Physics & Astrophysics Colloquium

Integral Equation Theory for Classical Fluids with Pressure and Free Energy Consistency

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4:00 PM Friday, March 10, 2023, Room 211, Witmer Hall

Abstract:
An integral equation theory is a powerful approach to simple liquids due to its low computational cost and the fact that theory is thermodynamically complete. Although this equation is exact, it must be coupled with an approximate closure equation, which introduces path-dependence and thermodynamic inconsistencies. In particular, pressure and free energy inconsistencies introduce severe inaccuracies and limit the usefulness of this approach. Therefore, we proposed a new closure approximation that simultaneously enforces both pressure and free energy consistencies and tested it for a single-component Lennard-Jones fluid in terms of the Ornstein-Zernike integral equation theory. We present numerical results for the Helmholtz free energy, pressure, and excess chemical potential for some values of reduced densities and temperatures. Moreover, we discuss some results for excess chemical potential for hard-sphere atomic/molecular fluids and solute-solvent system using different approximations. Our results are in good agreement with available Monte-Carlo data.

Refreshments at 3:30 PM in Witmer Hall, Room 215

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