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Simulation of hydrogen plasma with cluster multi-range interpolation

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Abstract

In the present work, we use the recently developed cluster multi-range interpolation (CMRI) (Valuev 2005 *Comput. Phys. Commun.* **169** 60) of interaction potentials to simulate hydrogen plasma using molecular dynamics (MD). The interpolation is based on variational mixing of cluster connectivity within a given system of electrons and ions described by coordinates of the particles. The use of potential interpolation based on connectivity allows us to treat the collisions of small numbers of particles (up to two ions and three electrons together) by more accurate empirical models and treat such processes as ionization or molecule formation by means of MD simulation on single-valued smooth approximate N-particle potential energy surfaces. The construction of the scheme and the results of equilibrium MD simulations are discussed. Energy spectra and particle pair correlation functions are compared between the current CMRI model and two classical models with pair pseudopotentials.

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1. Interpolation scheme

Effective pair potentials [2–5] used in molecular dynamics (MD) simulations of plasma do not allow us to describe bound states correctly, thus limiting the applicability of MD to the classical region. Interaction models constructed by explicitly using chemical composition or *ab initio* models like QMC are not suitable for dynamical simulations. Bonded interaction models for small numbers of electrons and protons (H, H_2-like structures) can be constructed as semi-empirical or *ab initio* potentials. In the current work, we use the interpolation approach (many-dimensional switching function) allowing us to combine bonded $U^N(\mathbf{R})$ and non-bonded $U^{\mathrm{NB}}(R_{ab})$ descriptions into a single smooth many-particle total energy function. The potential energy for a set of particles is given by cluster multi-range interpolation (CMRI) [1]:

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$$U(\mathbf{R}) = \sum_S P_S(\mathbf{R}) U_S(\mathbf{R}), \tag{1}$$

$$U_S(\mathbf{R}) = \sum_{C_S} U^{N_{C_S}}(\mathbf{R}) + \sum_{C_S^1 \neq C_S^2} \sum_{a \in C_S^1, b \in C_S^2} U^{\mathrm{NB}}(R_{ab}), \tag{2}$$

$$\sum_S P_S(\mathbf{R}) = 1, \tag{3}$$

where S indexes cluster connectivity configurations, C_S indexes all aggregate clusters in configuration S, N_{C_S} is the number of atoms in cluster C_S, $U^N(\mathbf{R})$ are the bonded potentials for N bound particles, $U^{\mathrm{NB}}(R_{ab})$ are the pair additive non-bonded potentials for particles a and b, R is a set of particle coordinates, R_{ab} is the distance between particles a and b, $P_S(\mathbf{R})$ are the smooth weight functions. The CMRI algorithm explicitly considers bonding configurations S that can be achieved in the system. Each configuration consists of a number C_S of particle clusters which are located using distance criteria. The interaction of particles within clusters is calculated using the bonded model and the interaction between clusters is described by a non-bonded pair potential. Weights P_S are assigned for each configuration, which depend on 'bonds' between particles and bond transition function $p(R_{ab})$. The configuration weight P_S is a product $P_S = \prod_{i=1}^{N_{\mathrm{bonds}}} w_i$ where $w_i(R_{ab}) = p_i(R_{ab})$ if the bond i exists (bonding case) and $w_i(R_{ab}) = 1 - p_i(R_{ab})$ if the bond i does not exist in configuration S. Although the number of all possible bonding configurations for a many-particle system may be tremendously large, the algorithm selects the significant configurations only, thus limiting the number of items in the sum (1). In the current work, we use a very simple symmetric local weight function:

$$p(r) = \begin{cases} 1, & r \in (-\infty; r_0 - d] \\ 1 - \dfrac{1}{2}\left(1 - \cos\left(\dfrac{\pi(r - r_0 + d)}{2d}\right)\right)^n, & r \in (r_0 - d; r_0] \\ \dfrac{1}{2}\left(1 - \cos\left(\dfrac{\pi(r_0 - r + d)}{2d}\right)\right)^n, & r \in (r_0; r_0 + d] \\ 0, & r \in (r_0 + d; +\infty). \end{cases} \tag{4}$$

Its parameters determine the transition region location r_0, half-width d and transition steepness n. These parameters of the model are selected to specify the distance range which is problematic for quasi-classical description and where potential interpolation is needed (figure 1(*a*)).

2. Hydrogen plasma with ionization and bound states

For describing interactions at small distances, the following primitive models were used. Interaction between two protons surrounded by one, two and three electrons is described by Morse potentials fitting equilibrium energies and distances of molecules/ions H_2^+, H_2 and H_2^- correspondingly. Interaction energy in clusters of more than two protons or containing more than three electrons is set prohibitively large (+10 eV/particle) for the test purposes of this model (metallic region is not described). We assume a flat electron energy potential surface of 1–3 electrons bound around 1–2 protons at small distances (no e–e interaction in atoms or molecules). Interaction between all particles at large distances is described by the Coulomb potential, for clusters containing protons and electrons, the electron charge is considered to be centred at protons (full screening in this test model). Potential curves obtained from the above interpolation model are shown in figure 1(*b*). The left part of the graph represents electron separation from a cluster (atom or ion), proton separation is on the right.

