Quantum Rotations in Methyl Iodide (CH_3I)

An experimental investigation using the
High-Flux Backscattering Spectrometer and Filter Analyzer Spectrometer

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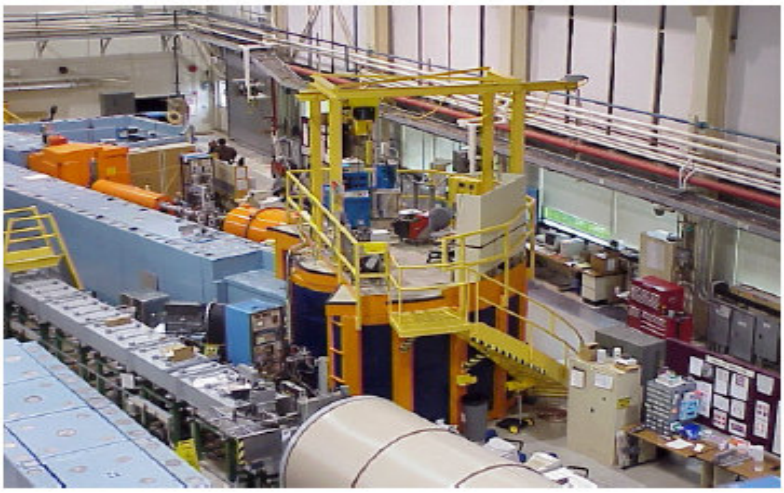


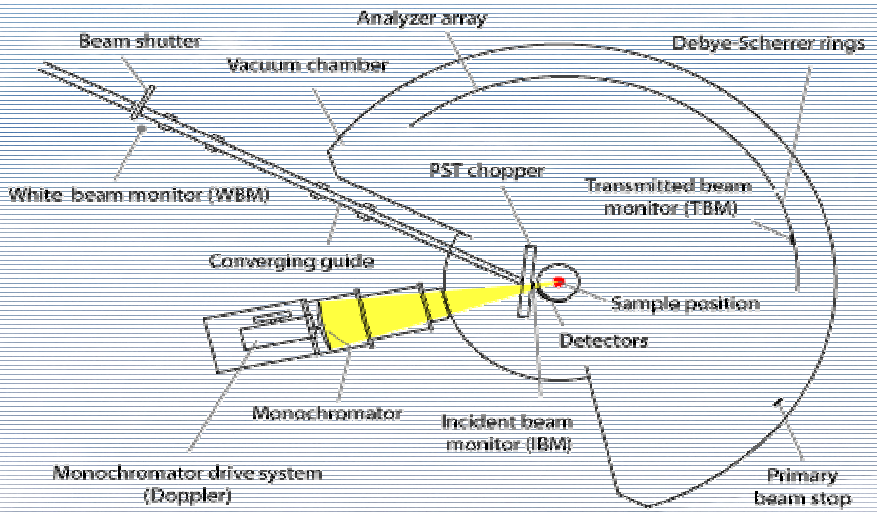
Backscattering

$$\frac{\delta\lambda}{\lambda} = \frac{\delta d}{d} + \frac{\delta\theta}{\tan\theta}$$

Maximum resolution requires that neutrons scatter off of both the monochromator and analyzer with a 2θ of 180

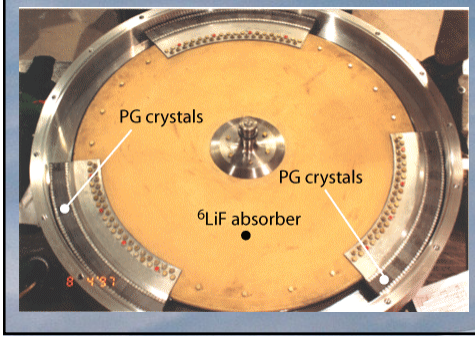
HFBS uses the (111) plane of Silicon due to its low δd

