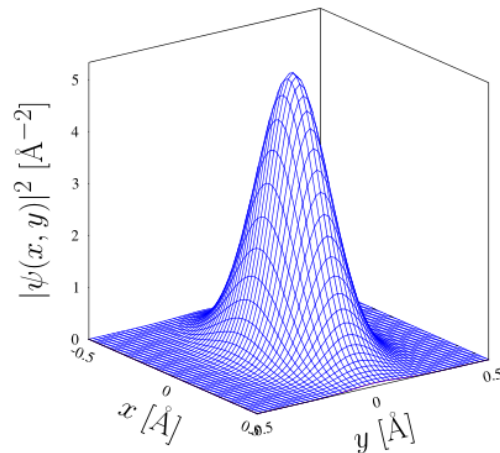
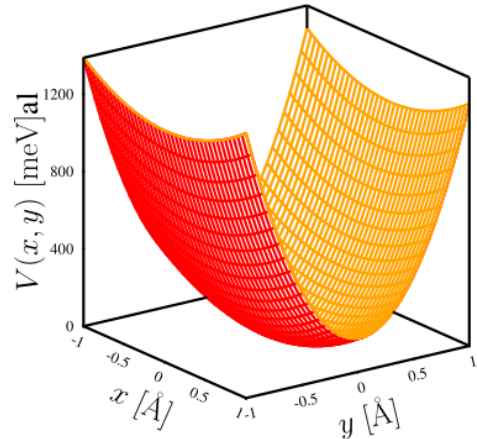


# Nuclear kinetic energy from vibrational modes

### Harmonic Potential

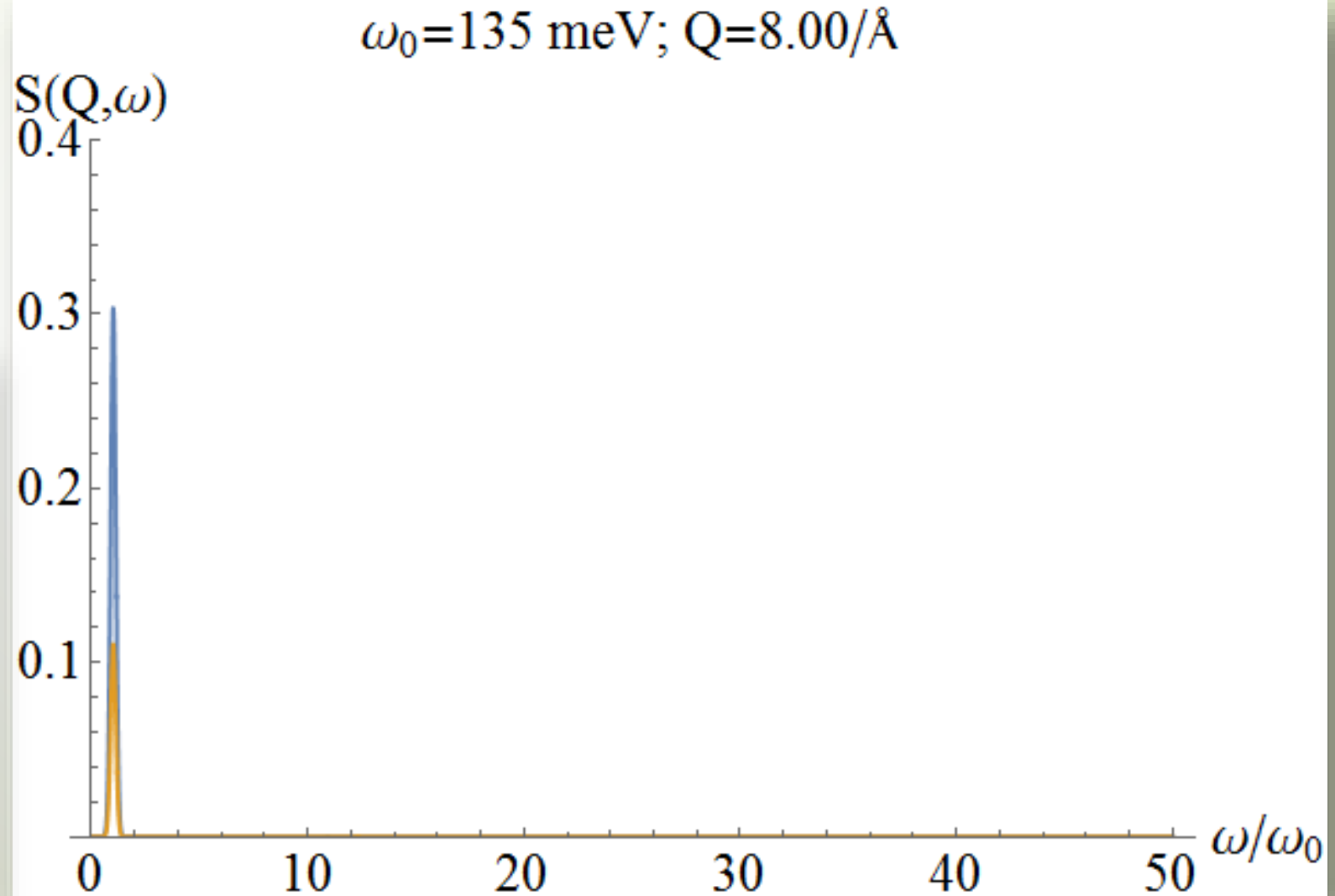
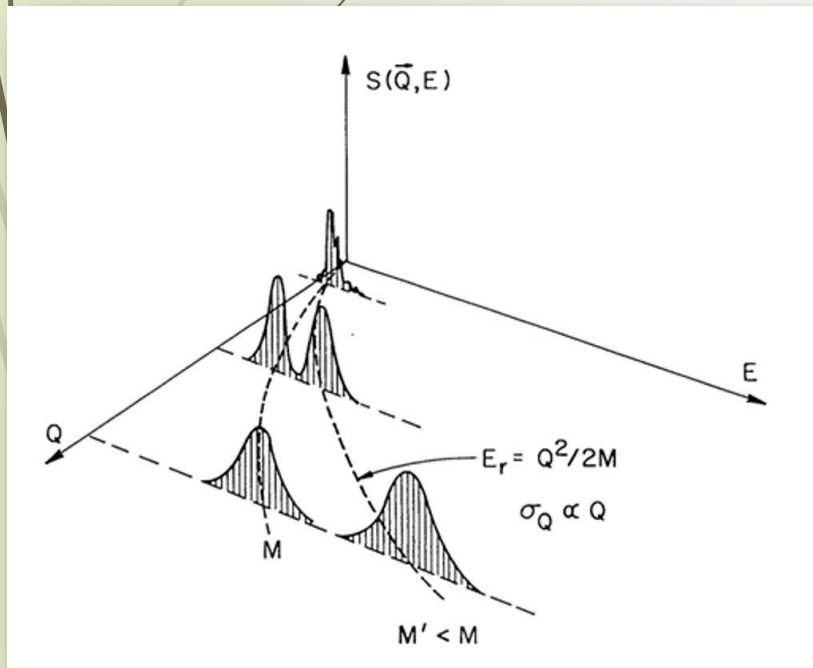


