Microscopic Dynamics of Liquid and Solid Hydrogen

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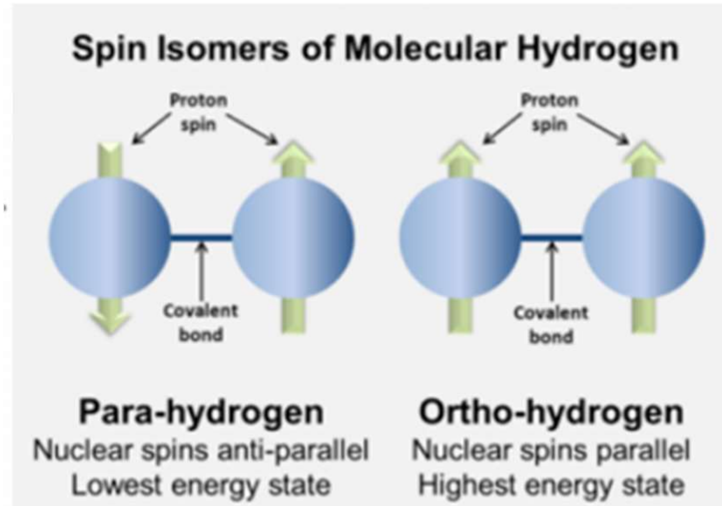
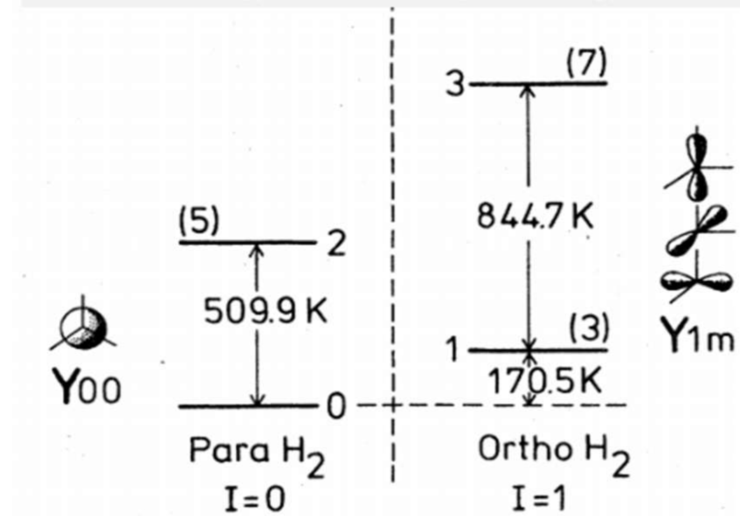
Why Hydrogen?

- Forms a quantum fluid and solid in nature
- Two nuclear spin isomers
- Large quantized rotational levels
- Can be modeled from first principles



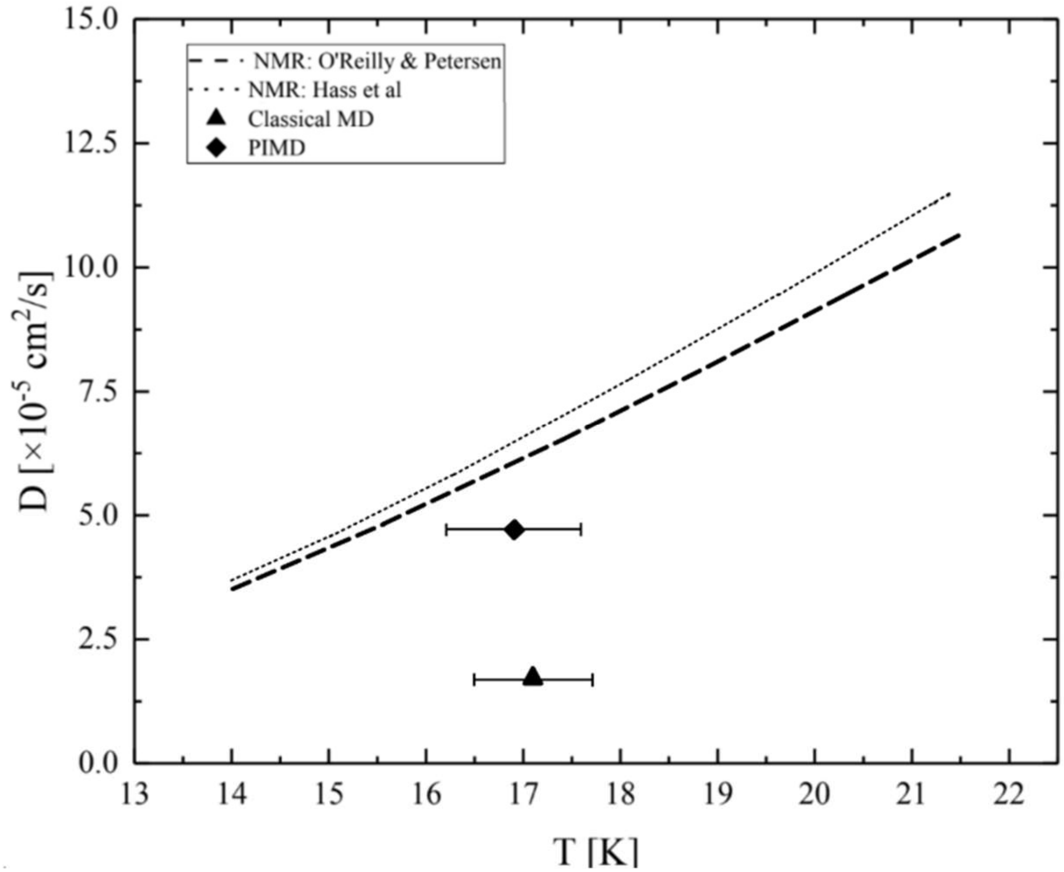


A presentation in three parts

- Diffusion of liquid normal hydrogen
- Molecular mean square displacement of solid para hydrogen
- Applications of research studies in an introductory physics classroom.

