

Abstract Submitted
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Path Integral Sampling Techniques JENNIFER BARRY, AMY BUG,
Swarthmore College — In this study, we evaluate several Monte Carlo methods with the goal of simulating a light particle in a fluid. We present a simulation that allows Metropolis sampling, Wang-Landau sampling, or multicanonical sampling for a Lennard-Jones fluid within a canonical or grand canonical ensemble. We compare these methods and show that the results from each are self-consistent. We also present a simulation that performs Metropolis Path Integral Monte Carlo or Wang-Landau Path Integral sampling for a light particle. Simulating a quantum particle in a simple harmonic potential, we demonstrate that our results match analytical calculations for finite bead numbers. The two sampling methods yield results that are in agreement for the light particle interacting with the fluid via a potential meant to represent He within Ar. Finally, we show benchmarks that indicate how the performance of Wang-Landau and Metropolis sampling compare for these systems where efficient means of equilibration and sampling are needed.

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