Monte Carlo sampling with Tensor Network States

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DMRG achieved one of the major step in simulating of strongly correlated systems

DMRG: variational method within the class of MPS

DMRG can be generalized to deal with 2D systems: A family of variational ansatze has been proposed including PEPS, MERA and iPEPS

Figure 6. Convergence of relative errors $\Delta x = |x_{\text{iPEPS}} - x_{\text{QMC}}|/|x_{\text{QMC}}|$ with bond dimension $M$. Monte Carlo results from $^{[40,41]}$ are taken as exact. For the definition of the magnetization, refer to the text.

$M = 0.35$(iPEPS) 
$M = 0.307$(SSE) 
$\Delta M = 0.043$


FIG. 20. (color online) The ground state energy of the Heisenberg model on a honeycomb lattice as a function of the bond dimension $D$ obtained by the SRG with $D_{\text{cut}} = 130$.

$M = 0.3098$(SRG) 
$M = 0.2681$(MC) 
$\Delta M = 0.0417$


Figure 9. Staggered magnetization of the dimerized Heisenberg model as a function of the coupling ratio. $J/J' = 1$ corresponds to the isotropic Heisenberg model, while $J/J' = 0$ corresponds to isolated dimers on every second horizontal bond.

$M = 0.35$(iPEPS) 
$M = 0.307$(SSE) 
$\Delta M = 0.043$

FIG. 21. (color online) The staggered magnetization as a function of $D$ for the Heisenberg model on a honeycomb lattice.

FIG. 20. (color online) The ground state energy of the Heisenberg model on a honeycomb lattice as a function of the bond dimension $D$ obtained by the SRG with $D_{\text{cut}} = 130$. 

$M = 0.3098$(SRG) 
$M = 0.2681$(MC) 
$\Delta M = 0.0417$
Method of PEPS ansatz often comes with very large complexity scaling with $D$

- PEPS with variational minimization of the ground state energy $\sim D^{12}$
- iPEPS with time evolution $\sim \chi^3 D^4$
- TERG contraction of square lattice $\sim \chi^6$
- TERG contraction of honeycomb lattice $\sim \chi^5$

$\chi$ is the Schmidt coefficients kept (also referred as $D_{cut}$)

A square root speed up is obtained by using importance sampling over physical indices, which is first shown for MPS and string bond state.

• We use poorman’s update (the simple update) introduced by Xiang et al. to obtain the tensor describing the ground state of AF Heisenberg model on square lattice.


• We use importance sampling QMC method to evaluate finite size energy and staggered magnetization for square lattices with periodic boundary condition. Especially, we choose TERG method to approximately contract a tensor network.

The poorman’s update

\[ \sqrt{\Lambda_i} \quad \sqrt{\Lambda_n} \]
\[ \sqrt{\Lambda_j} \quad \sqrt{\Lambda_m} \]
\[ \sqrt{\Lambda_k} \quad \sqrt{\Lambda_l} \]

\[ R_L R_R = U \Lambda V^T \]

this trick basically reduces the cost from \( D^9 \) to \( D^5 \)
TERG algorithm

\[ T^B_{ijkl} = \sum_\alpha S^1_{ij\alpha} S^3_{kl\alpha}, \]
\[ T^A_{jkli} = \sum_\alpha S^2_{jk\alpha} S^4_{li\alpha}, \]
\[ T'_{\alpha\beta\gamma\delta} = \sum_{ijkl} S^2_{jk\alpha} S^3_{kl\beta} S^4_{li\gamma} S^1_{ij\delta}. \]
QM sampling

\[
\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\sum_{\sigma} W^2(\sigma) \sum_{\sigma'} \frac{\langle \sigma | H | \sigma' \rangle W(\sigma')}{W(\sigma)}}{\sum_{\sigma} W^2(\sigma)}
\]

\[
W(\sigma) = t \text{Tr}\{T^{s_1} T^{s_2} \cdots T^{s_N}\}, \quad |\sigma\rangle \equiv |s_1, s_2, \cdots, s_N\rangle
\]

\[
P = \min \left[ 1, \frac{W^2(\sigma')}{W^2(\sigma)} \right], \quad \frac{W(\sigma')}{W(\sigma)} = \frac{g'}{g} \prod_{q,p} \frac{f'_{q,p}}{f_{q,p}}
\]

\[
g \equiv t \text{Tr}\{T^{1, nr} T^{2, nr} T^{3, nr} T^{4, nr}\}, \quad f_{q,p} \equiv \max\{|T^q_{ijkl}|\}
\]
The finite size magnetization errors are 0.003(2) and 0.013(2) at $D=16$ for a system of size $L=8,16$ respectively. Finite $D$ extrapolation provides exact finite size magnetization for $L=8$, and reduces the magnetization error to 0.005(3) for $L=16$. 

$$C^\alpha(L/2, L/2) = \frac{1}{L^2} \sum_i S^\alpha(i_x, i_y) S^\alpha(i_x + \frac{L}{2}, i_y + \frac{L}{2}), \quad M^2 = \sum_\alpha C^\alpha(L/2, L/2).$$