### Multivariate Potential

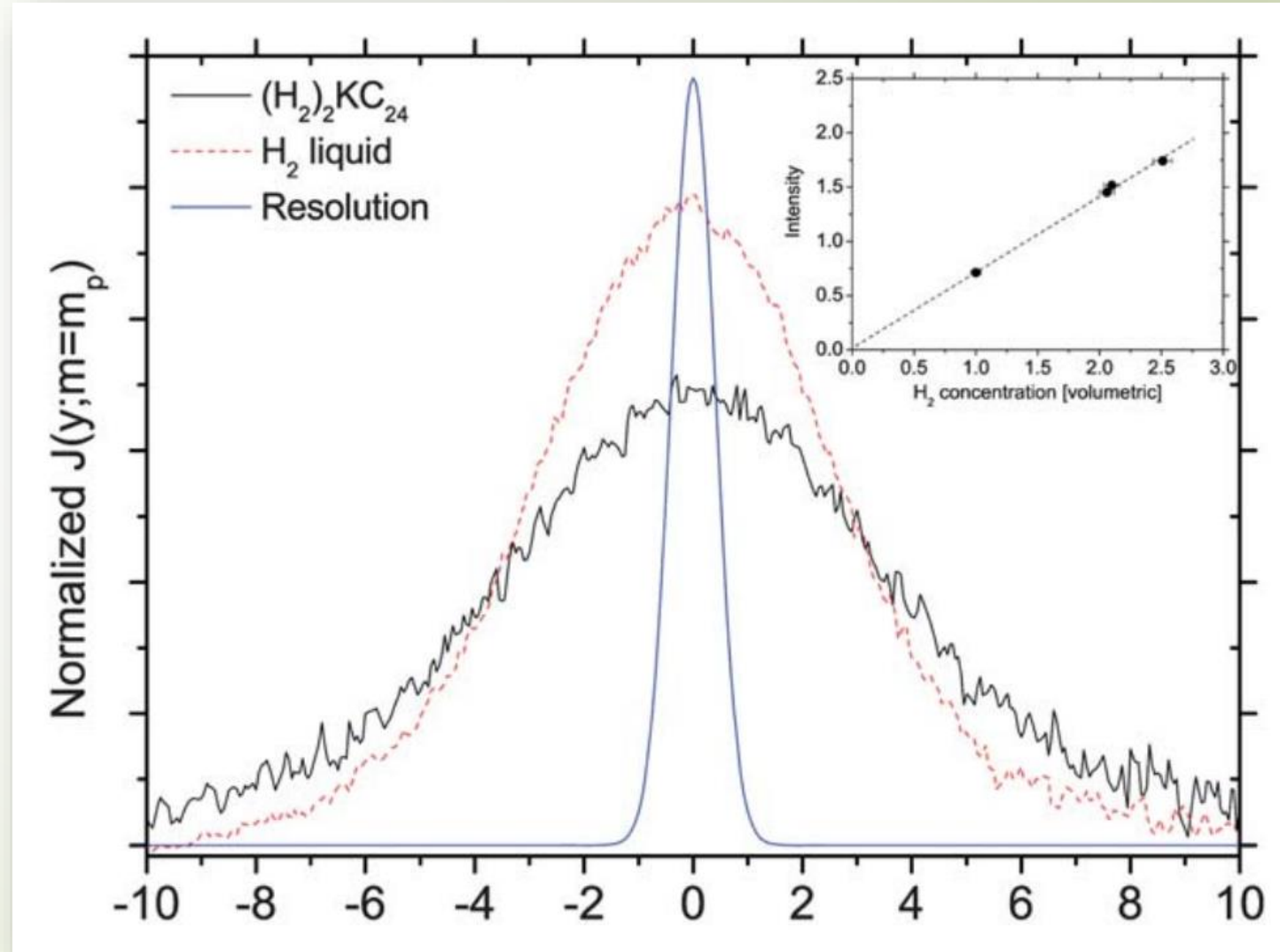
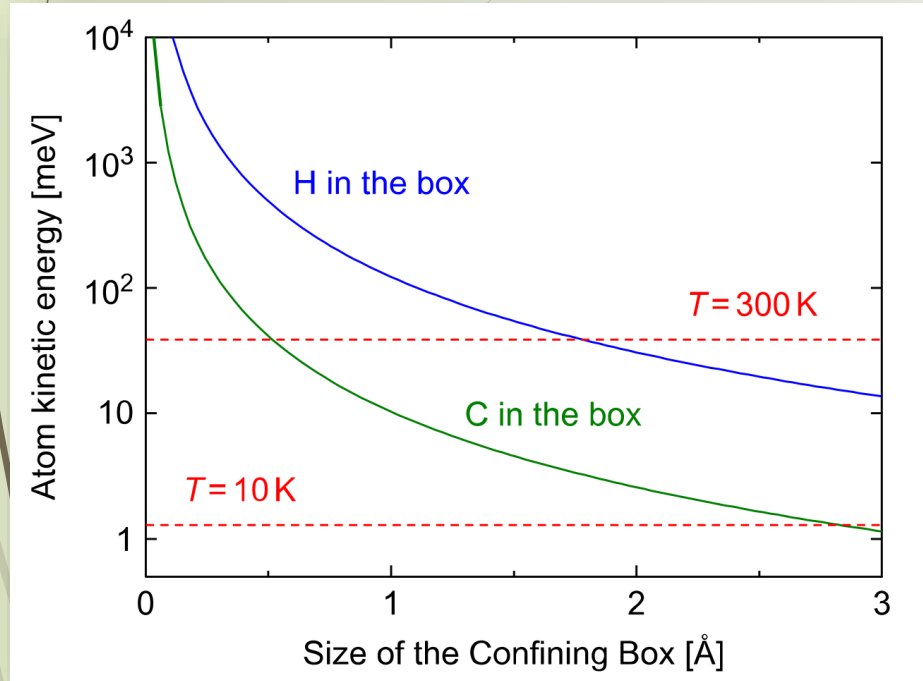


$$3 \int \frac{\hbar\omega}{4} g_M(\omega) \coth\left(\frac{\hbar\omega}{2k_B T}\right) = \frac{\hbar^2 \sigma^2}{2M}$$

