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Title: Wave Packet Molecular Dynamics with Packet Splitting

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The method of Wave Packet Molecular Dynamics Method (WPMD) is used in the dynamic simulations of many-electron systems. It may be considered as a robust mapping of the quantum many body problem onto a set of "classical" equations of motion with fixed number of dynamic variables. The antisymmetrized version of WPMD (AWPMD) allows one to construct trial many-electron wavefunction taking electron spins into account, for example, taking Hartree-Fock approximation. In this contribution we present recently developed split-packet version of WPMD. In this formulation each electron is represented by multiple Gaussians, with mixing coefficients playing the role of additional dynamic variables. The resulting set of equations of motion is constrained by the norm conservation requirements for each electron and for the whole wave function. It is solved dynamically or by Monte Carlo sampling. The new method was recently implemented into LAMMPS molecular dynamics package in its fully antisymmetrized formulation. The split packet method has larger flexibility and much better accuracy than the original WPMD with a single Gaussian per electron. We demonstrate its ability to reproduce binding energies for atoms and molecules with accuracy increasing with the number of Gaussians. We also consider a problem of ionization of atoms by an external electric field, where the split packets provide a basis for quantum branching. The results for Hydrogen ionization agree well with direct numerical solution of the Schroedinger equation. The computational scalability of the WPMD algorithm depends on the approximation level for the quantum problem. The antisymmetrized version is the most computationally demanding (scales as ~N^4 with the number of particles). The strategy of improving scalability is discussed based on diagonal Coulomb interaction prevailing for large systems. Computational details and the implementation of WPMD into the LAMMPS code will be presented briefly.