SSE and Projector Quantum Monte Carlo

Pranay Patil
Department of Physics
Boston University

November 29, 2018

Quantum Monte Carlo for Spin Systems

- Stochastic Series Expansion: Used to calculate observable expectation values ($Tr(O_1 e^{-\beta H})$)

- Projector QMC: Used to calculate expectation values in the ground state: $\langle \psi_g | O | \psi_g \rangle$.

- Broad idea is to map the quantum system to a larger classical system on which we can perform Monte Carlo simulations.

- Has been applied sucessfully to many magnetic systems and this method has the ability to reach sizes far beyond the abilities of the traditional method of exact diagonalization.

- We will illustrate in some detail the workings of Projector QMC here.

Projector QMC

- Before setting up the simulation, we must ensure that the all energies have the same sign and the ground state energy has the highest magnitude of all. This can always be done by adding an appropriate constant to the Hamiltonian.

- We start with a trial wavefunction $|\psi_t\rangle$ and we can show that the ground state can be written as $|\psi_g\rangle = H^m |\psi_t\rangle$ for large m.
  $$\langle\psi_g|O|\psi_g\rangle = \langle\psi_t|H^m O H^m|\psi_t\rangle$$
 $$\hat{H} = \sum_i \alpha_i \hat{P}_i$$

- This implies:
  $$\langle\psi_t|H^m O H^m|\psi_t\rangle = \sum_s \prod_i \alpha_i(s) \langle P_1(s)P_2(s)...O...P_{2m}(s)\rangle$$

  where the sum is over all possible strings.

- This set of all possible strings is too large to exactly enumerate for even small sizes and we must resort to Monte Carlo sampling of these strings using the coefficients in the sum as the weights.

1D Transverse Field Ising Model Projector QMC

- $H = -\sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x$

- The magnetization ($\frac{(\sum M_i^z)^2}{N^2}$) drops from 1 to zero as the transverse field gets stronger due to a phase transition to a paramagnetic phase. Can be seen through QMC for a range of sizes.
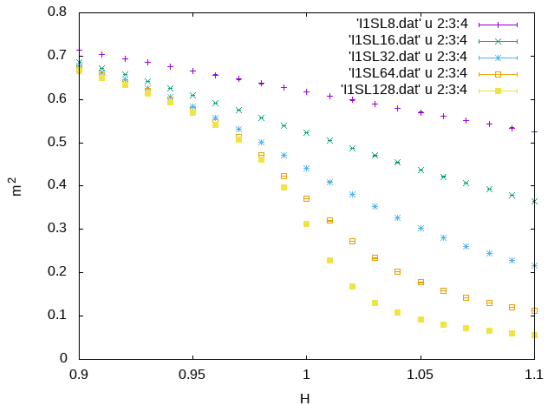
Limitations of this flavour of QMC

▶ Some models suffer from the "sign porblem" which implies that a classical model cannot be found.

▶ Some models without the sign problem may suffer from ergodicity issues as it is difficult to design quickly equilibrating updates.

▶ Nevertheless, it is being used heavily to understand the thermodynamic behaviors of many magnetic and electronic systems.