Quantum Symmetry from Enhanced Sampling: A First Exploration

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The simulation of Fermi systems at finite temperature has always posed great difficulties to the point that most of the research work in the field has been focused on finding valid approximations[1]. This is caused by the Fermi "minus" sign problem that introduces a generally unknown nodal surface in the density matrix to be sampled. This problem is so severe that even two-particle systems can be challenging, if not impractical to study with a straightforward approach based on brute-force sampling. We will thus consider systems composed of two particles, and propose a method, exact in principle, where the properties of a Fermi system are obtained through the computation of a free energy difference from a Path Integral Molecular Dynamics simulation of distinguishable particles. This free energy difference will be computed with Metadynamics[2], and will be used to obtain local properties such as the energy, the density, and the radial distribution function of the particles. We test the robustness of the results with different interactions and in particular for the case of two electrons confined in a harmonic potential, a model for a quantum dot where both theoretical and experimental data is available to compare with. The possibility to scale this method to three and more particles will be discussed.

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[2] A. Barducci, G. Bussi, and M. Parrinello, *Phys. Rev. Lett.* **100**, 020603 (2008).