# Multi Phonon Expansion towards the IA



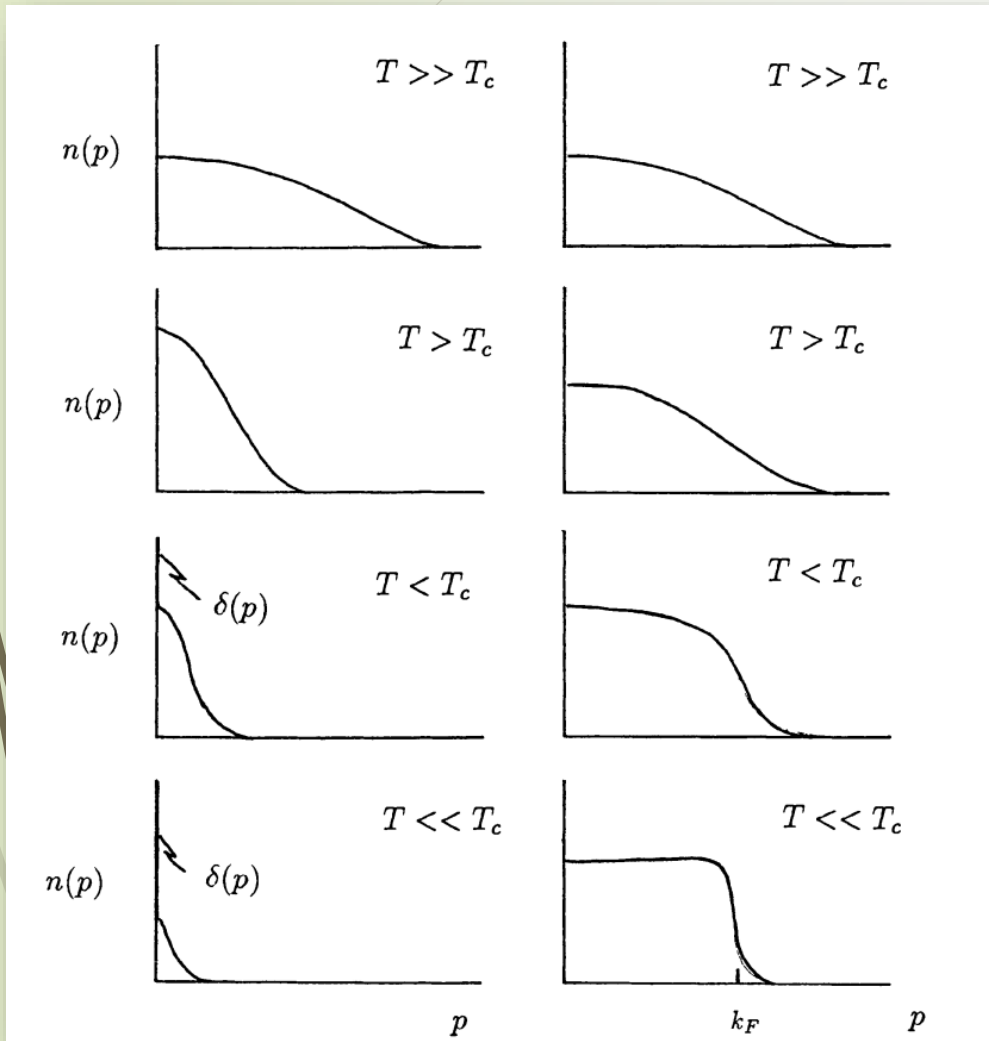
# Effect of confinement



*M Krzystyniak, MA Adams, A Lovell, NT Skipper, SM Bennington, J Mayers, and F Fernandez-Alonso; Faraday Discussions 151 (2011)*



## Effect of statistics: Bose/Einstein vs Fermi/Dirac

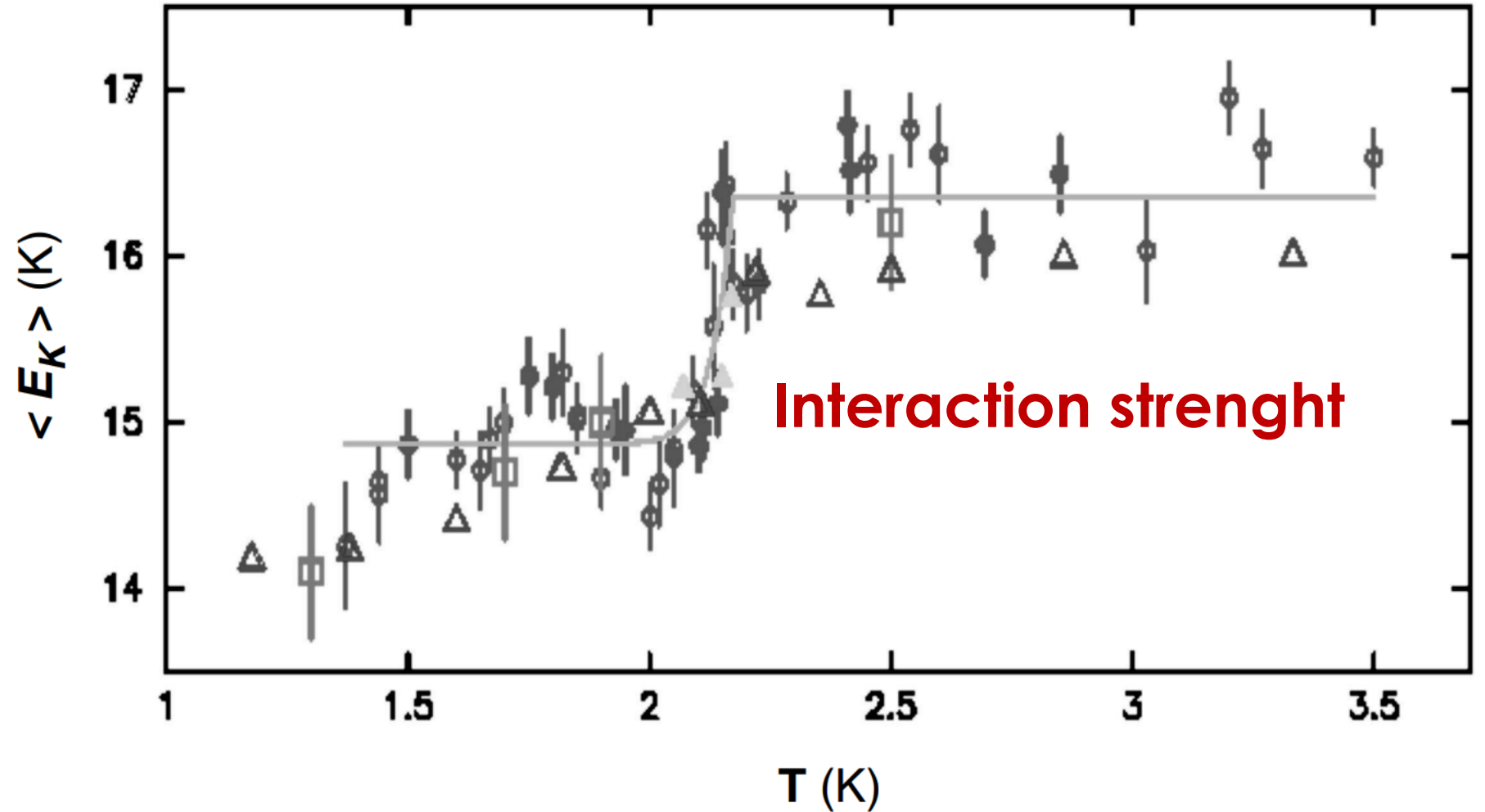


At low temperature, a gas of identical Bosons tends to condensate in the minimum energy state ( $p=0$ ).

