

# Classical Molecular Dynamics of an Ideal Fermi Gas for Calculating Thermodynamic Properties

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This work presents a classical molecular dynamics approach for simulating the thermodynamic properties of an ideal degenerate Fermi gas. The key idea is to express the density matrix of non-interacting fermions in determinant form and then rewrite the configurational weight of the quantum system in a Boltzmann-like form. This makes it possible to introduce an effective many-body pseudopotential defined as the logarithm of the determinant, which yields a positive weight and allows the system to be sampled through Newton's equations of motion in an auxiliary classical system. A similar idea was introduced in Ref. [1].

Simulations in the canonical ensemble, performed with LAMMPS and a Nosé-Hoover thermostat, show that the method reproduces the energy, pair correlation function, and static structure factor in very good agreement with analytical results [2], including in the strongly degenerate regime. Although the approach is limited to static properties and cannot describe quantum dynamical behavior, it enables simulations of systems with up to about one thousand fermions, exceeding the typical capabilities of conventional quantum methods. The work was supported by the Foundation for the Advancement of Theoretical Physics and Mathematics "BASIS" (Grant No. 23-1-5-119-1).

[1] Miura S and Okazaki S 2000 *The Journal of Chemical Physics* **112** 10116–10124 ISSN 0021-9606 URL <https://doi.org/10.1063/1.481652>

[2] Kozharin A S and Levashov P R 2021 *Contributions to Plasma Physics* **61** e202100139 e202100139 ctp.202100139