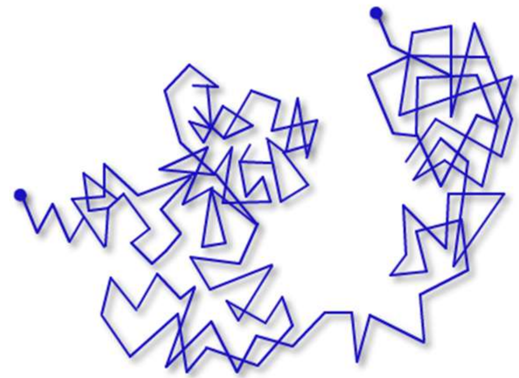
Motivation for the study of liquid H_2 diffusion

- Large zero-point energy contribution
- Theoretical calculations are not fully in agreement with experiment.
- Neutron scattering as a new experimental technique



Neutron Scattering and Diffusive Dynamics of Low temperature Hydrogen

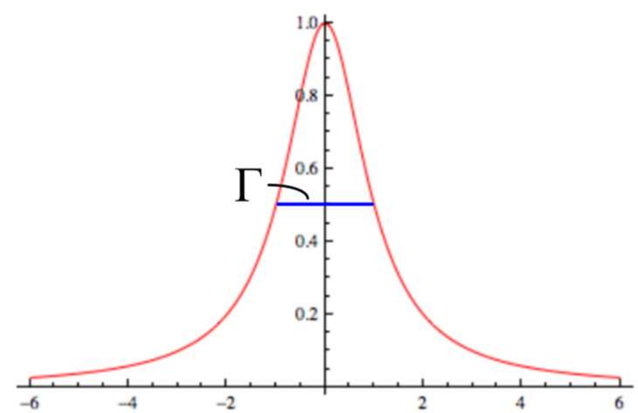
- Why neutron scattering?



Structure Factor:

$$S_{inc}(Q,\omega) = \frac{1}{\pi\hbar}\frac{DQ^2}{\omega^2+(DQ)^2}$$

$$\Gamma_{fwhm} = 2\hbar DQ^2$$



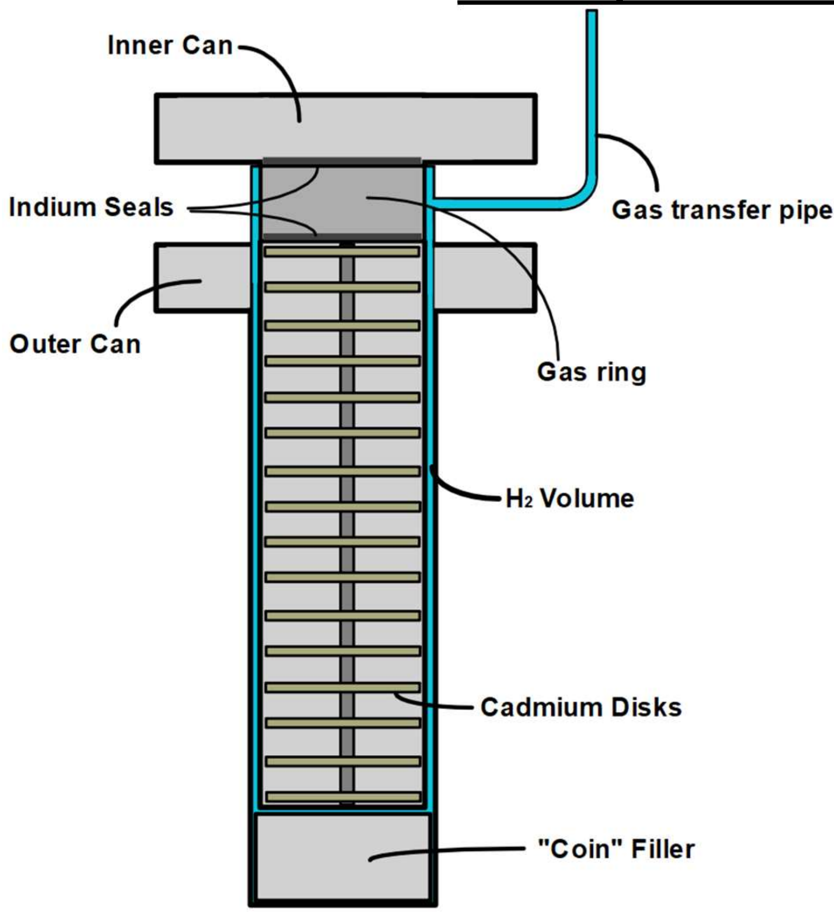
Our instrument: The disk chopper spectrometer (DCS)