On the other hand, a gas of identical fermions tends to occupy all available states (exclusion principle) up to a Fermi energy state.



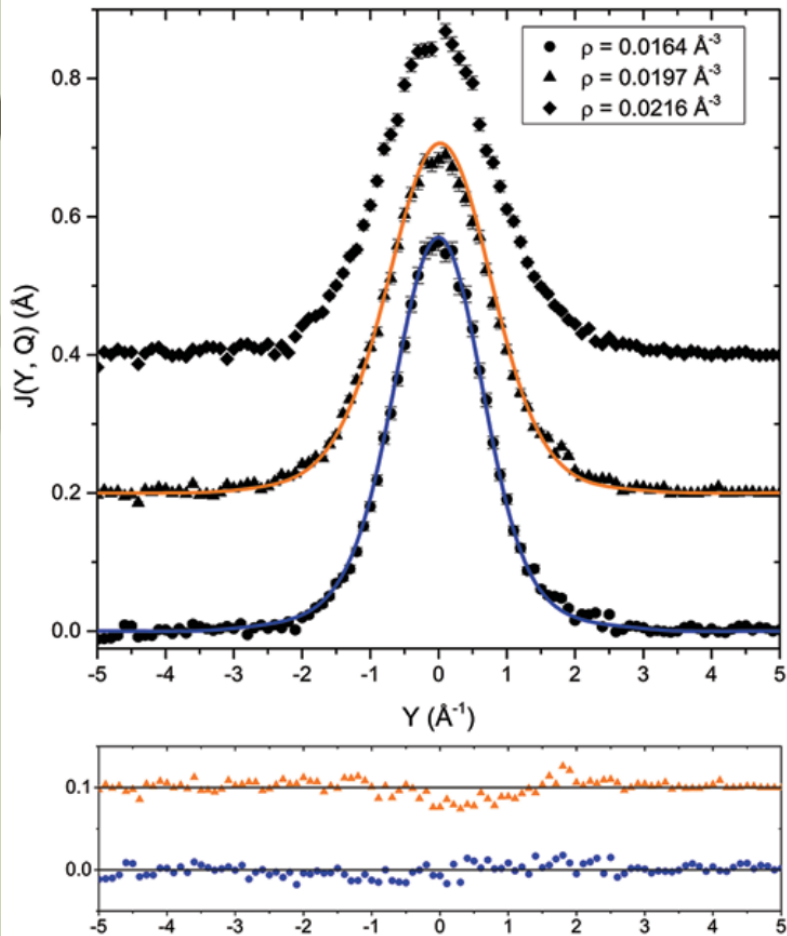
# Effect of statistics: $^4\text{He}$ (Bosons) below $T_c$



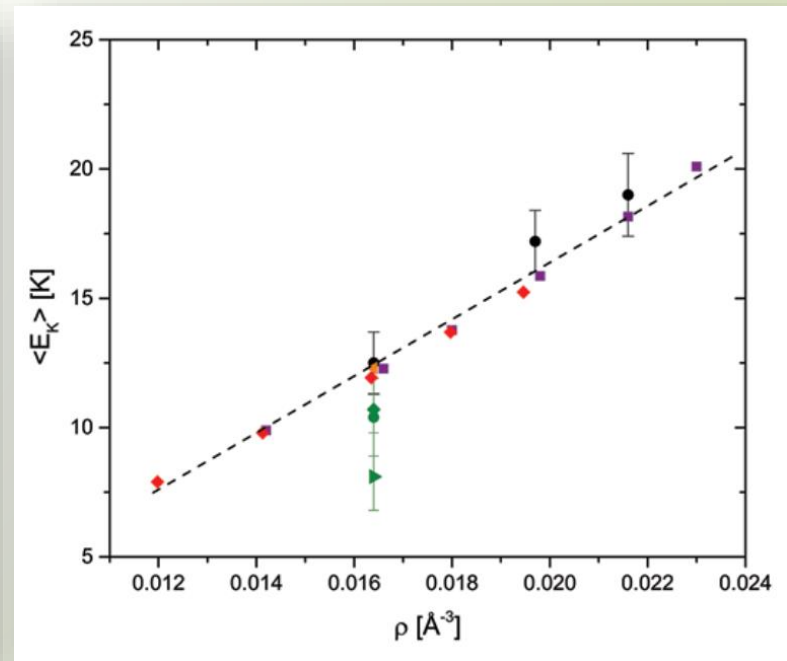
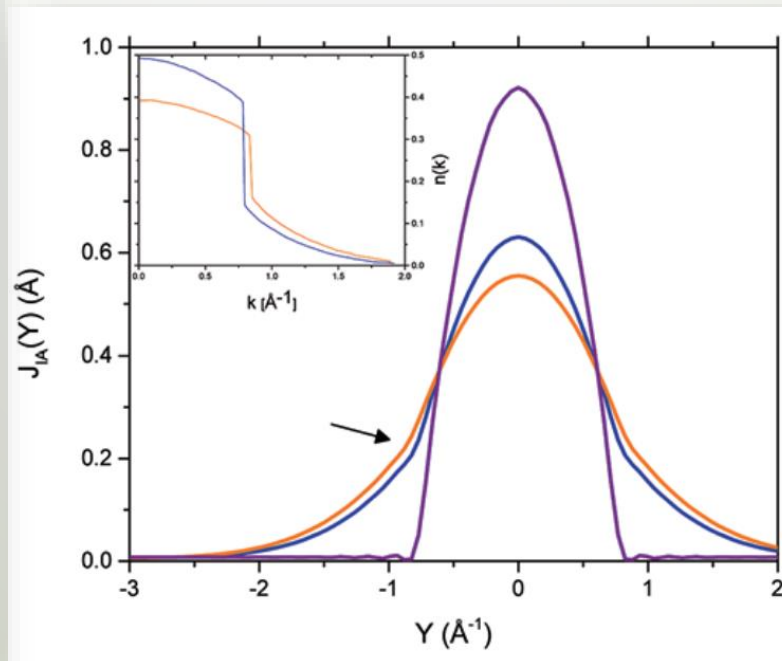
*C Andreani, D  
Colognesi, J Mayers,  
G F Reiter, and R  
Senesi; Advances in  
Physics, (2005)*

