Steady state formulation of inchworm Quantum Monte Carlo

Andre Erpenbeck¹, Emanuel Gull¹, and Guy Cohen²

¹Department of Physics, University of Michigan, 450 Church Street, Ann Arbor, 48109, USA ²School of Chemistry, Tel Aviv University, Tel Aviv 6997801, Israel

This is the companion poster for the talk with the same title, where we present an inchworm Quantum Monte Carlo method that is directly formulated in the steady-state. Until now, numerically exact real time Monte Carlo methods simulated steady-state dynamics by propagating from a tractable initial condition to long times. The computational cost for accessing nonequilibrium steady-states in these methods is often prohibitive. We overcome this issue by reformulating the inchworm equations such that they can directly be solved for the steady-state. We demonstrate the performance of our steady-state inchworm Quantum Monte Carlo method by comparison with analytical results and other numerically exact techniques and showcase its usage within dynamical mean field simulations. The steady-state inchworm Quantum Monte Carlo method closes the gap between short-time dynamics and the long-time behaviour and extends the regime of applicability for nonequilibrium Monte Carlo methods as impurity solvers within quantum embedding schemes.