Title: Efficient Bosonic and Fermionic Sinkhorn Algorithms for Non-Interacting Ensembles in One-body Reduced Density Matrix Functional Theory in the Canonical Ensemble

Abstract: One-body Reduced Density Matrix Functional Theory (1-RDMFT) is a promising method for treating strongly correlated systems, as well as systems at finite temperature. In this talk I introduce 1-RDMFT in the canonical ensemble and then proceed to approximate the interacting ensemble by a non-interacting ensemble that maximizes the entropy, independently of temperature. [1] Bosonic and Fermionic Sinkhorn algorithms are derived and used to invert the relationship between the Natural Orbital Occupation Numbers (NOONs) and the effective orbital energies of the non-interacting ensemble. Both the Bosonic and Fermionic Sinkhorn algorithms are shown to perform well in reproducing the NOONs of simulated distributions and the ground-state NOONs of H2O and H2. In the case of H2 the resulting non-interacting entropy and non-interacting approximation to the interaction energy are studied within several wavefunction subspaces as the bond length varies. This provides several new starting points for approximations of the interaction energy, also at zero-temperature. Connections to entropically-regularized Multi-Marginal Optimal Transport (MMOT) are highlighted that may prove interesting for future research.

1. D.P. Kooi. Efficient Bosonic and Fermionic Sinkhorn Algorithms for Non-Interacting Ensembles in One-body Reduced Density Matrix Functional Theory in the Canonical Ensemble. arXiv:2205.15058