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Convergence Study of the Path Integral Monte Carlo Technique for a Quantum Particle in a Supercritical Fluid TERRENCE REESE, Southern University and A&M College, BRUCE MILLER, Texas Christian University — A quantum particle (qp) in a fluid near the liquid vapor-critical point creates a volume of altered density in which it becomes localized. In previous research we have used the Path Integral Monte Carlo (PIMC) technique to investigate the properties of the qp-fluid molecule system. The path integral formulation represents the quantum particle as a closed chain of P classical particles in which the quantum spread of the qp is manifest in the spread of the chain. This formulation allows classical Monte Carlo techniques to be used to compute quantum mechanical equilibrium values. In this work we will explore the convergence of the PIMC technique for a qp equilibrated in a Lennard-Jones fluid whose characteristics resemble Xenon. The computations were done for two densities of the fluid at 300 and 340K. The correlation function, the number of independent samples and the radius of gyration were computed. The autocorrelation function for the pick-off decay rate was computed for increments of 500 and 5000. It was discovered that for the lower density the computed values of the pick-off decay rate became independent within an increment of 500, while near the critical density an increment of more than 1000 was required for the values to become uncorrelated.

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