# Effect of statistics: $^3\text{He}$ (Fermions) below $T_c$

Liquid  $^3\text{He}$ :  $Q = 27.5 \text{ \AA}^{-1}$ ;  $T = 500 \text{ mK}$



$$J(y) = 2\pi\hbar \int_{|\hbar y|}^{\infty} p n(p) dp$$



# How to select epithermal energies

$$\sigma = \gamma \Lambda^2 / \Delta \nu_s = \frac{\Lambda^2}{\pi} S \frac{\Gamma_s \Gamma}{(\nu - \nu_0)^2 + \Gamma^2}.$$

APRIL 1, 1936

PHYSICAL REVIEW

VOLUME 49

## Capture of Slow Neutrons

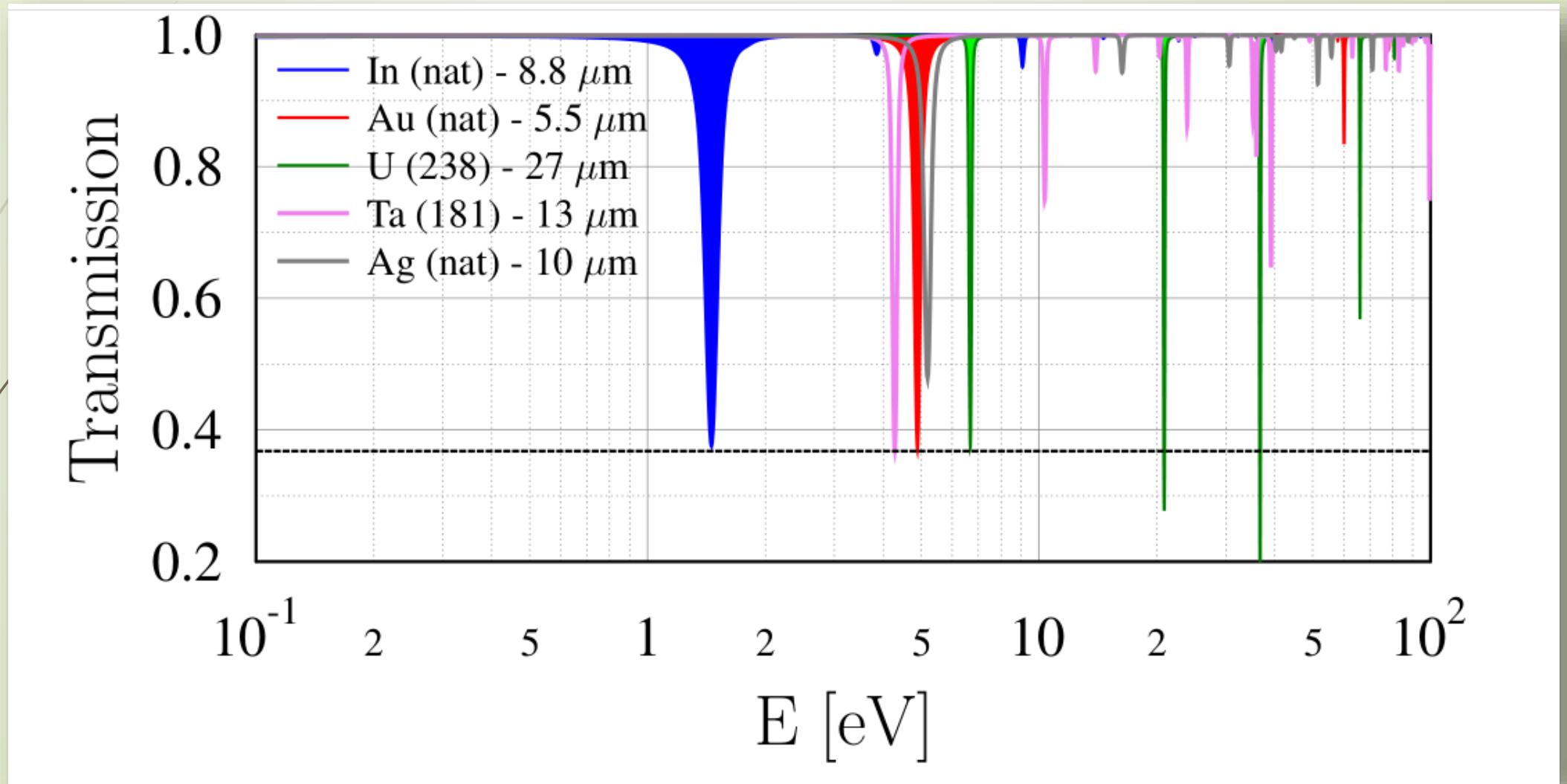
G. BREIT AND E. WIGNER, *Institute for Advanced Study and Princeton University*

(Received February 15, 1936)

Current theories of the large cross sections of slow neutrons are contradicted by frequent absence of strong scattering in good absorbers as well as the existence of resonance bands. These facts can be accounted for by supposing that in addition to the usual effect there exist transitions to virtual excitation states of the nucleus in which not only the captured neutron but, in addition to this, one of the particles of the original nucleus is in an excited state. Radiation damping due to the emission of  $\gamma$ -rays broadens the resonance and reduces scattering in comparison with absorption by a large factor. Interaction