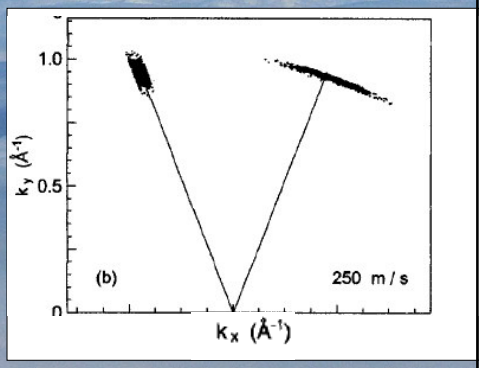
HFBS Spectrometer



PST Chopper

Increases neutron flux
by a factor of 4.2





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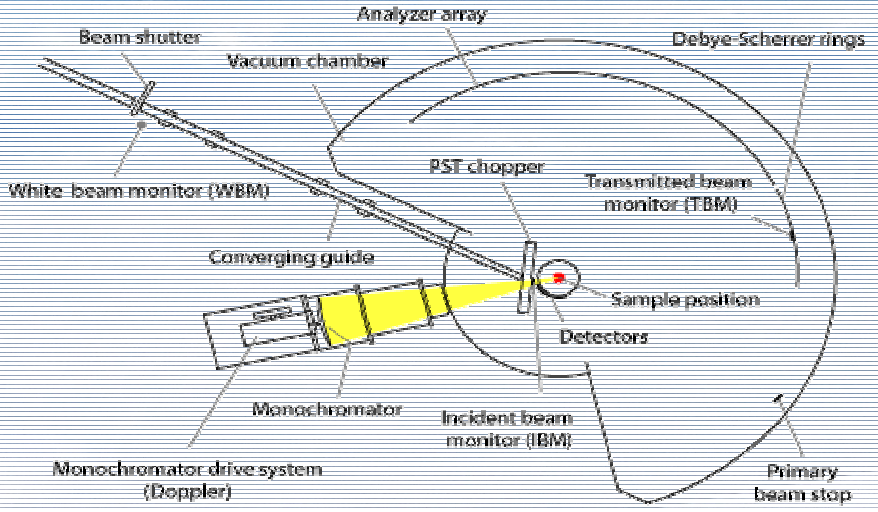
HFBS Spectrometer



Instrument Specifications

Dynamic Range

$-35\mu eV < \omega < +35\mu eV$

$0.25\text{Å}^{-1} < Q < 1.75\text{Å}^{-1}$

$\tau \approx 0.1 - 1ns$

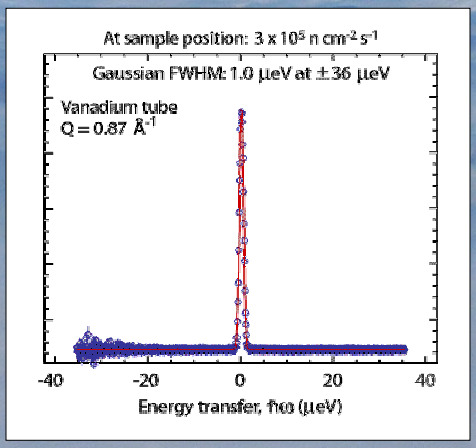
Resolution

$\delta\omega < 1\mu eV\,(FWHM)$

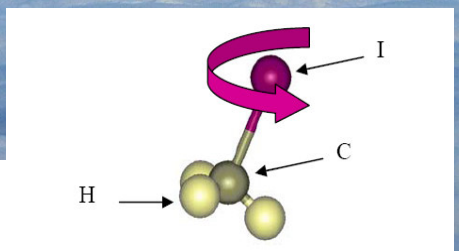
$\delta Q = 0.1 - 0.2\text{Å}^{-1}$

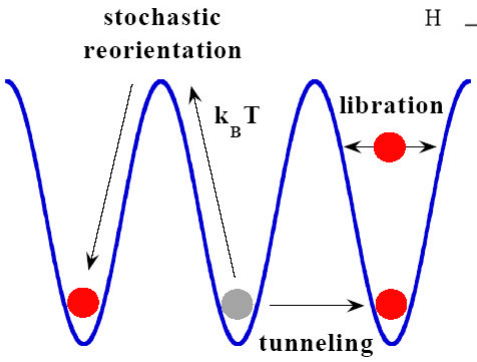
Incident Flux: $1.43 \times 10^5 \frac{n}{cm^2 s}$

