THERMODYNAMIC PROPERTIES OF NEON: LESSONS FOR THE DEVELOPMENT OF INTERMOLECULAR POTENTIALS FOR MODERATELY STRONG QUANTUM FLUIDS

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ABSTRACT

Neon occupies a special place among fellow members of the stable and naturally occurring noble gas family. It is very much smaller than argon, krypton and xenon but considerably larger than helium. It is well established [1] that the properties of the larger noble gases can be treated as classical particles and, similarly, the quantum nature of helium is beyond doubt. In contrast, the quantum nature of neon remains contentious. In this work, we discuss recently obtained results [2], which shed light on the nature of intermolecular interactions in neon and their influence on macroscopic thermodynamic properties. This is achieved by using both conventional Monte Carlo (MC) and path integral Monte Carlo (PIMC) simulations [3], in conjunction with a variety of intermolecular potentials that are coupled to the Feynman-Hibbs (FH) term [4] to account for quantum effects. Key thermodynamic properties of neon such as the isobaric and isochoric heat capacities have been reported and compared with experimental data for the entire range of liquid densities from the triple point to the critical point (e.g., see Figure 1).

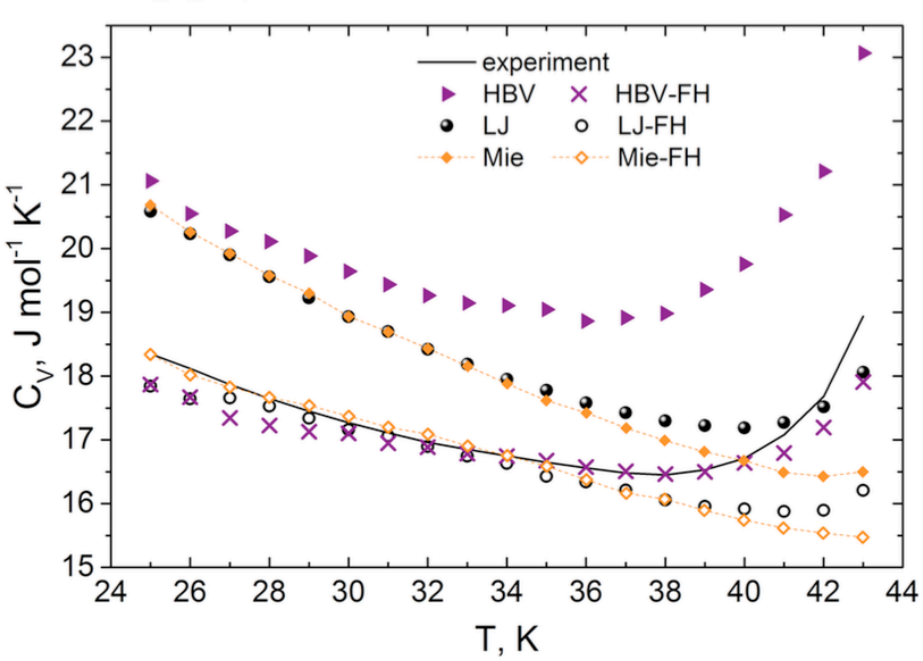

Figure 1: Comparison with experiment of the isochoric heat capacity of neon predicted by alternative intermolecular potentials.

The Feynman-Hibbs (FH) quantum correction results in significant improvements in the accuracy of predicted thermodynamic properties. For example, the new FH version of the Hellmann-Bich-Vogel [5] potential (HBV-FH) predicts isochoric heat capacity to an accuracy of 1.4% over the entire range of liquid densities. The results indicate how some conventional intermolecular potentials can be systematically improved to account for moderately strong quantum systems. The approach has the advantage of being both computationally less expensive and less error prone than PIMC calculations.

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