Diffusive time scales: ~10^{-12}s

$\lambda_{incident} = 6$ Å

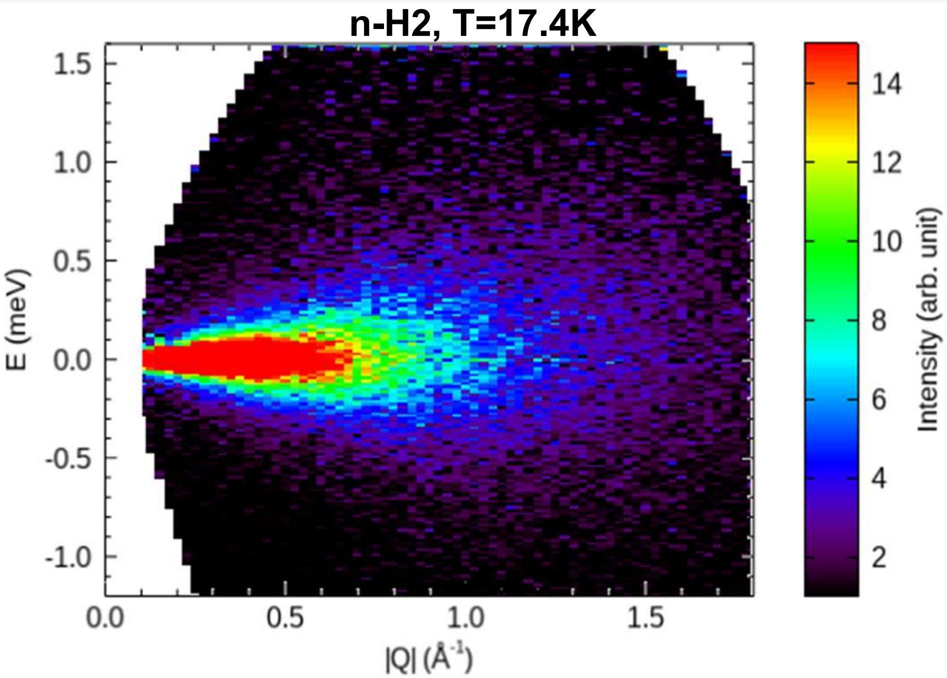
Resolution ~ $30 \mu eV$

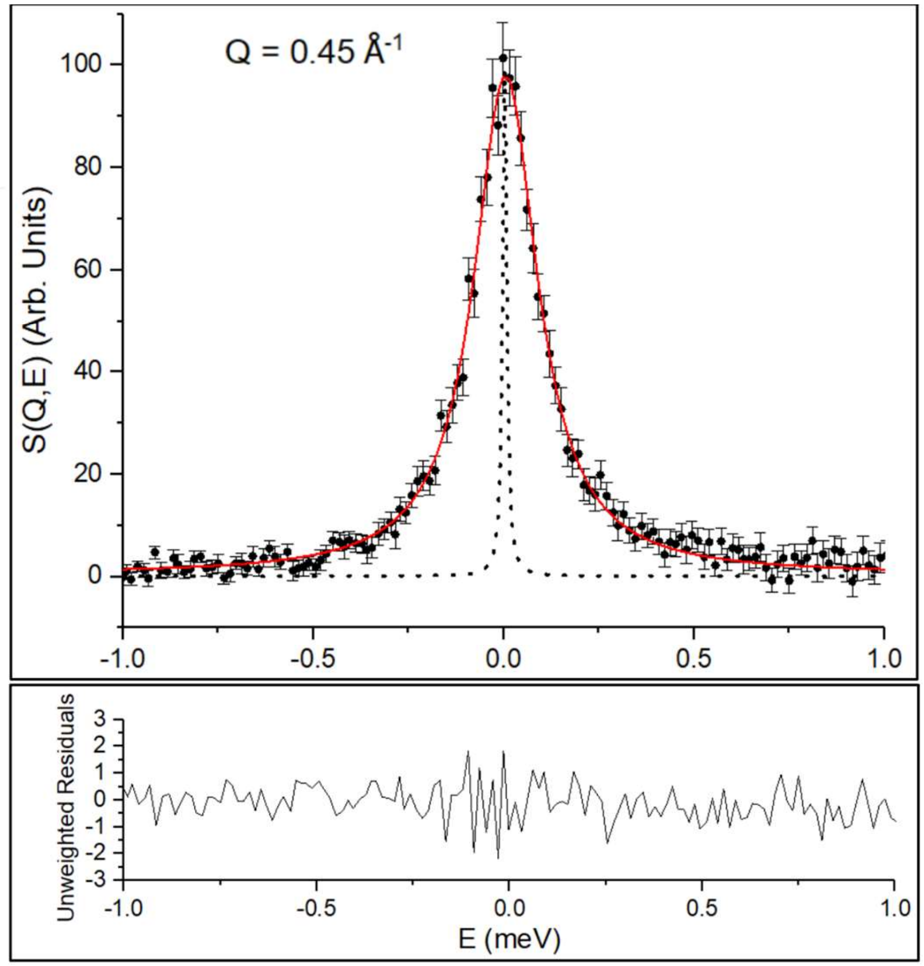
Sample Environment



- We collected data over a 5 temperatures between 15.4 K and 20.4 K.
- We also performed measurements of the empty can background, darkcounts, and vanadium resolution.

