MOLECULAR DYNAMICS SIMULATION OF NON-DEGENERATE HYDROGEN PLASMA USING A MODIFIED KELBG PSEUDOPOTENTIAL WITH LONG-RANGE INTERACTIONS

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This study presents the results of quasi-classical simulations of the thermodynamic properties of non-degenerate hydrogen plasma at moderate coupling. The primary focus is on developing a method that accurately accounts for both the long-range nature of Coulomb interactions and quantum effects, including the Pauli exclusion principle and the uncertainty principle.

At the core of this research is the derivation of the Kelbg-AAE pseudopotential for a two-component Coulomb system [1], based on the angular-averaged Ewald potential (AAEP) [2]. This approach provides an explicit expression for the pseudopotential [1], incorporating long-range Coulomb interactions via the Ewald summation method. The analytical simplicity of AAEP also allows for an explicit representation of the corresponding Coulomb density matrix.

To improve the accuracy of electron-proton and electron-electron interactions at strong coupling, temperature-dependent corrections have been incorporated into the pseudopotential at short distances using an improved Kelbg pseudopotential [3]. Additionally, an effective electron size has been introduced for particles with the same spin projection. This ensures agreement with the Pauli exclusion principle, preventing plasma collapse and the formation of unphysical clusters [3] at temperatures below the characteristic molecular formation threshold of 50 kK.

The developed method has been implemented in the KelbgLIP package [4], which computes pseudopotentials for all interaction types in the system (electron-electron with different spin projections, electron-proton, and proton-proton). It also facilitates quasi-classical molecular dynamics simulations using the LAMMPS package. In this study, we computed the energy, pressure, and radial distribution functions for non-degenerate hydrogen plasma over a wide temperature range (from 600 kK to 1 kK) while maintaining a fixed degeneracy parameter at 0.01. The formation of atoms, molecules, and other hydrogen complexes was observed, and their composition was analyzed as a function of the coupling parameter.

The results are in good agreement with path integral Monte Carlo simulations [5]. However, the proposed method requires significantly fewer computational resources, allowing simulations of thousands of particles and enabling calculations in the thermodynamic limit. The work is supported by the Russian Science Foundation (project No. 24-19-00746).

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