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Confining Boundary Conditions For Simulation of Electron-Ion Plasma by Antisymmetrized Wave Packet Molecular Dynamics

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Abstract content
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The method of Wave Packet Molecular dynamics is an approximate quantum method for numerical simulation of many-particle dynamics. In this method single electron wave functions are expanded in a set of floating Gaussian wave packets (WP). A trial many-body wave function is constructed depending on the quantum statistical properties of the simulated ensemble, for example for fermions (electrons) a single Slater determinant antisymmetrized product is usually used for each spin projection. The resulting equations of motion follow from the variational principle.
In this work we study a system of electrons in a 3D confinement potential constructed from harmonic walls and a flat floor in each spatial direction.

The unlimited broadening of the Gaussian wave packets and underestimation of the electron-electron and electron-ion collision frequencies is known to be the major problems of the WPMD method [4] when applied to many-particle systems with homogeneous density, for example plasma systems. We show however that the method is able to excellently describe the thermodynamics of a confined fermionic system. The infinite WP broadening is directly related to the infinite statistical sum in an unconstrained system and does not appear in the confined system. For example, the nearest image boundary conditions guarantee the periodicity of expectation values but do not limit the number of allowed states in the simulated system.
We show that for the confined electron-ion system the AWPMD model does not suffer from the unlimited wave packet broadening problem and the electron wave packet parameters perform finite ergodic motion in the available system phase space. The implementation of the proposed model to simulation of the extended warm dense matter is presented.

Primary author: Dr VALUEV, Ilya (Kintech Lab Ltd.)

Co-author: Mr LAVRINENKO, Yaroslav (JIHT RAS)

Presenter: Dr VALUEV, Ilya (Kintech Lab Ltd.)

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