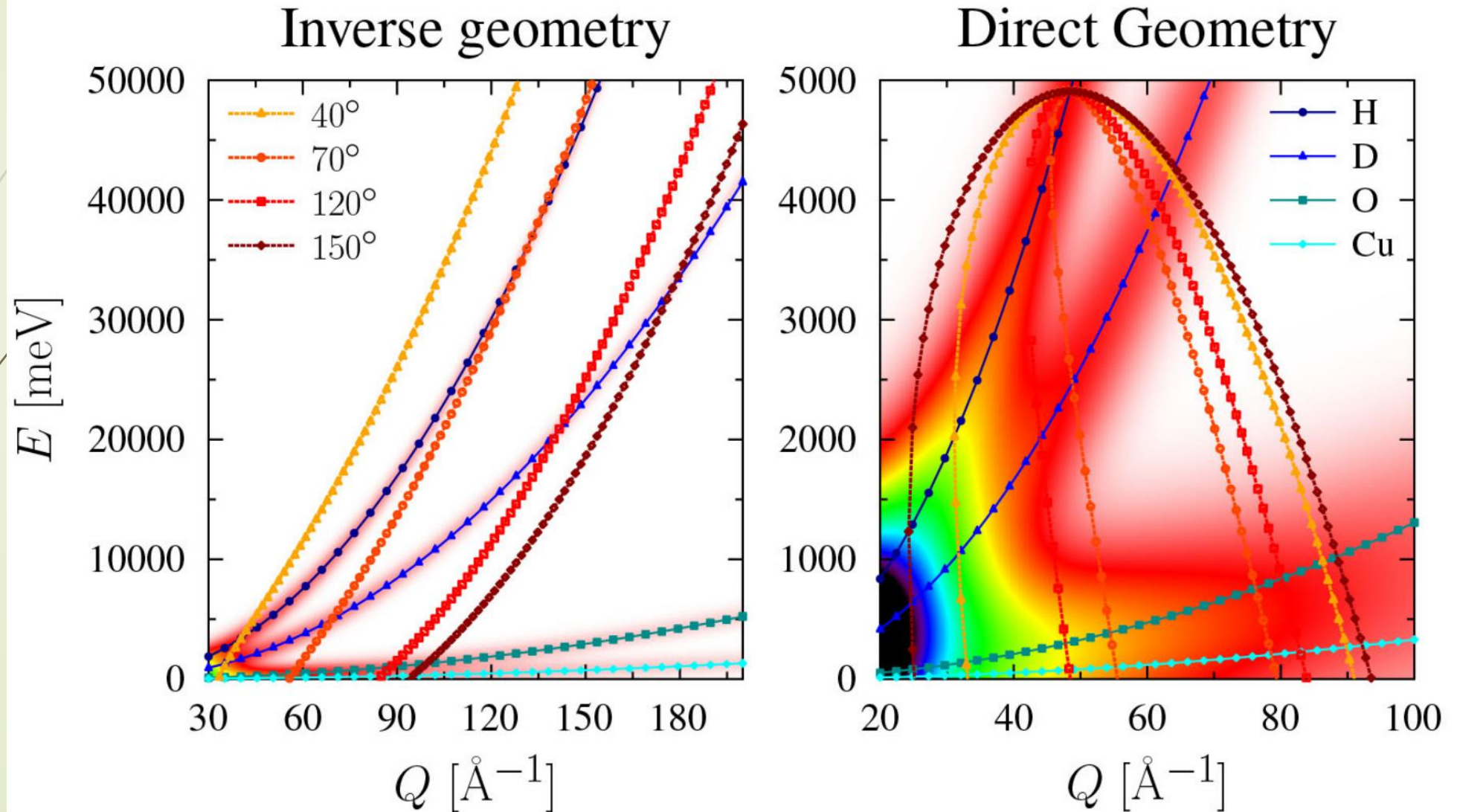
with the nucleus is most probable through the  $s$  part of the incident wave. The higher the resonance region, the smaller will be the absorption. For a resonance region at 50 volts the cross section at resonance may be as high as  $10^{-19}$  cm<sup>2</sup> and  $0.5 \times 10^{-20}$  cm<sup>2</sup> at thermal energy. The estimated probability of having a nuclear level in the low energy region is sufficiently high to make the explanation reasonable. Temperature effects and absorption of filtered radiation point to the existence of bands which fit in with the present theory.

# How to select epithermal energies

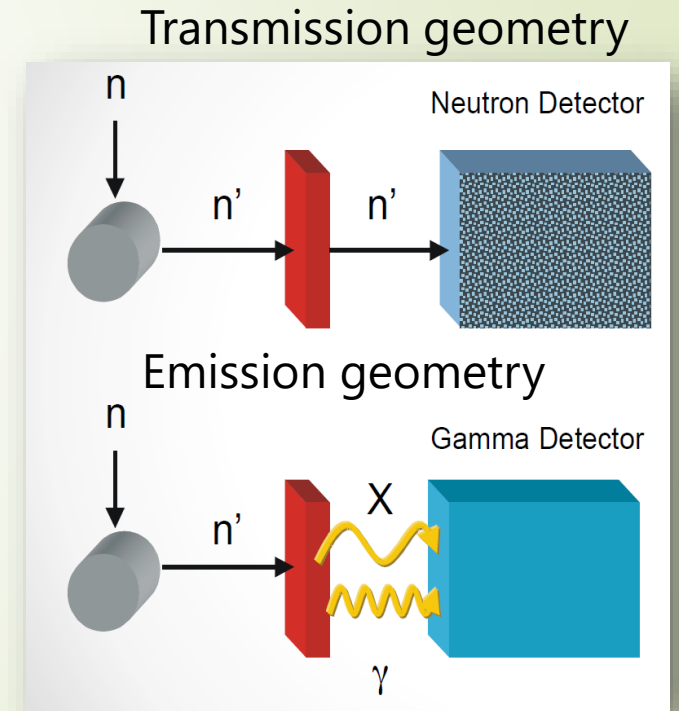
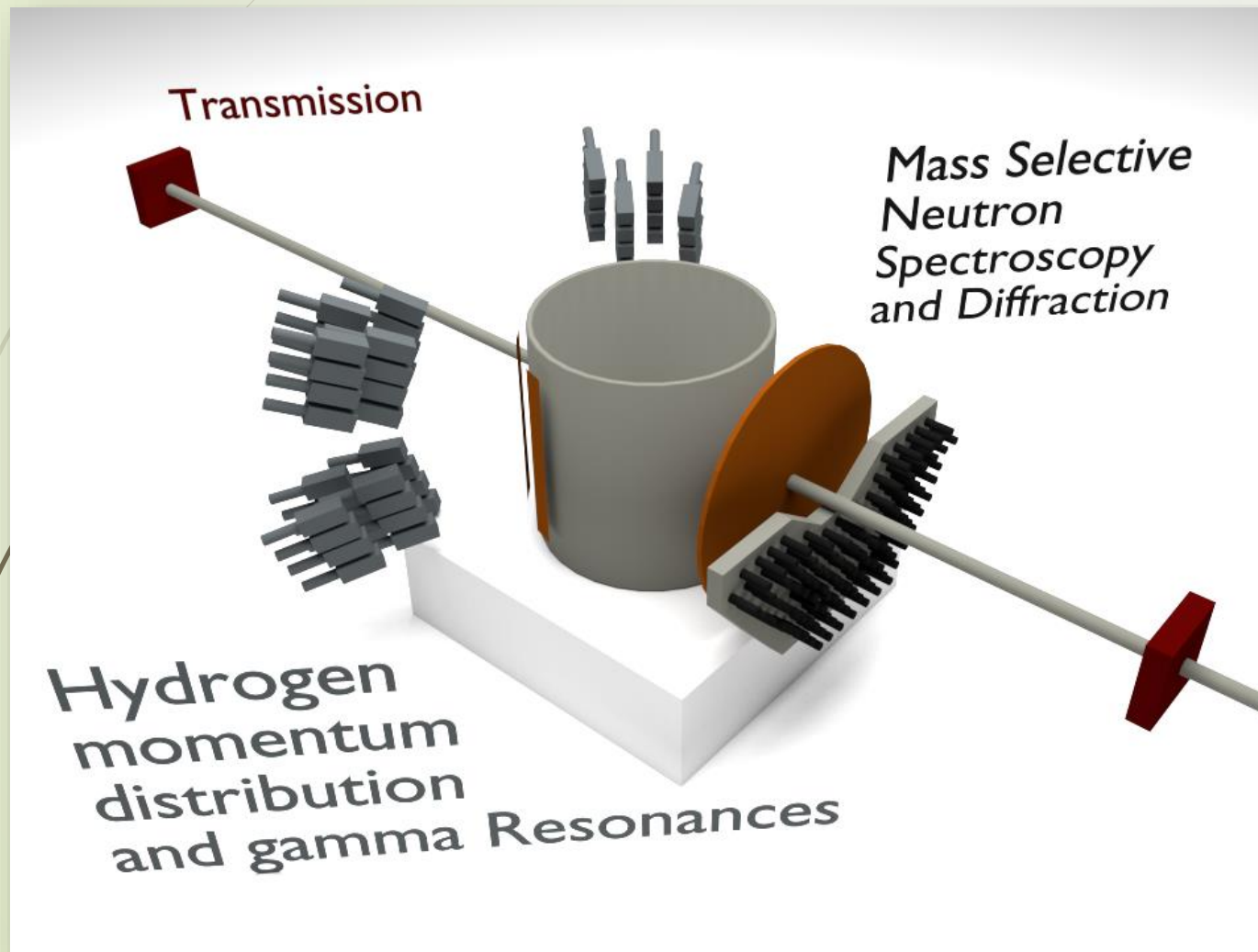




