Simulations of nonideal plasmas and warm dense matter by the methods of wave packet dynamics

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The method of wave packet molecular dynamics (WPMD) for studying nonideal plasmas and warm dense matter is overviewed. This method is based on the representation of electrons as Gaussian wave packets with variable width. It extends the classical molecular dynamics where the electron-electron and ion-electron interactions are defined by semi-empirical pseudopotentials. Various modifications of the WPMD method are considered including AWPMD with antisymmetrization of the multi-electron wave functions, Electron Force Field (eFF) with parametrization of s- and p-electrons, Split-WPMD with multiple Gaussians per electron, and a new WPMD-DFT approach where the exchange and correlation effects are treated using an additional energy term taken from DFT [1, 2]. The issues of the wave packet broadening and the use of different boundary conditions are discussed.

The application of the wave packet methods is demonstrated by simulations of shock-compressed deuterium and helium. The compression isentropes and the deuterium Hugoniot adiabat are calculated by WPMD-DFT and compared with experimental data and other simulation approaches including eFF, AWPMD, QMD, and PIMC. It is shown that the WPMD-like methods are applicable to simulations of nonequilibrium states and electron-ion relaxation processes.

[1] Lavrinenko Y S, Morozov I V and Valuev I A 2019 *Contrib. Plasma Phys.* **59** e201800179

[2] Lavrinenko Y, Levashov P R, Minakov D V, Morozov I V and Valuev I A 2021 *Phys. Rev. E* **104** 045304