Width Spreading and Tests of Wave Packet Molecular Dynamics

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We examine three aspects of wave packet molecular dynamics (WPMD): wave packet spreading, the versatility of the isotropic Gaussian basis, and the interpretation of WPMD data. It is commonly known in the WPMD community that at large temperatures isotropic Gaussian wave packets have divergent widths. We quantify the unphysicality of this behavior by calculating radial distribution functions at many temperatures and densities, and compare to quantum statistical potential and path integral Monte Carlo results. We also make direct comparisons with a numerically exact time-dependent Schrödinger equation solver to determine deficiencies in the basis by studying a single quantum electron traveling through a static classical dense plasma. Another aspect is the validity of standard calculation methods. Central to these quantum computations are the ensemble explored by WPMD and its ergodic properties.

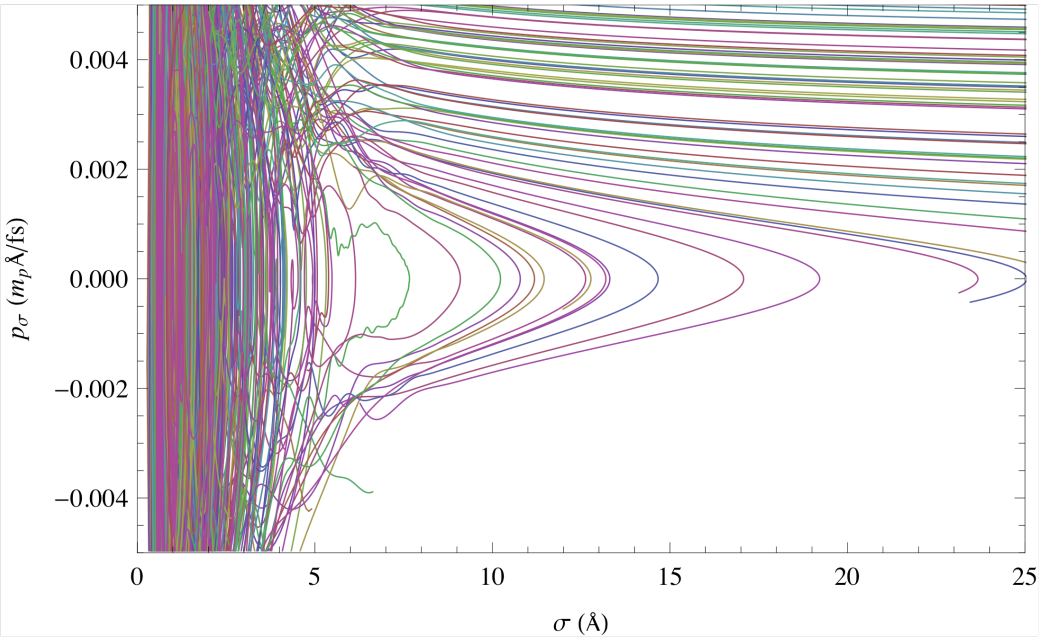

Figure 1: Generalized phase space of the wave packet widths and their conjugate momenta of a WPMD simulation at T = 46 eV and n = 10^{24} cm^{-3} during 17 fs of a 1000 particle simulation.