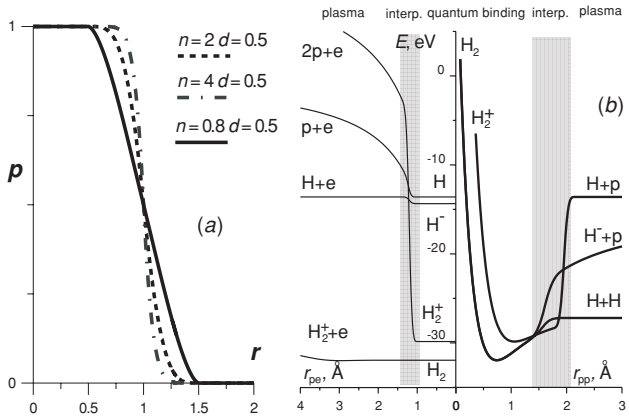

Figure 1. (*a*) Local switching function for different parameters, (*b*) potential curves for hydrogen resulting from CMRI-potential surface with switching parameters: $r_0(\mathrm{e,p}) = 1.2$ Å, $d(\mathrm{e,p}) = 0.2$ Å, $r_0(\mathrm{p,p}) = 1.6$ Å, $d(\mathrm{p,p}) = 0.4$ Å, $n = 2$.

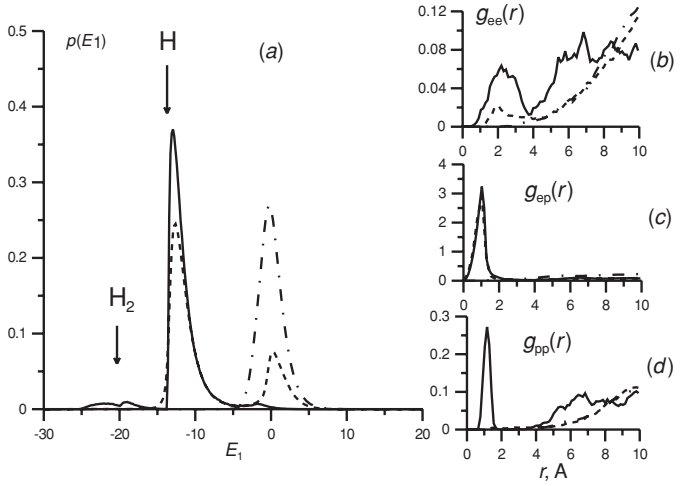

Figure 2. Energy spectra $p(E_1)$ (*a*) and pair correlation functions ((*b*), (*c*) and (*d*)) for equilibrium hydrogen plasma systems with $\Gamma_e = 1$ and different effective potentials, $T = 10\,000$ K. (——) CMRI potential, (- - - -) Coulomb potential (cut-off −13.5 eV), (— · —) Coulomb potential (cut-off $-3T$).

3. MD simulations

The CMRI-smoothed hydrogen potential is used for a system of 20 electrons and 20 protons with nearest image periodic boundary conditions. The system is equilibrated by a Monte Carlo procedure to a given Γ (plasma nonideality parameter) and T (temperature) values and then a molecular dynamics run is performed. Initial conditions were Maxwellian velocity distribution and either atomic hydrogen or random particle coordinate distribution. Comparison of simulations with different effective potentials is shown in figures 2 and 3. The main aim of the comparison was to track the appearance of bound states for different effective potentials [6]. Two quantities were used for this purpose: (1) single-particle energy $E_1 = U_1 + E_{\mathrm{kin}}$ is the interaction energy of one selected particle with all others in the system plus kinetic energy of

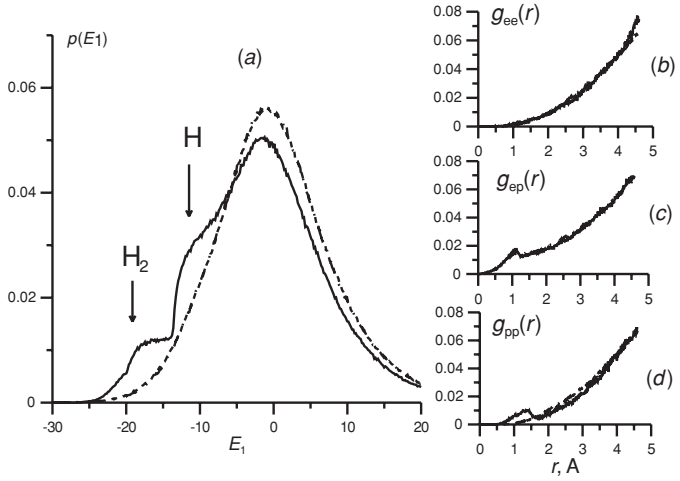

Figure 3. Energy spectra $p(E_1)$ (*a*) and pair correlation functions ((*b*), (*c*) and (*d*)) for equilibrium hydrogen plasma systems with $\Gamma_e = 1$ and different effective potentials, $T = 50\,000$ K. (——) CMRI potential, (- - - -) Coulomb potential (cut-off -13.5 eV), (— · —) Coulomb potential (cut-off $-3T$).

the particle. The spectra of E_1 is used to distinguish between free and bound states by energy; (2) pair correlation functions $g_{ee}(r)$, $g_{ep}(r)$, $g_{pp}(r)$ are the probabilities of finding a particle of any given species (e, p) at a distance r from another particle. We compare the CMRI potential which explicitly includes molecular and atomic bound states with (a) the Coulomb potential with e–p interaction cut-off of $-3T$ and (b) the Coulomb potential with e–p interaction cut-off of -13.5 eV. The potential (a) is designed to take only free electron states into account [5], potential (b) assumes a 'classical' bound state with the energy equal to the hydrogen ground state energy.

4. Conclusions

The new interpolation method for constructing smooth effective interaction potentials for MD simulations of nonideal plasma is proposed. Explicit inclusion of bound states is possible with the new scheme. The future work will be concentrated on developing more advanced primitive bonded models, improvement of CMRI performance to treat larger numbers of particles and simulations to obtain the hydrogen equation of state and dynamical properties.

Acknowledgments

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