E_f=2.08meV

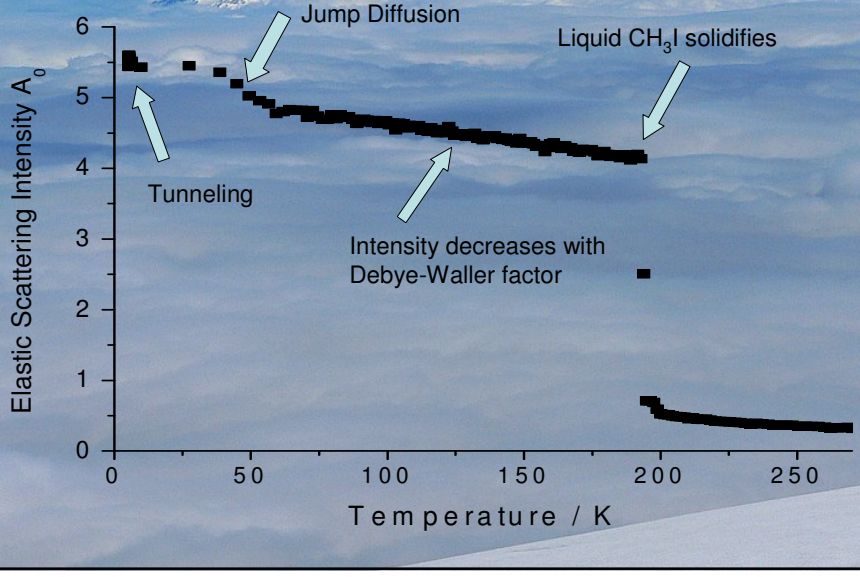


Quantum Rotations in Methyl Iodide

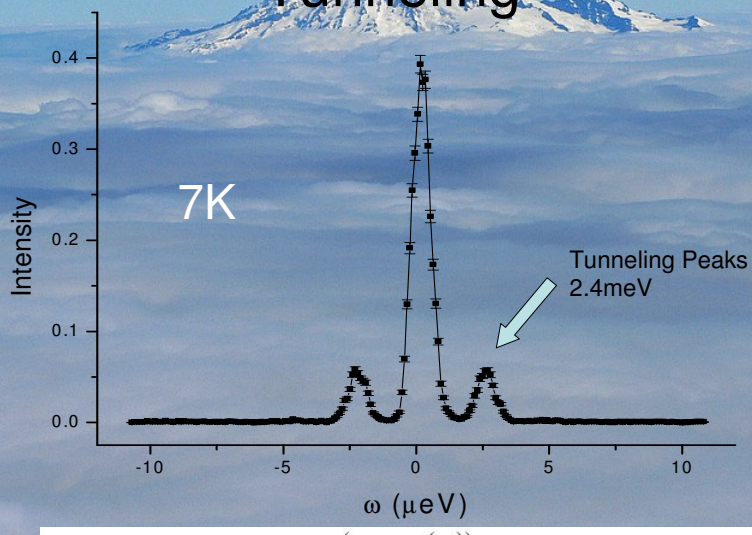




Elastic Scattering

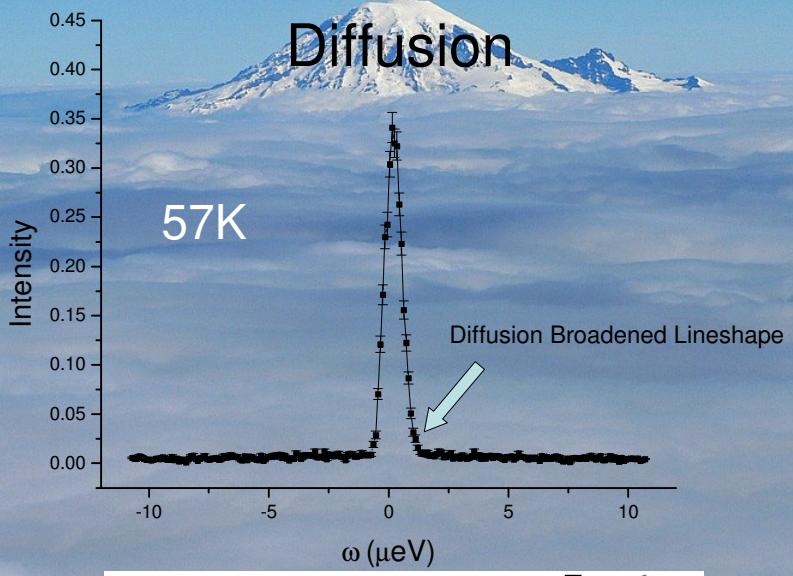


Tunneling

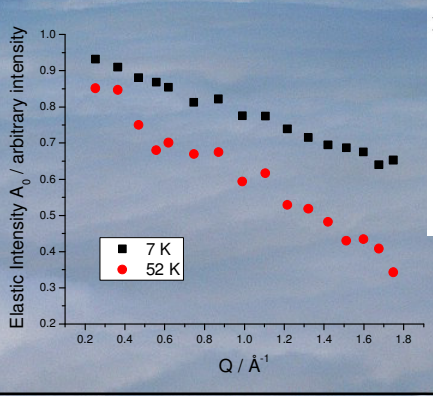


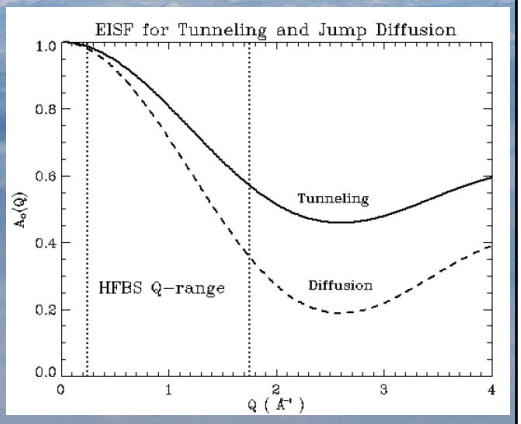
$$S(Q,E) = A_0(Q)\delta(E) + \frac{(1 - A_0(Q))}{2}[\delta(E - E_t) + \delta(E + E_t)]$$

