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Effective momentum-dependent potentials for atomic bound states and scattering in strongly coupled plasmas A. CHRISTLIEB, G. DHARUMAN, J. VERBONCOEUR, Michigan State University, M.S. MURILLO, New Mexico Consortium — Modeling high energy-density experiments requires simulations spanning large length and time scales. These non-equilibrium experiments have time evolving ionization and partial degeneracy, obviating the direct use of the time-dependent Schrodinger equation. Therefore, efficient approximate methods are greatly needed. We have examined the accuracy of one such method based on an effective classical-dynamics approach employing effective momentum dependent potentials (MDPs) within a Hamiltonian framework that enables large-scale simulations. We have found that a commonly used formulation, based on Kirschbaum-Wilets MDPs [1] leads to very accurate ground state energies and good first/second-ionization energies. The continuum scattering properties of free electrons were examined by comparing the momentum-transfer cross section (MTCS) predicted by KW MDP to a semi-classical phase-shift calculation. Optimizing the KW MDP parameters for the scattering process yielded poor MTCSs, suggesting a limitation of the use of KW MDP for plasmas. However, our new MDP yields MTCS values in much better agreement than KW MDP.[1] Phys. Rev. A 51, 266 (1995)

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