Towards Temperature-Dependent DeePMD Potential for Hydrogen Plasma

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Path-integral Monte Carlo and other quantum simulation methods provide accurate descriptions of hydrogen plasma but are computationally prohibitive for large-scale or long-time molecular dynamics (MD). In contrast, classical MD is highly efficient yet relies on effective interaction models that often fail to capture essential quantum constraints—most notably the Pauli exclusion principle. Machine learning potentials, such as DeepMD [1], offer a promising route to bridge this gap: by training on high-quality reference data, they can reproduce quantum-level accuracy at MD cost. In this work, we take key steps toward a DeepMD potential for hydrogen plasma, focusing on two critical physical ingredients: (i) explicit temperature dependence inherited from the underlying Kelbg pseudopotential [2, 3], and (ii) proper treatment of long-range Coulomb interactions via periodic Ewald summation. We show that omitting the latter leads to systematic errors, while its inclusion ensures physical consistency and stability. Training on data in the range $T = 24$–97 kK ($\Gamma = 0.1$–0.5) yields excellent accuracy: $R^2 = 0.967$ for energy and $R^2 = 0.987$ for forces, confirming the viability of machine-learned potentials for efficient, large-scale simulations of hydrogen plasma.

[1] Wang H, Zhang L, Han J *et al.* 2018 *Computer Physics Communications* **228** 178–184
[2] Kelbg G 1963 *Annalen der Physik* **467** 219–224
[3] Filinov A V, Golubnychiy V O, Bonitz M, Ebeling W and Dufty J W 2004 *Phys. Rev. E* **70**(4) 046411 URL `https://link.aps.org/doi/10.1103/PhysRevE.70.046411`