Accurate first-principles singlet and triplet forces built upon the two-particle density matrix

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A consistent theory for the numerical calculation of effective potentials and forces in the two-component system of protons and electrons based on the density matrix is presented. We provide precise calculations for the two-particle system, investigating the parametric convergence and explaining the choice of all numerical parameters. We rigorously include the two-particle exchange of interacting fermions. Therefore, effective potentials and forces represent the singlet and triplet states. The triplet density matrix vanishes in the $r \to 0$ limit, while the effective potential and force are infinite, consistent with the Pauli exclusion principle. The limits are derived analytically and reproduced numerically.
Finally, our density-matrix-based forces and effective potentials are close to the improved Kelbg pseudopotential and force, including when the latter account for the two-particle exchange (in the kinetic energy part). By this comparison, we reveal that the problem of unphysical complex formation in the molecular dynamics simulations of a hydrogen plasma at $T < 52$ kK [1, 2], existing for more than 20 years, is due to the application of the two-particle approximation to the many-body problem. The two-particle approximation cannot describe molecular formation.

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[2] Demyanov G S and Levashov P R 2025 *Physics of Plasmas* **32** 123901 ISSN 1070-664X URL `https://doi.org/10.1063/5.0298952`