Metallic Hydrogen: A Liquid Superconductor?

Craig M. Tenney, Zachary F. Croft, and Jeffrey M. McMahon*
Department of Physics and Astronomy, Washington State University

WASHINGTON STATE UNIVERSITY

Introduction

Background

In 1935, Wigner and Huntington predicted[1] that high pressures would dissociate molecular hydrogen into an atomic, metallic phase.

Theoretical arguments suggest[2] that (solid) metallic hydrogen should be a high-temperature superconductor:

- The ions in the system are protons; their small mass should cause the vibrational energy scale of the phonons to be high.
- The electron–ion interaction is due to the bare Coulomb attraction; the electron–phonon coupling should thus be strong.
- The electronic density of states at the Fermi surface should be large; and the Coulomb repulsion between electrons low.

Such arguments further suggest[3] that metallic hydrogen may be superconducting even in the liquid phase:

- The superconducting critical temperature (in the solid) is expected to be greater than the melting temperature.
- The phonon spectrum should be similar in both the solid and liquid phases.
- Disorder doesn't inhibit superconductivity.

Recent calculations[4,5] support these arguments.

Motivation

Determining whether liquid metallic hydrogen is a high-temperature superconductor is important for several reasons:

- **Fundamental physics**: There is no known liquid superconductor. Such would constitute a new state of matter.
- **Planetary physics**: Gas giants (planets) are comprised primarily of liquid metallic hydrogen.
- **Applications**: High- and room-temperature superconductors would have significant applications in energy, electronics, etc.

Methods

General approach

1. Simulate liquid metallic hydrogen.
2. Calculate phonons (spectrum).
3. Calculate electron–phonon coupling.
4. Calculate superconducting critical temperature.

Liquid Structure

In an ordinary **liquid**, atoms do not show any form of long-range order.

Qualitatively, this is seen in liquid metallic hydrogen:

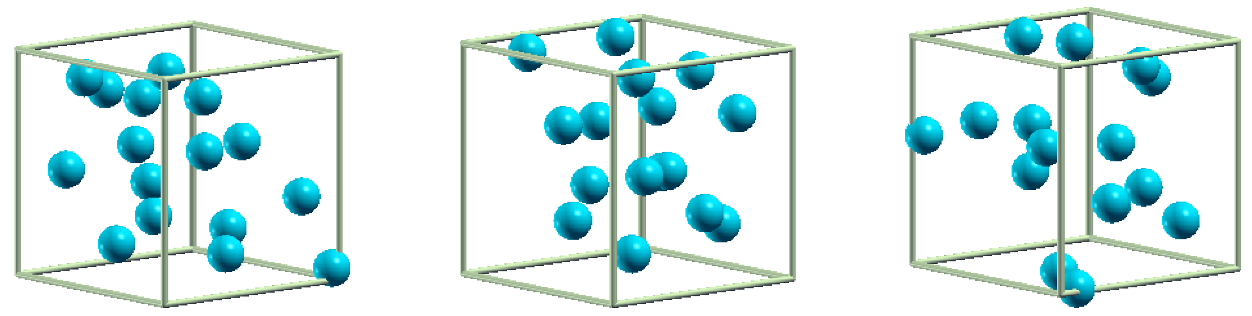

Figure: Snapshots from dynamical simulations, at 550 GPa and 500 K.

Quantitative measures, however, show anomalous local structure:

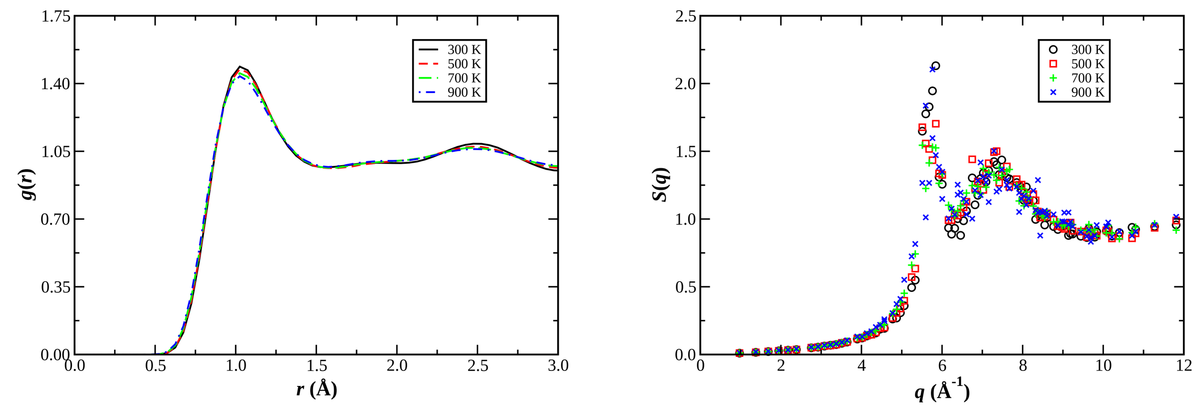

Figure: Structural measures, at 500 GPa.

