SIMULATION OF HYDROGEN PLASMAS USING THE IMPROVED KELBG PSEUDOPOTENTIAL IN THE QUASICLASSICAL MOLECULAR DYNAMICS FRAMEWORK

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In this work, we present a quasi-classical molecular simulation of a two-component plasma in the weak degeneracy regime and over a wide range of coupling parameters. We use the improved Kelbg pseudopotential [1], which allows us to take into account the quantum uncertainty principle and an accurate treatment of bound state formation, as well as the Pauli principle to prevent electrons with the same spin from being in the same state. We also use an improved Kelbg-AAE pseudopotential [2], which allows us to take into account interactions with all periodic images.

We compare our results with the Path integral Monte-Carlo simulations by Filinov and Bonitz [3], examine the stability of a hydrogen plasma, solving the problem of cluster formation under 50 kK [4], and investigate the dependence of equilibrium pressure (accounting volume effects [5]) and energy on the number of particles. The obtained data confirm the efficiency of the pseudopotential description of the system with strong long-ranged interactions. The work was supported by the Foundation for the Advancement of Theoretical Physics and Mathematics "BASIS" (Grant No. 23-1-5-119-1).

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