# Geometry and Impulse Approximation

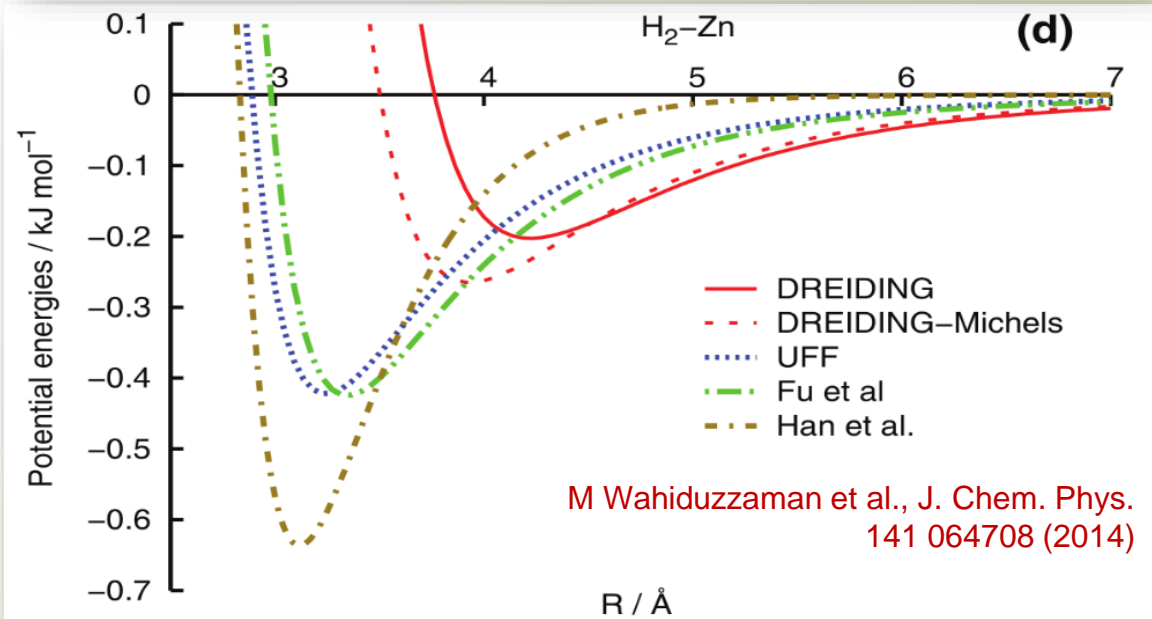
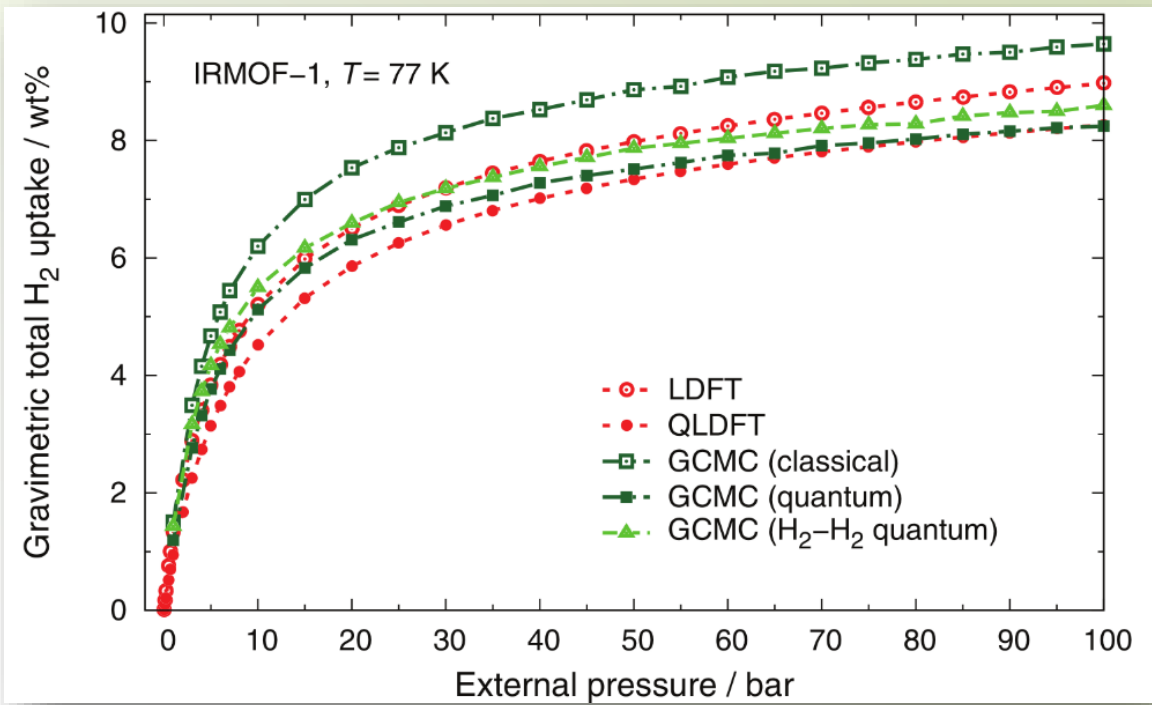
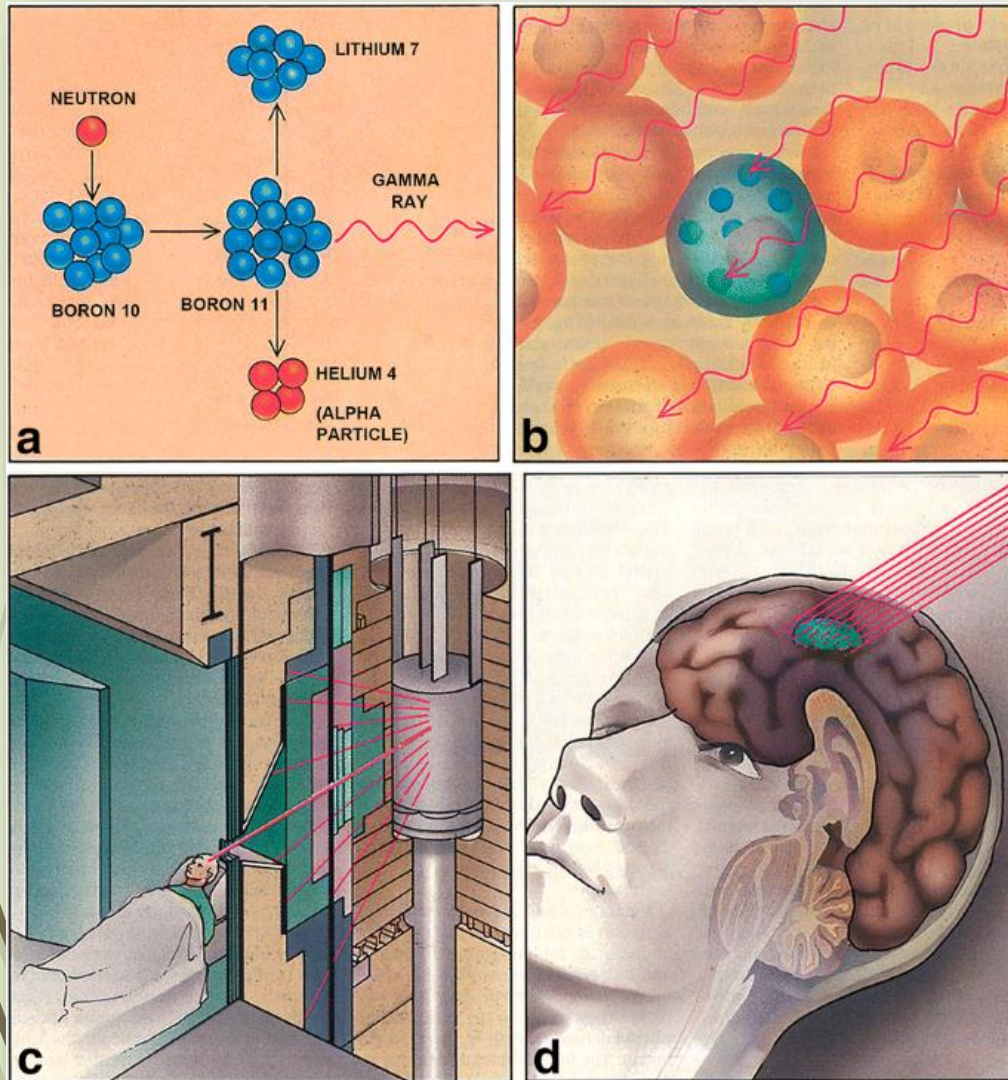