Phonons

Phonon spectra calculated from dynamical simulations are similar to those from (static) snapshots:

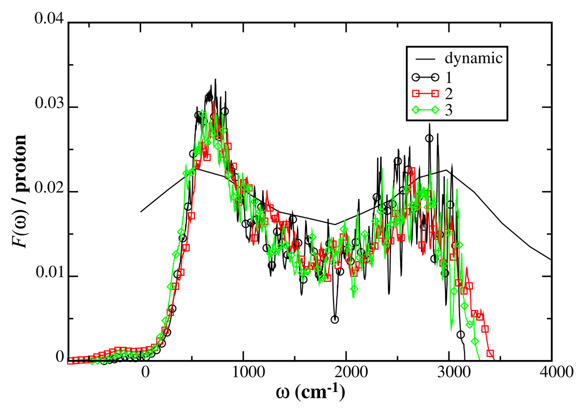

Figure: Phonon density of states $F(\omega)$.

Electron–Phonon Coupling

The bare Coulomb attraction results in large **electron–phonon coupling**:

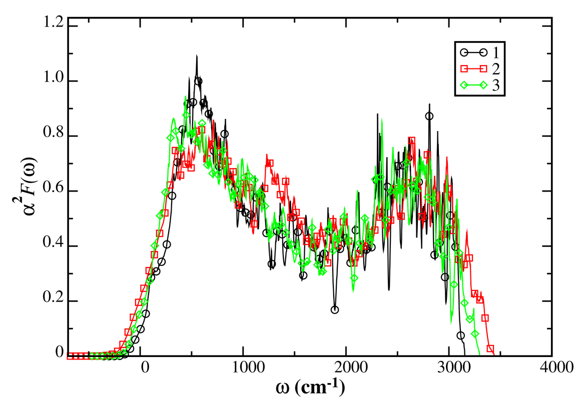

Figure: Electron–phonon spectral function $\alpha^2F(\omega)$.

Superconductivity

The prior features result in high-temperature **superconductivity**:

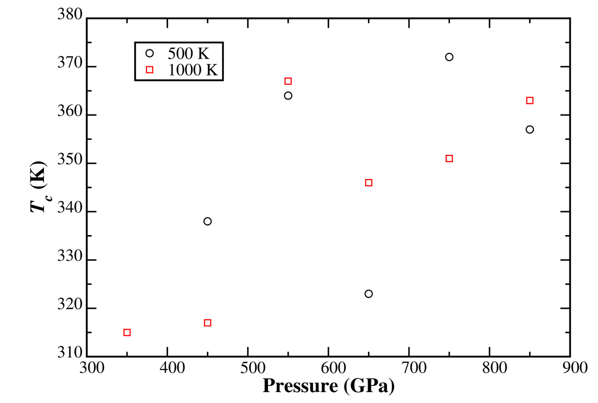

Figure: Superconducting critical temperatures T_c.

Note: These temperatures are above those calculated[5] for melting.

Concluding Remarks

Summary

- Liquid metallic hydrogen *is* a high-temperature superconductor
- … (above the melting temperature[5]).

Future work

- Determine and analyze the uncertainties in the calculations.

Acknowledgments

Startup support:

WASHINGTON STATE UNIVERSITY
Department of Physics and Astronomy

References

1. E. Wigner and H. B. Huntington, *J. Chem. Phys.* **3**, 764 (1935)
2. N. W. Ashcroft, *Phys. Rev. Lett.* **21**, 1748 (1968)
3. J. E. Jaffe and N. W. Ashcroft, *Phys. Rev. B* **23**, 6176 (1981)
4. J. M. McMahon and D. M. Ceperley, *Phys. Rev. B* **84**, 144515 (2011)
5. J. M. McMahon *et al.*, *Submitted* (2017)

https://labs.wsu.edu/mcmahon/
*jeffrey.mcmahon@wsu.edu