3rd Asia-Pacific Conference on Plasma Physics, 4-8,11.2019, Hefei, China

Quantum simulation of structure and thermodynamic properties of dense hydrogen

Dongdong Kang
Department of Physics, National University of Defense Technology
e-mail (speaker): ddkang@nudt.edu.cn

The nuclei in quantum many-body systems at finite temperatures are usually treated as classical particles based on Newton equation. This probably leads to inaccurate results for light-atom systems under low temperatures and high pressures. The reason is when the thermal de Broglie wavelength of particles is comparable with the distance between them, the quantum effects such as quantum tunneling and zero-point motion cannot be neglected. Feynman's path-integral formulation of quantum statistical mechanics supplies the possibility for the computer simulation of quantum many-body systems at finite temperatures.

Structure and thermodynamic properties of dense hydrogen are of fundamental significance in astrophysics, planetary science and inertial confinement fusion, and importance for determining the structure and evolution of these astrophysical objects. Due to the low mass, hydrogen is expected to exhibit significant nuclear quantum effects, especially under low temperatures and high pressures [1]. To consider nuclear quantum effects (NQEs), we investigated structure, transport properties, melting behavior and liquid-liquid phase transition of dense hydrogen using ab initio path integral molecular dynamics (PIMD) simulations. The electronic interactions are calculated by density functional theory. The results show that the nuclear quantum nature significantly affects the structure and transport properties [2,3]. With the inclusion of NQEs, the radial distribution functions are obviously broadened. Due to the lower collision cross sections, the self-diffusion is largely higher while the shear viscosity is notably lower than the results without the inclusion of NQEs. The electrical conductivity is also significantly affected by NQEs.

The melting temperature of dense hydrogen was investigated using the two-phase approach based on the PIMD with the Yukawa potential describing the interaction between ions. The results show that the NQEs have a significant impact on the melting of dense hydrogen, which largely lower the melting temperature by ~10% at the density range of 10-1000 g/cm^3. PIMD simulations driven by orbital-free density functional theory are applied to study NQEs on equation of states and structure of two-temperature warm dense hydrogen [4]. NQEs on structure and thermodynamic properties of the two-temperature systems are systematically evaluated. In addition, the liquid-liquid phase transition of dense liquid hydrogen at megabar pressures is also significantly affected by NQEs [5].

References

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