Kelbg pseudopotential with Ewald summation technique for strongly coupled weakly degenerate hydrogen plasma simulations

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The solution of the Blöch equation in first-order perturbation theory [1] yields a pseudopotential for simulating the thermodynamic properties of two-component Coulomb systems. The Ewald potential that accounts for the Coulomb long-range interaction has a complex form, which prevents finding an analytical solution. The angular-averaged Ewald potential (AAEP) has a very simple form [2], so a pseudopotential can be obtained in direct analytic form [3]. This pseudopotential can be used to perform quasi-classical simulations of the plasma's thermodynamic properties [4]. This work provides a step-by-step derivation of the Kelbg-AAE pseudopotential for a two-component Coulomb system [2]. Solving the Blöch equation with the AAEP yields an improved Kelbg pseudopotential [4], which accounts for the Coulomb long-range electron-proton interaction in hydrogen plasma [5]. Similarly, we calculate a pseudopotential for the interaction between electrons, accounting for its spin. In order to examine strong coupling regimes at low degeneracy, it is important to introduce effective electron repulsion to account for the Pauli exclusion principle. This modification account for finite size of electrons, preventing the formation of unphysical clusters at temperatures lower than the dissociation temperature of the hydrogen molecule [4]. The work is supported by the Russian Science Foundation (project No. 24-19-00746).

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