HIGH ACCURACY MOLECULAR DYNAMICS SIMULATIONS OF ELECTRON-ION TEMPERATURE RELAXATION IN NONIDEAL PLASMAS

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In this work, we prepare a simulation framework for a high-accuracy numerical study of electron-ion temperature relaxation in nonideal (strongly coupled) plasmas. The existing relaxation rate theories require either parameter selection or some pre-knowledge of the electron-ion correlation functions and effective interaction potentials [1]. This makes nonequilibrium classical and quantum molecular dynamics simulations a crucial stage in the study of energy transfer rates [2].

We begin by revisiting the classical molecular dynamics simulations of a system of equally charged particles with different masses on a neutralizing background. We accurately simulate this simple ab-initio (parameterless) system with controlled precision in terms of number of particles, mass ratio and energy convergence. The predictions for the equally charged system are compared to the previous simulations and theories, which are reproduced with higher accuracy.

We also perform a series of classical molecular dynamics simulations of the system of oppositely charged particles with the corrected Kelbg potential based on the quantum statistical approach. The differences and similarities between the same-charge and opposite-charge systems are analyzed.

One of the goals of this work is to support future studies of the electron-ion relaxation rate by quantum simulations with the help of the recently developed WPMD-DFT approach [3].

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