Path Integral representation of quantum particles in fluids: Convergence of observables TERREBCE REESE, Southern University and A&M College, BRUCE MILLER, Texas Christian University — In previous work the Path Integral Monte Carlo (PIMC) technique was used to simulate a low mass quantum particle (qp) in a dense Lennard-Jones 6-12 fluid having the thermodynamic properties of Xenon. Because of the difference in thermal wavelengths between the qp and the fluid molecules, the fluid molecules can be treated classically. This combination of using quantum mechanics for the qp and classical mechanics for the fluid molecules is known as a hybrid model. In the path integral formulation the qp is represented as a closed chain of P classical particles where the quantum uncertainty in the position of the qp is manifested by the finite spread of the polymer chain. The PIMC technique allows standard classical Monte Carlo techniques to be used to compute quantum mechanical equilibrium values like the ortho-Positronium pick-off decay rate. Here we compare the convergence of PIMC for different thermodynamic states, including one near the liquid-vapor critical point of the fluid. We employ the correlation function of the iterated quantum observables to estimate the number of statistically independent configurations in a run and provide an estimate of the standard error.

Terrence Reese
Southern University and A&M College