Modeling quasielastic broadening

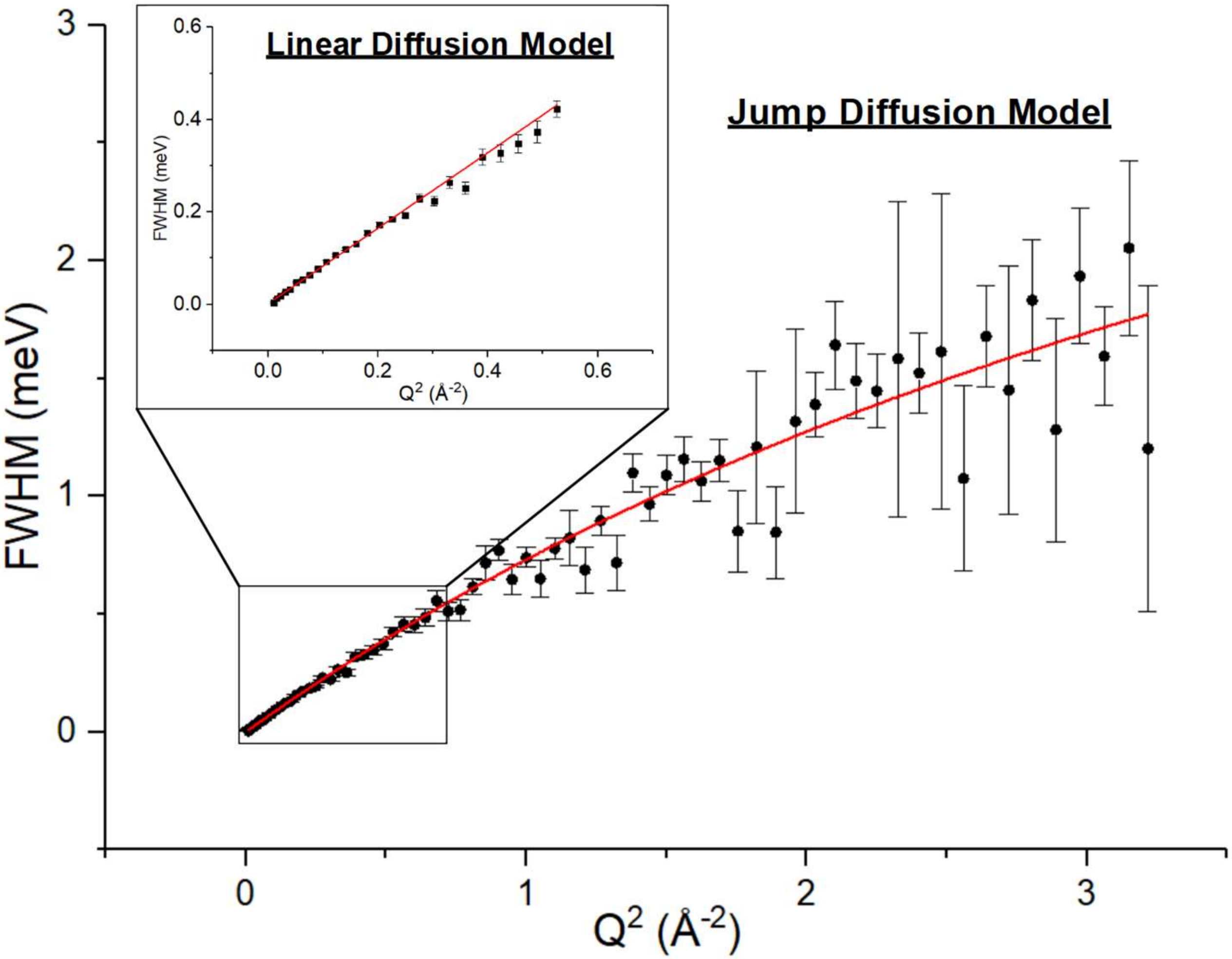




$$\Gamma_{fwhm} = 2\hbar D Q^2$$

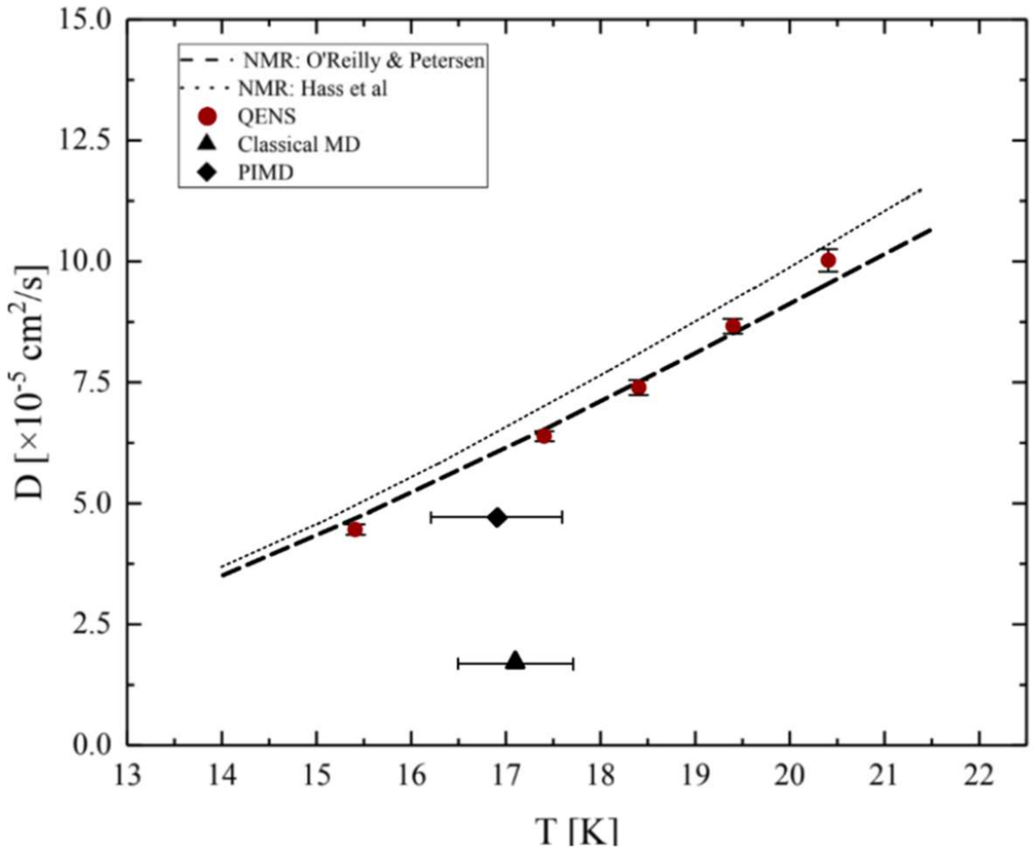
Modeling Q dependence

$$\Gamma_{fwhm} = 2\hbar D Q^2$$

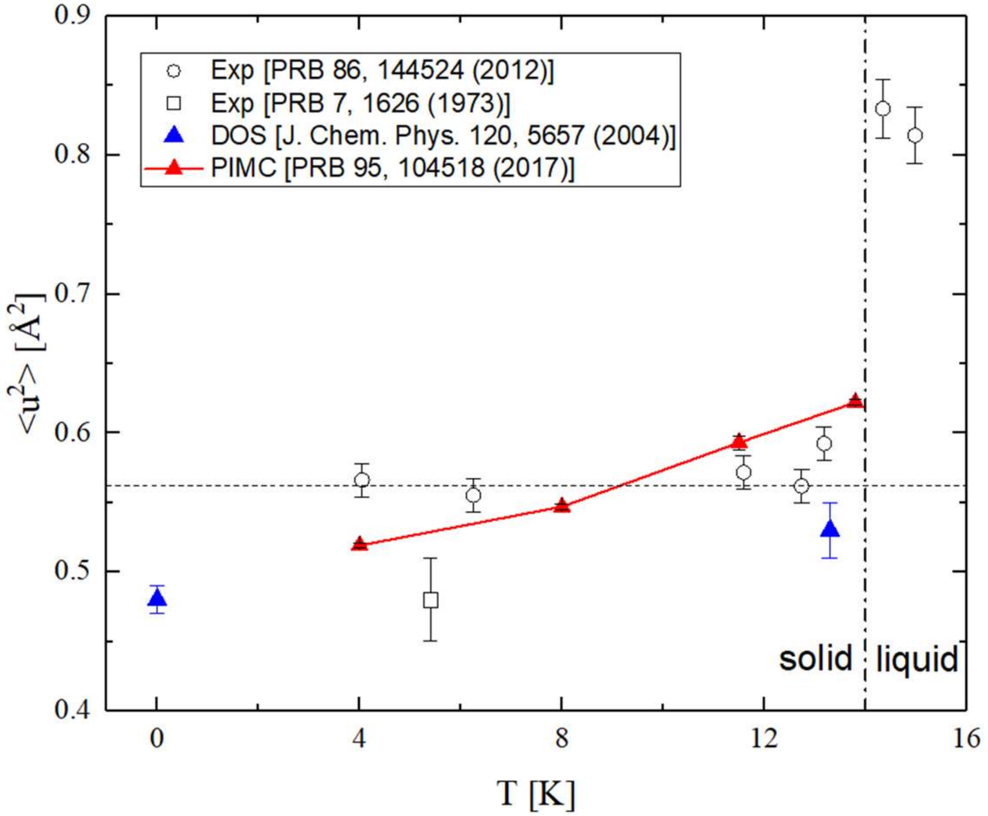


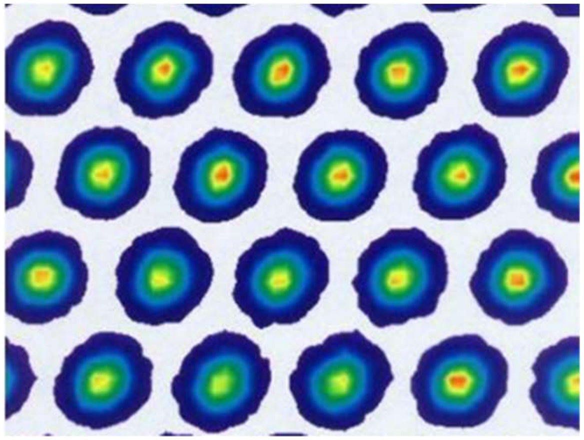
Modeling Temperature Dependence and Conclusion

- Our results provide independent experimental confirmation
- Suggests the need for improved PIMD approximations.



Motivation for the study of dynamics of solid p-H_2



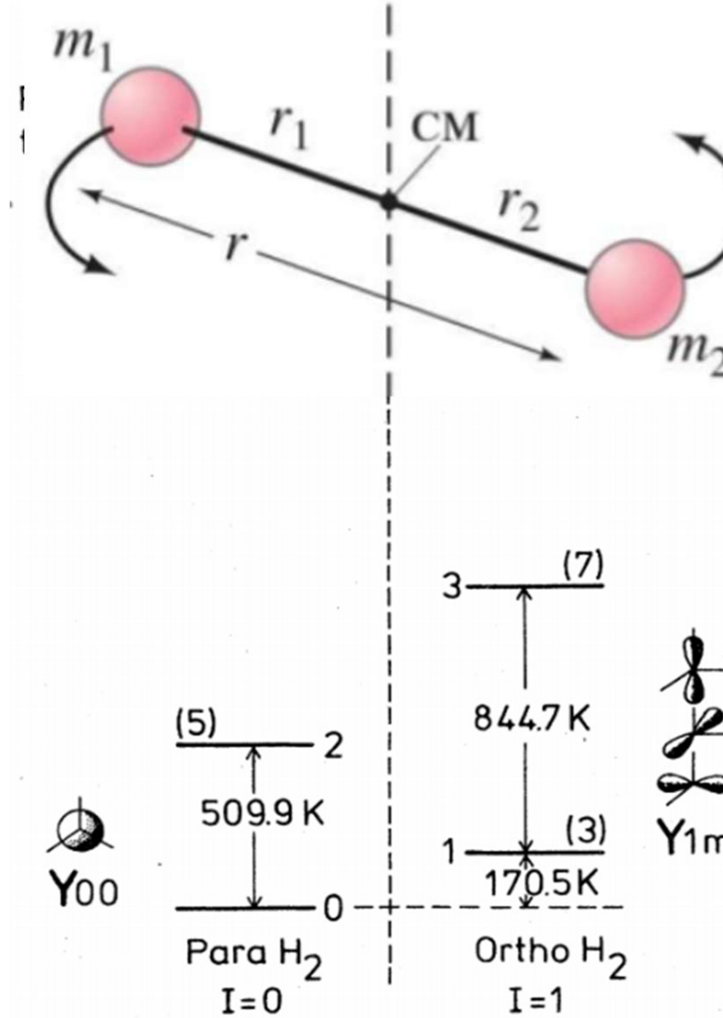


- Experimental results show no qualitative temperature dependence
- Theory predicts T-dependence approaching melting temp.
- What is the contribution of zero-point vs. thermal energy to the vibration of solid H_2?

Mean Squared Displacement of solid $p\text{-}H_2$

- Large zero-point contributions limit bragg peak diffraction techniques normally used to measure $\langle \mu^2 \rangle$
- The rotational line has a contribution from $\langle \mu^2 \rangle$ that we can utilize.

$$I(Q) \sim j_1^2(Qa) \cdot e^{-\left(\frac{\langle \mu^2 \rangle}{3}\right)Q^2}$$