# The VESUVIO Spectrometer (ISIS)

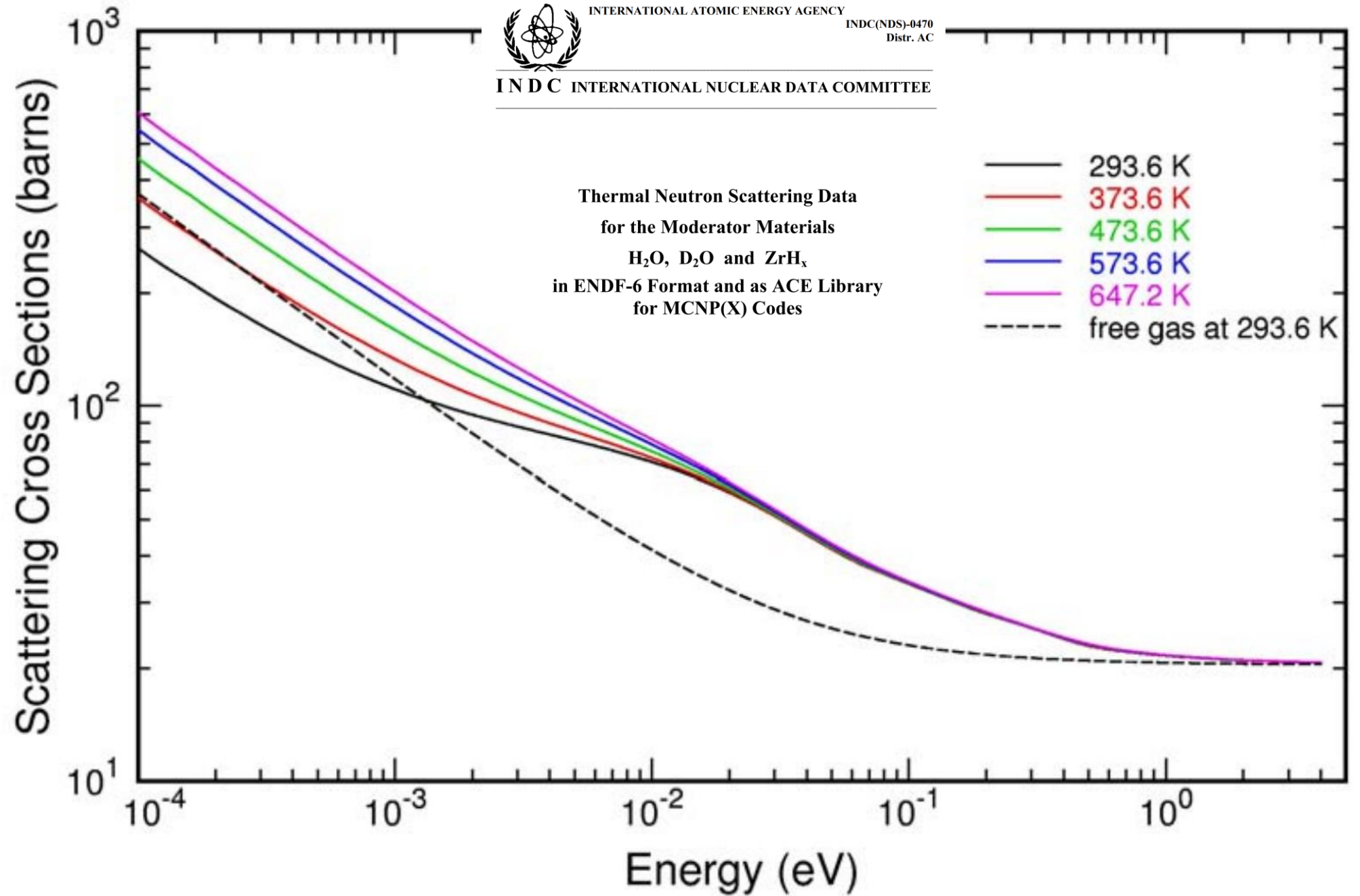




# Applications



M Wahiduzzaman et al., *J. Chem. Phys.*  
141 064708 (2014)





# Thanks

