Account for bound states in atomistic plasma model using split-WPMD method

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The method of Wave Packet Molecular Dynamics (WPMD) [1-6] is an approximate quantum method for simulation of nonideal plasmas and warm dense matter. In WPMD, antisymmetrized Gaussian wave packets are used to represent electrons and point-like particles represent the ions. The quantum model corresponds therefore to a single-determinant (Hartree-Fock) approximation. In this model both thermodynamic properties such as equation of state for plasma and dynamic quantities may be calculated.

As shown by previous research [3] the original WPMD model, where each electron is represented by a single Gaussian, may largely underestimate the role of bound states and therefore the plasma ionization degree.

In the present work we propose a model based on Split-WPMD approach [3,4]. In the current implementation each electron is represented by two Gaussians, one of which remains attached to one of the ions and the other is free to move. The balance between two parts is controlled by a coefficient, which is treated as a new dynamic variable in the variational approach. Note that after anti-symmetrization electrons may be regarded as equivalent, and the identity connection between the electron density attached to a particular ion and its free counterpart is lost.

Although the new model appears to be more computationally demanding since singularities may appear in the system Norm matrix and require special treatment, it helps to obtain more realistic ionization degrees, especially for lower plasma density.

Using a hydrogen plasma as an example we demonstrate that the new model is capable of describing the whole range of bound states that may appear in hydrogen starting from the molecular gas at low temperatures and densities to the partially ionized plasma whith substantial presence of neutral atoms and molecular ions.

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