The method of Wave Packet Molecular Dynamics for warm dense matter and nonideal plasma simulations

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Interaction of strong laser pulses and particle beams with condensed matter produce special (extreme) states of the mater such as warm dense matter and nonideal plasmas. Study of particle dynamics at such states can hardly be done analytically and require appropriate computer simulation techniques.

The method of molecular dynamics (MD) is widely used to study nonideal plasmas with electrons and ions treated classically. At the same time the use of electron-ion pseudopotentials in the classical MD simulations restricts the applicability of this method to high temperatures, high ionization degrees and near equilibrium states. relaxation rates.

Computational methods based on the Density Functional Theory (DFT), applied to both warm dense matter and plasma simulations, are much more computationally demanding than the classical MD. Moreover, these methods are mostly not capable to handle the dynamics of electrons.

The Wave Packet Molecular Dynamics/Wave Packet Mote-Carlo methods (WPMD/WPMC) introduce quantum features in terms of classical electron dynamics. Within these methods the ions are treated classically whereas the electron quantum dynamics is approximated by propagation of wave packets [1], parameterized by a small number of dynamic variables. The exchange interaction between electrons of the same spin in the Hartree-Fock limit can be taken into account using antisymmetrized wave packets [2].

Poor accuracy for electronic bound states at ions and spreading of wave packets for weakly bound electrons are known problems of the existing WPMD models for nonideal plasmas [3,4]. We address both issues using a new technique based on multiple Gaussian expansion of the single-electron wave function, which is called Split Wave Packet Molecular Dynamics (SWPMD) [5]. Calculations of the ground state energies of small atoms and molecules show that this method provides better accuracy than the original WPMD. Representing an electron by at least three Gaussians results in the ground state energy for H and He to be within 1% error compared to the exact values.

The main feature of SWPMD is the ability to study electron dynamics taking into account the wave function branching. As a test case we consider tunnel ionization of simple atoms in a short laser pulse. It is shown that the SWPMD results are in a good agreement with more accurate quantum-mechanical calculation methods. Other dynamical events such as electron-ion scattering and propagation of and electron in the nonideal plasma are considered [5].

References

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