PIMC for Heavy Atoms with Pseudo-Hamiltonians

Kenneth P. Esler Jr., Bryan K. Clark and David M. Ceperley

Department of Physics, University of Illinois at Urbana-Champaign
Urbana, IL, USA

Decades ago, local pseudopotentials (LPPs) proved quite successful in density functional calculations which contained heavy atoms. These were supplanted by nonlocal pseudopotentials (NLPPs), which were more accurate, but lost the desirable property of locality. In 1989, Bachelet, Ceperley, and Chiocchetti[1] introduced pseudo-Hamiltonians (PHs), which added flexibility to the local PP by adding a position-dependent mass tensor. This improved on the accuracy of LPPs, while retaining locality.

Path Integral Monte Carlo (PIMC) is tool proven to simulate many-body quantum systems at finite temperature. It provides exact equilibrium results for bosons and very high-accuracy results for fermions. The problems assoiciated with introducing NLPPs into PIMC have prevented the method from being used in systems containing all but the lightest elements. Here, we introduce a method utilizing PHs in PIMC for simulation for simulations containing heavy atoms, and a corresponding suite of codes for

- the construction of BCC PHs
- the computation of pair density matrices from the PHs
- path integral Monte Carlo simulation
- statistical analysis of results and HTML report generation
- visualization of the simulation

This suite will be released as open-source when it has reached production quality. We present some preliminary results from the simulation of sodium.

References

[1] G.B. Bachelet, D.M. Ceperley, and M.G.B. Chiocchetti, Phys. Rev. Let. **62**, 2088 (1989)