Diffusion

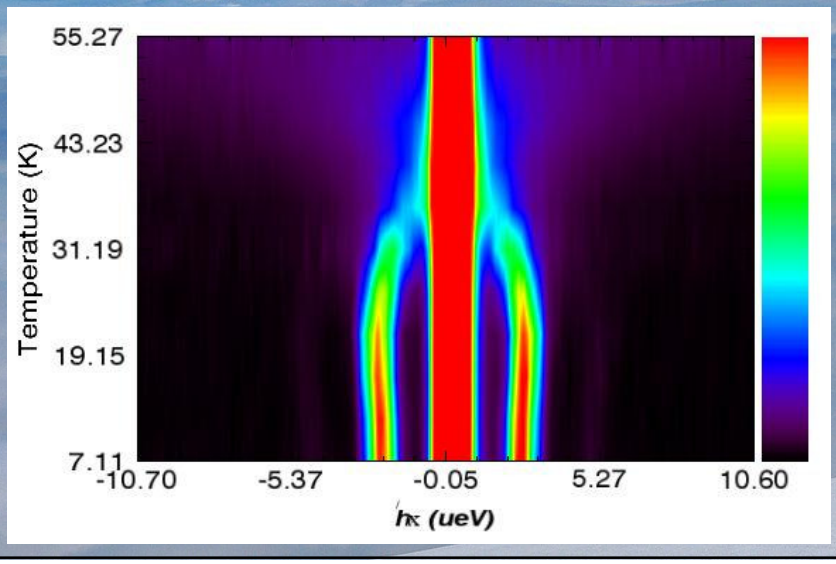


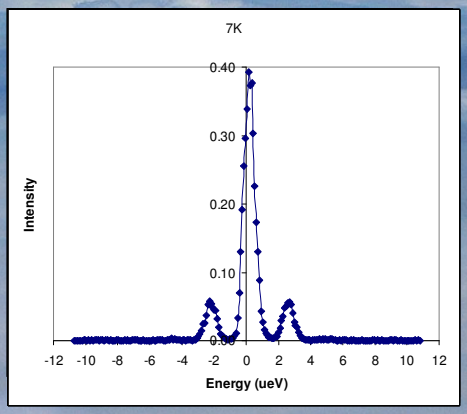
$$S(Q,E) = A_0(Q)\delta(E) + (1 - A_0(Q))\frac{\Gamma}{\pi}\frac{1}{E^2 + \Gamma^2}$$





Temperature Dependence: Diffusion to Tunneling





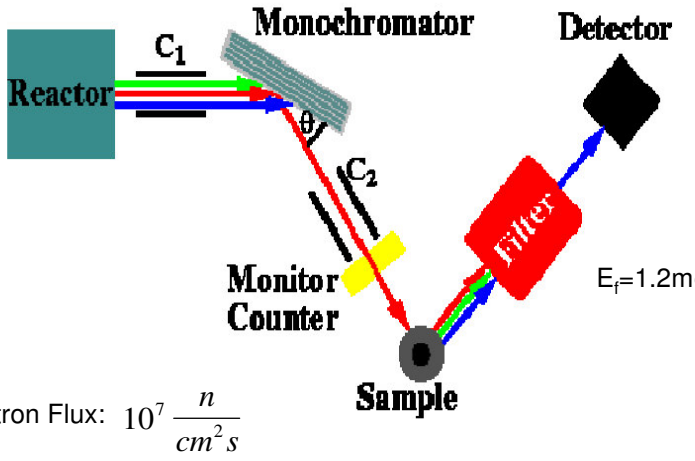
Tunneling energy of 2.4μeV is Q-independent

