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Wave packet spreading and localization in electron-nuclear scattering ANDREAS MARKMANN*, Chemistry, Yale, P.E. GRABOWSKI*, Computational Physics, LANL, I.V. MOROZOV, I.A. VALUEV, Inst. High Temp., Moscow, Russia, C.A. FICHTL, Computational Physics, LANL, V.S. BATISTA, Chemistry, Yale, F.R. GRAZIANI, LLNL, M.S. MURILLO, Computational Physics, LANL, CIMARRON COLLABORATION — The wave packet molecular dynamics (WPMD) method solves the time-dependent Schrödinger equation via a variational approximation. Application to high-temperature dense plasmas has yielded diverging electron width (spreading) with diminished electron-nuclear interaction. This was previously ascribed to a shortcoming of WPMD and has been counteracted by heuristic additions to the model. We employ various methods to determine if spreading continues to be predicted. Single electron scattering on a periodic array of statically screened protons is used as a model problem for comparison via the numerically exact split operator Fourier transform method, the Wigner trajectory method, and the time-dependent variational principle (TDVP). Within the TDVP, we use as ansätze the standard form of WPMD, a single Gaussian wave packet (WP), as well as the split WP method, a linear combination of Gaussian WPs. Spreading is predicted by all methods, so is not the cause of unphysical diminishing interactions in WPMD. Instead, the Gaussian WP's inability to reproduce breakup of the density into fragments localized near ions is responsible for the deviation between methods. Hence, extensions of WPMD must include a mechanism for breakup.
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