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Comparisons of Different Particle-Chain Methods for Path Integral Monte Carlo Methods TERRENCE REESE, Southern Unversity and A&M College, BRUCE MILLER, Texas Christian University — In previous work we have used Path Integral Monte Carlo methods to simulate a Positronium atom in a Lennard-Jones fluid. Trial positions are created for sub-chains of particles on the polymer chain to allow for proper exploration of the configuration space. Different methods can be used to determine how the different chains are selected. In this report we compare the results from simulations of Positronium in Xenon at 300 and 340K using our leap frog method and another method where the selection of the sub-chains for trial movements is done randomly. The results indicate that a random selection of sub-chains leads to more accurate simulation results at higher densities.

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