

Abstract Submitted
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Comparison of Correlation Functions for Path Integral Formulation of Ortho-Positronium in Dense Fluids TERRENCE 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 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 using quantum mechanics for the qp and classical mechanics for the fluid molecules is a hybrid model. The path integral formulation represents a qp as a closed chain of P classical particles in which the quantum uncertainty in the position of the qp is manifested in the finite width 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. The Correlation Function, $C(k)$, is the mean of the product of the difference of a variable, at the times j and $j+k$, with the average value of that variable divided by the variance. The correlation length, k , at which $C(k)$ becomes zero, indicates the number of passes before values of the independent variable become statistically independent. The Correlation Function versus the correlation length has been plotted for the decay rate covering different polymer segment lengths, temperatures, densities, and fluid molecule numbers. The number of statistically independent configurations has also been computed for each thermodynamic system.

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