Path Integration, Lexicographic Symmetrization, and Derivative-Free Energy Estimation Within the Stochastic Representation of Wavefunctions

Liam Bernheimer[1] **and Guy Cohen**[1,2]

[1] *School of Chemistry, Tel Aviv University, Tel Aviv 6997801, Israel*
[2] *The Raymond and Beverley Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel*

Describing the ground states of continuous, real-space quantum many-body systems, like atoms and molecules, is a significant computational challenge with applications throughout the physical and chemical sciences. Recent progress was made by variational methods based on machine learning (ML) ansatzes. However, since these approaches are based on energy minimization, ansatzes must be twice differentiable. This (a) precludes the use of many powerful classes of ML models; and (b) makes the enforcement of bosonic, fermionic, and other symmetries costly. Furthermore, (c) the optimization procedure is often unstable unless it is done by imaginary time propagation, which is often impractically expensive in modern ML because computation time scales cubically with the number of parameters. We recently introduced a new approach to problem (c): the idea of stochastic representation of wavefunctions (SRW). There, at each stage, ML is used to perform regression on a set of stochastically sampled points; then new points at a later imaginary time are obtained from the resulting model by local applications of the propagator. SRW makes it viable to reliably perform imaginary time propagation at scale, and makes some headway towards the solution of problem (b), but remains limited by problem (a). Here, we show that performing imaginary time propagation within SRW by path integration overcomes all three problems. To demonstrate the effectiveness of this method, we apply it to generalized "Hooke's atoms": interacting fermions and bosons in a harmonic well. We show that our results are consistent with existing state-of-the-art approximations, and explore the effect of particle statistics on the density in the weakly interacting regime. We then continue to stronger interactions, where we investigate the crossover from the Fermi liquid to the Wigner molecule within a closed-shell system. Our results shed new light on the competition between interaction-driven symmetry breaking and kinetic-energy-driven delocalization in the intermediate regime.