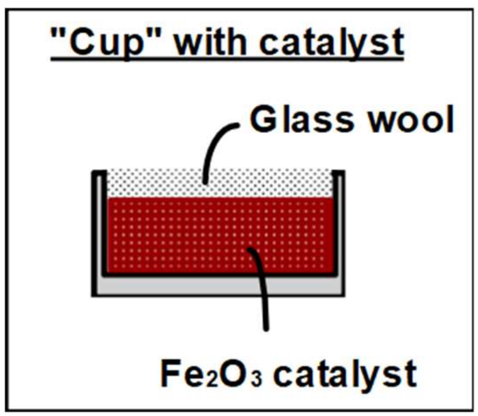
Scattering on the DCS

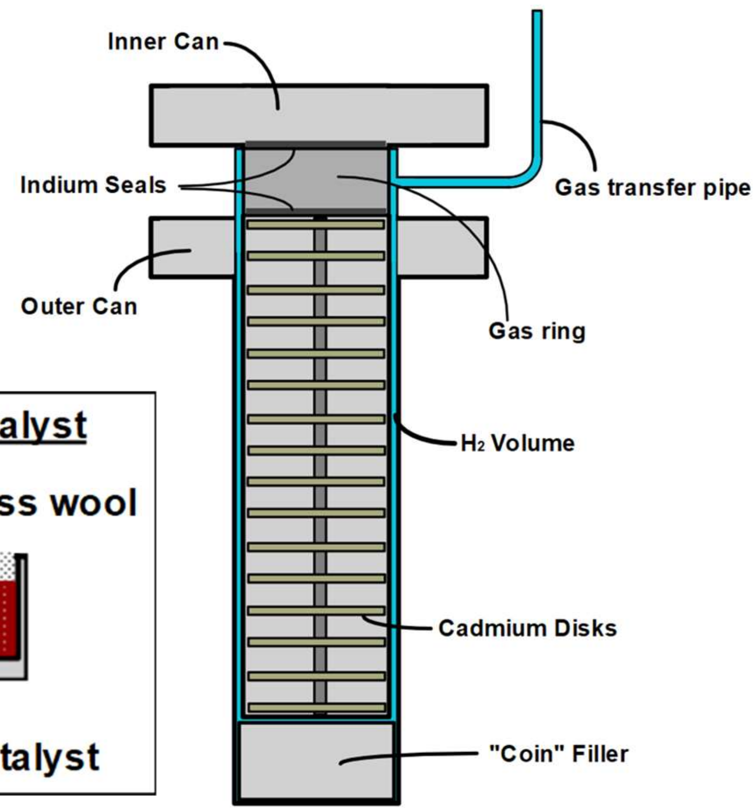
$$\lambda_{incident} = 1.81\ \text{Å}$$

- Expected J0->1 rotational line at 14.7 meV

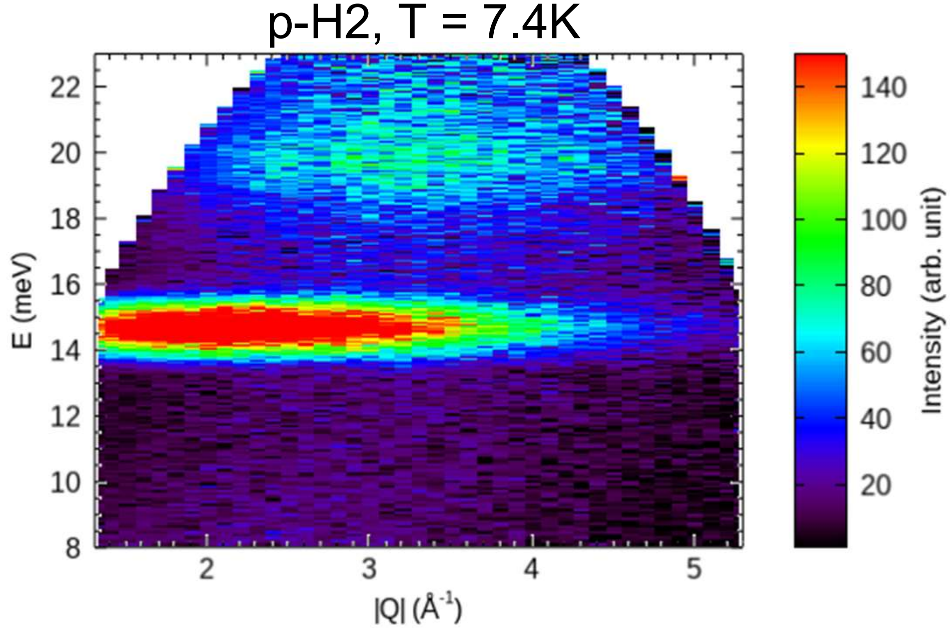
- Ortho to Para conversion

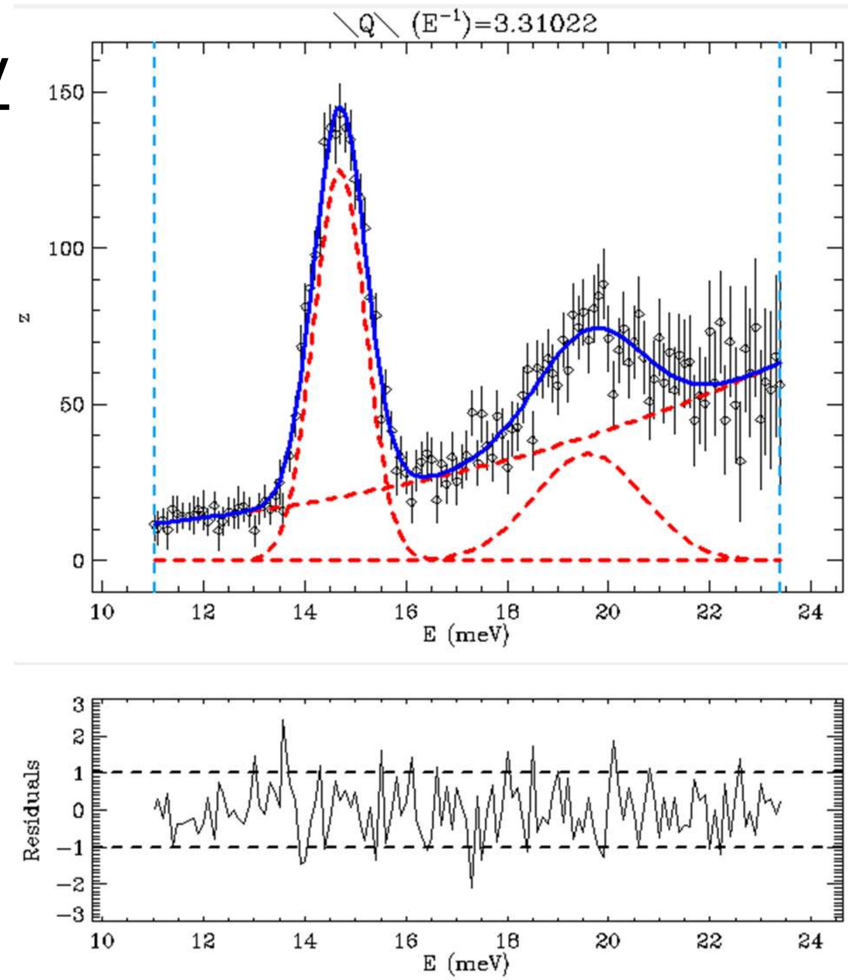
- Temperature range 1.5 K to 13.7 K





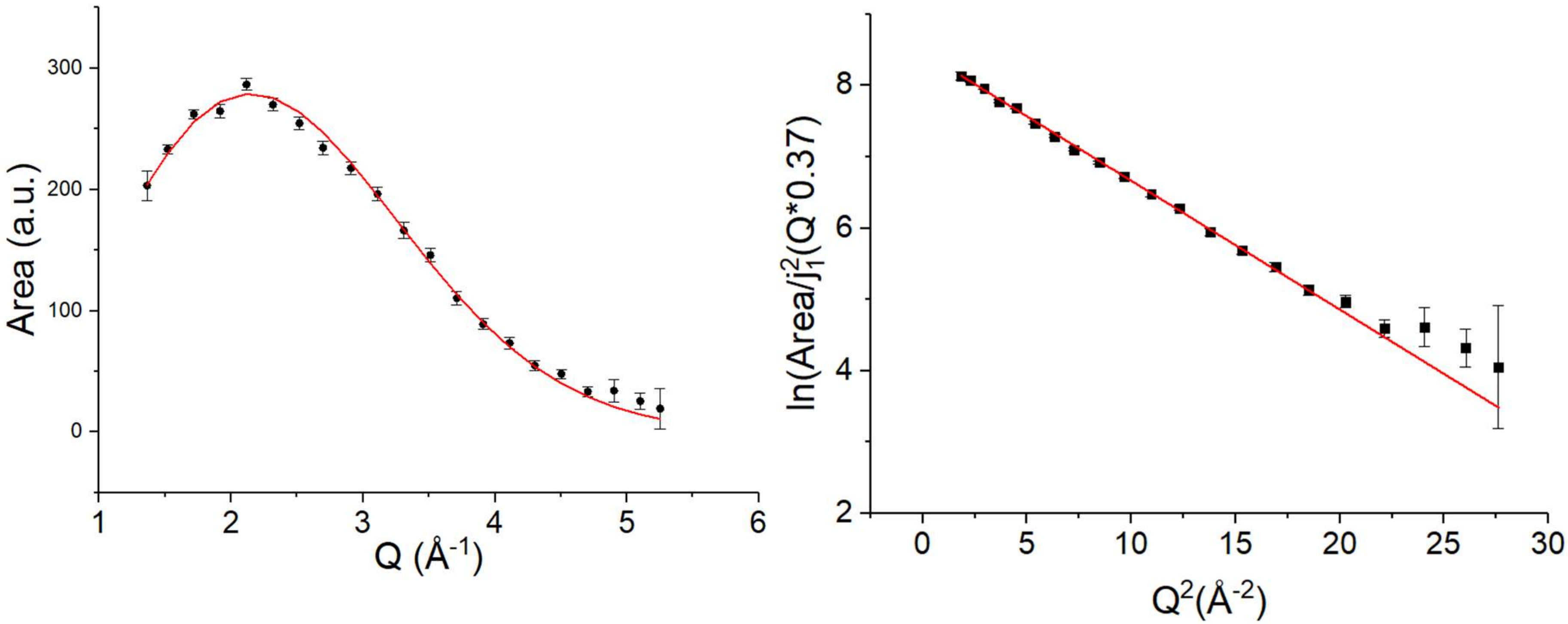
Modeling Rotation Line Energy





$$I(Q) \sim j_1^2(Qa) \cdot e^{-(\frac{<\mu^2>}{3})Q^2}$$

