Auxiliary Field Quantum Monte-Carlo using Tensor Network States

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Imaginary time evolution

- If we take an arbitrary state:

  \[ |\psi_T\rangle = \sum_i c_i |\psi_i\rangle \quad \text{with} \quad \hat{H} |\psi_i\rangle = E_i |\psi_i\rangle \]

  and propagate it in imaginary time:

  \[ e^{-\tau \hat{H}} |\psi_T\rangle = \sum_i e^{-\tau E_i} c_i |\psi_i\rangle, \]

  higher energy components are suppressed.

- For long enough times and \( \langle \psi_0 | \psi_T \rangle \neq 0 \):

  \[ |\psi_0\rangle \propto \lim_{\tau \to \infty} e^{-\tau \hat{H}} |\psi_T\rangle \]

- Problem: naive propagation has exponential cost.
Introducing Auxiliary Fields

• Take a Heisenberg model with arbitrary interactions $J_{ij}$:

$$\hat{H} = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad \text{with} \quad J_{ij} = \sum_k \lambda_k v_i^k v_j^k$$

• The Hamiltonian can be expressed as the sum of squared one-site operators:

$$\hat{H} = \frac{1}{2} \sum_k \lambda_k v^2_k \quad \text{with} \quad \mathbf{v}^k = \sum_i v_i^k \mathbf{S}_i$$

• Now we can approximate the propagator for a small time step as:

$$e^{-\delta \tau \hat{H}} \approx \prod_{k,r \in \{xyz\}} e^{\frac{1}{2} V_{kr}^2} + O(\delta \tau^2) \quad \text{with} \quad V_{kr} = \sqrt{-\delta \tau \lambda_k} \hat{\nu}_{kr}$$
Every individual term can be written as a gaussian integral:

\[ e^{\frac{1}{2}V^2_{kr}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{\sigma^2_{kr}}{2}} e^{\sigma_{kr} \hat{V}_{kr}} d\sigma_{kr} \]

If we represent the wave function by a large number of simple walkers:

\[ |\psi\rangle = \sum_{i=1}^{N_w} w_i |\Omega_i\rangle \]

we can evaluate the integral using Monte-Carlo.

Sample \( \sigma_{kr} \) from a normal distribution, and propagate the walkers:

\[ |\Omega^{(n+1)}_i\rangle = \prod_{kr} e^{\sigma_{kr} \hat{O}_{kr}} |\Omega^{(n)}_i\rangle \]

These propagators are just local spin rotations and do not increase the complexity of the walkers.
Importance sampling and the sign problem

- Statistical fluctuations will be very large since \( \sigma_{kx} \) is completely random. Improve by distorting normal distribution using trial wave function \( |\Psi_T\rangle \):

\[
\tilde{p}(\sigma_{kx}) = e^{-\frac{1}{2}\sigma_{kx}^2} \frac{\langle \Psi_T | \Omega^{(n+1)}_i \rangle}{\langle \Psi_T | \Omega^{(n)}_i \rangle} \rightarrow \text{Importance Sampling}
\]

- Sampling is completely symmetric in the phase of the walker, leading to a phase problem which is remedied by imposing the constraint:

\[
\Re \langle \Psi_T | \Omega^{(n+1)}_i \rangle > 0 \rightarrow \text{Constrained Phase}
\]

- Implemented approximately using *phaseless approximation* [S. Zhang et al. PRL 90, 136401].

- Introduces *bias* into result dependent on the quality of the trial wave function!
Matrix product states as trial functions

- Matrix product states (MPS) are a wave function ansatz:

\[ |\psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} [A^{\sigma_1} \ldots A^{\sigma_n}] |\sigma_1 \ldots \sigma_n\rangle \quad \text{with} \quad (A^{\sigma_i})_{jk} \quad D\text{-dim matrix} \]

that is systematically improved by increasing the bond dimension.

- By using MPS with increasing \( D \) as trial we can remove the bias introduced by the phaseless approximation.

- Proof of principle implementation of MPS-AFQMC on the 2D \( J_1 J_2 \) model, which is frustrated and has a sign problem.

- MPS are used for both the trial as the walker states, with different bond dimensions \( D_T \) and \( D_W \).
Influence of walker bond dimension: $4 \times 4$ $J_2 = 0$
Convergence with discarded weight: $4 \times 4$ $J_2 = 0.6$

![Graph showing the convergence of MPS-AFQMC, DMRG, and exact methods with respect to discarded weight.](image)

$E(D_T = \infty) = -8.4133 \pm 0.0014$
Convergence with $D_T: 10 \times 10$ $J_2 = 0.5$

![Graph showing convergence with $D_T$]
Improvement over DMRG for all $J_2$: $10 \times 10$
Conclusions

- MPS-AFQMC energy converges to the exact result as $D_T$ increases.

- The QMC walk always improves upon DMRG result, sometimes reducing the error up to a factor of 5. Result tracks the modulation of the trial error across the different regimes of $\frac{J_1}{J_2}$.

- No influence of $D_W$ on energy or statistics. Computational scaling of QMC is better than DMRG $O(D_T^2)$ vs. $O(D_T^3)$. 
Outlook

- MPS in principle not suited for 2D systems. Bond dimension needed for same accuracy scales exponentially with system size.

- PEPS are 2D generalization of MPS. Bond dimension needed for same accuracy is constant with system size.

- Problem: computationally very expensive to work with. High scaling with $D$ makes it hard to converge result.

- Using PEPS as a trial one could improve the result, increase effective $D$, without adding extra computational cost.