Correlated parameters in the quasi-classical treatment of atomic ground states using effective momentum dependent potentials for molecular dynamics simulation of strongly coupled plasmas[1] JOHN VERBONCOEUR, GAUTHAM DHARUMAN, Dept. of Electrical Engg., Michigan State University, East Lansing, MI, USA, ANDREW CHRISTLIEB, Dept. of Mathematics, Michigan State University, East Lansing, MI, USA, MICHAEL MURILLO, Computational Physics and Methods Group, Los Alamos National Laboratory, Los Alamos, NM, USA — Ground state energies and configurations of N, F, Ne, Al, S, Ar and Ca are obtained using a quasi-classical treatment with Kirschbaum-Wilets potentials [1]. The effect of phase space parameters on the ground state energy is studied in detail and compared with Hartree-Fock values. The phase space parameters that resulted in ground state energies comparable to Hartree-Fock values are found to be correlated and follow a pattern with atomic number which led to identifying a predictive capability in the model. The change in ground state configurations for different phase space parameters is studied and correlated with the corresponding change in ground state energies.

[1] C.L. Kirschbaum and L. Wilets, Phys. Rev. A 21, 834 (1980).

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