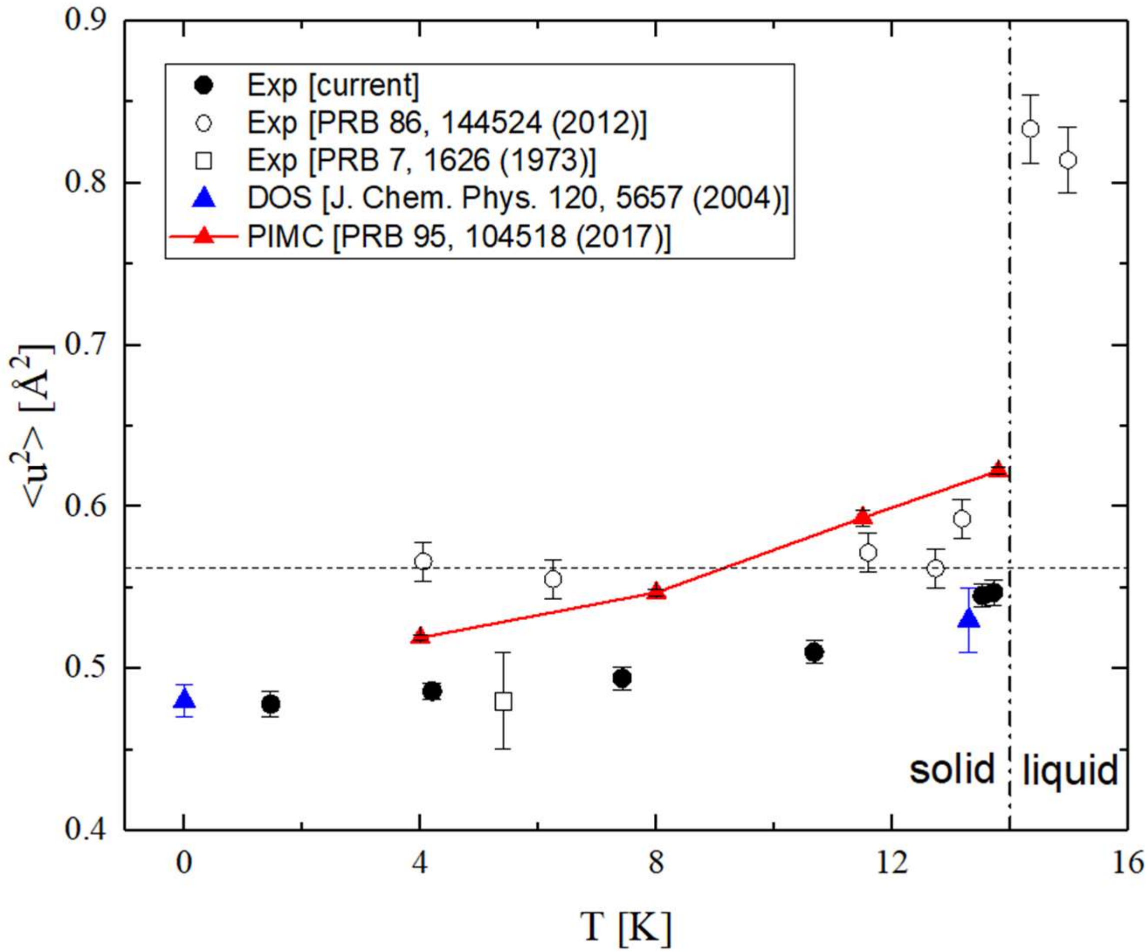
Modeling Q dependence



$$I(Q) \sim j_1^2(Qa) \cdot e^{-(\frac{<\mu^2>}{3})Q^2}$$

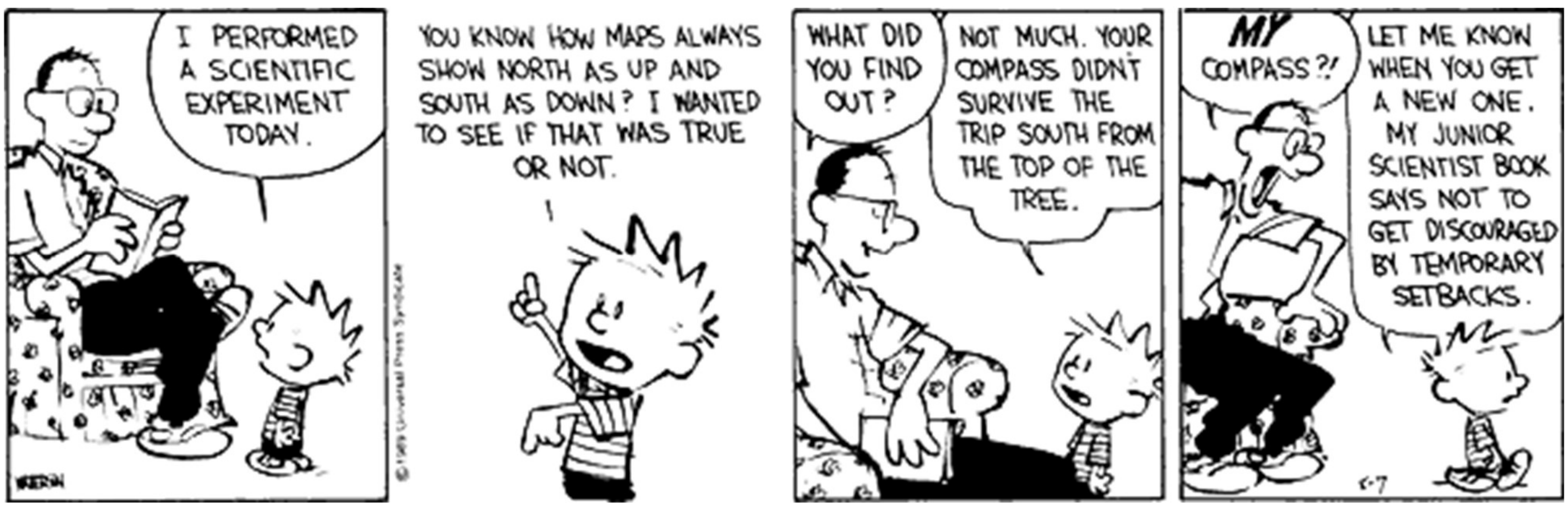
Conclusions

- Thermal contribution evident approaching melting point
- Disagreement with previous experiment
- Qualitative agreement with theoretical calculations.



What did I learn and experience?

- **My first professional research experience**
- **Diversity of science**
- **"In what units?"**
- **Engineer speak**