This tunneling energy indicates that the potential height V_3= 42meV

The separation between the J=1 and J=2 Librational levels is:

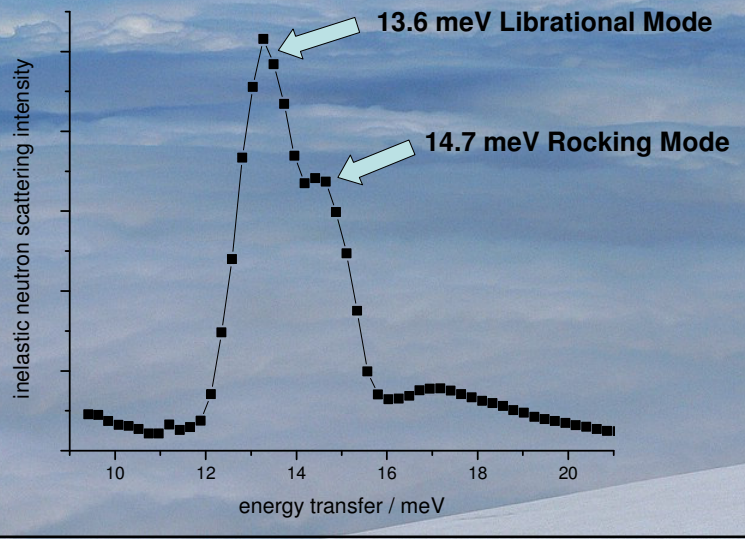
$$E_1 = 3\hbar\frac{\sqrt{V_3}}{2I} = 15.7meV$$

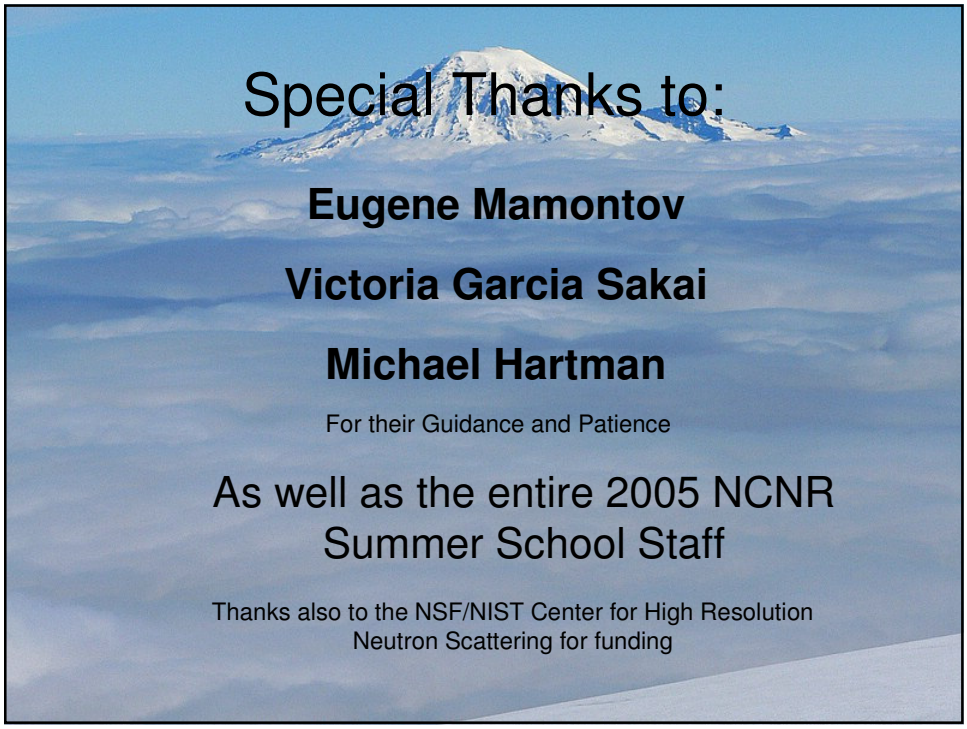
FANS Spectrometer



Neutron Flux: $10^7 \frac{n}{cm^2 s}$

Librational Modes

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