Simulations of the electron-ion relaxation in nonideal plasmas by the method of WPMD-DFT

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A new WPMD-DFT simulation approach [1] is applied to study the relaxation rate in nonideal plasmas for the electron number densities up to 10^{25} cm^{-3}. It is of great interest for analyzing the plasma generated by short laser pulses, particle beams, shock waves, etc.
The method of wave packet molecular dynamics (WPMD) is based on the representation of electrons as Gaussian wave packets whereas ions are treated as classical particles. Compared to the classical molecular dynamics, it improves the representation of electron-ion bound states without involving pseudopotentials and allows to account for electron degeneracy. In the latest modification of this method called WPMD-DFT, the exchange and correlation effects are determined by calculating the functional of the total electron density provided by the density functional theory (DFT) approach within the LSDA approximation. It provides an optimal balance between the code performance and precision of account for quantum effects compared to other WPMD modifications such as electron force field (eFF) and dynamics of antisymmetrized wave packets (AWPMD).
In this work, we apply WPMD-DFT to study the dependence of the electron-ion relaxation rate on the plasma nonideality parameter. The results are compared with various theoretical approaches and simulations by other methods including the classical molecular dynamics.

[1] Lavrinenko Y, Levashov P R, Minakov D V, Morozov I V and Valuev I A 2021 *Physical Review E* **104** 045304