- **Atmosphere of sharing**



Integrating research knowledge into physics labs

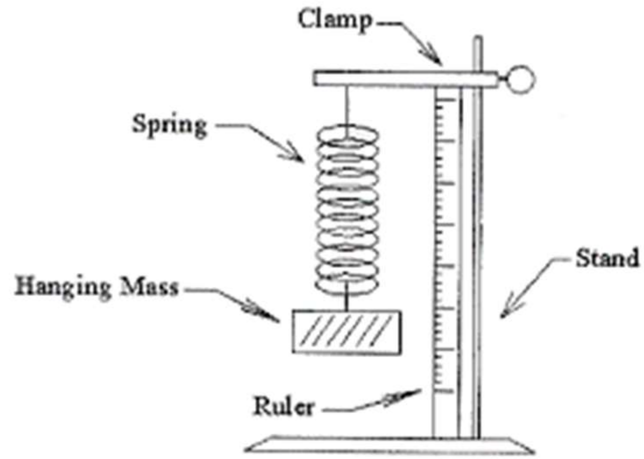
Pose an inquiry question with possible hypothetical hypotheses.

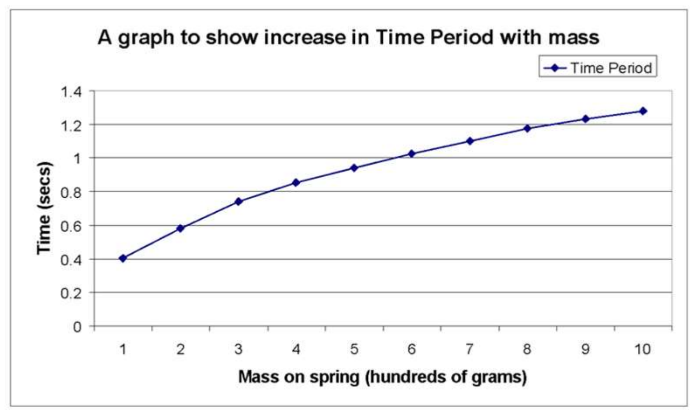
Students formulate their own experimental methodology

- Choose independent variable and controls
- Choose materials and measuring devices

Experimental uncertainties

Presentation of results and inferences.





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Questions?