Density-Matrix Renormalization Group for Quantum Spin Systems

Term Project for PHYS 580

Jin Xu
Graduate Student
Department of Physics, University of Alberta, Edmonton, T6G 2E1, Canada
Email: jin.xu@ualberta.ca

Quantum Spin Systems

Strongly correlated systems:

$$\hat{H}_{Hubbard} = -\sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^{\dagger} c_{j\sigma} + H.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$\hat{H}_{tJ} = -\sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^{\dagger} c_{j\sigma} + H.c.) + \sum_{\langle ij \rangle} J_{ij} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)$$

$$\hat{H}_{Heisenberg} = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Motivations to study quantum spin systems:

1. localized electronic spins in the Mott-insulators (high-Tc cuprates)

2. exotic ground states (quantum spin liquid)

3. quantum information & quantum computation (entanglement)

4. quantum many-body physics (phase transitions)

Numerical methods:

1. exact diagonalization(ED): small systems

2. quantum Monte Carlo(QMC): large system without frustration, non-fermionic

3. density-matrix renormalization group(DMRG): one-dimensional systems

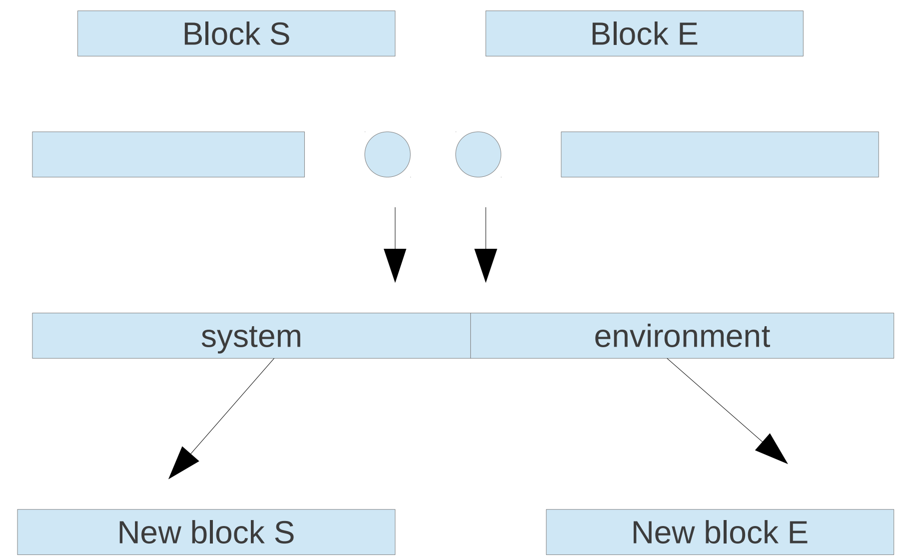
Density Matrices and DMRG Truncation

$$|\psi\rangle = \sum_{m^S=1}^{M^S} \sum_{\sigma^S=1}^{N_{site}} \sum_{\sigma^E=1}^{N_{site}} \sum_{m^E=1}^{M^E} \psi_{m^S \sigma^S \sigma^E m^E} |m^S \sigma^S\rangle |m^E \sigma^E\rangle = \sum_{i}^{N^S} \sum_{j}^{N^E} \psi_{ij} |i\rangle |j\rangle$$

$$\hat{\rho} = Tr_E |\psi\rangle\langle\psi|$$

$$\hat{\rho}|w_\alpha\rangle = w_\alpha |w_\alpha\rangle$$

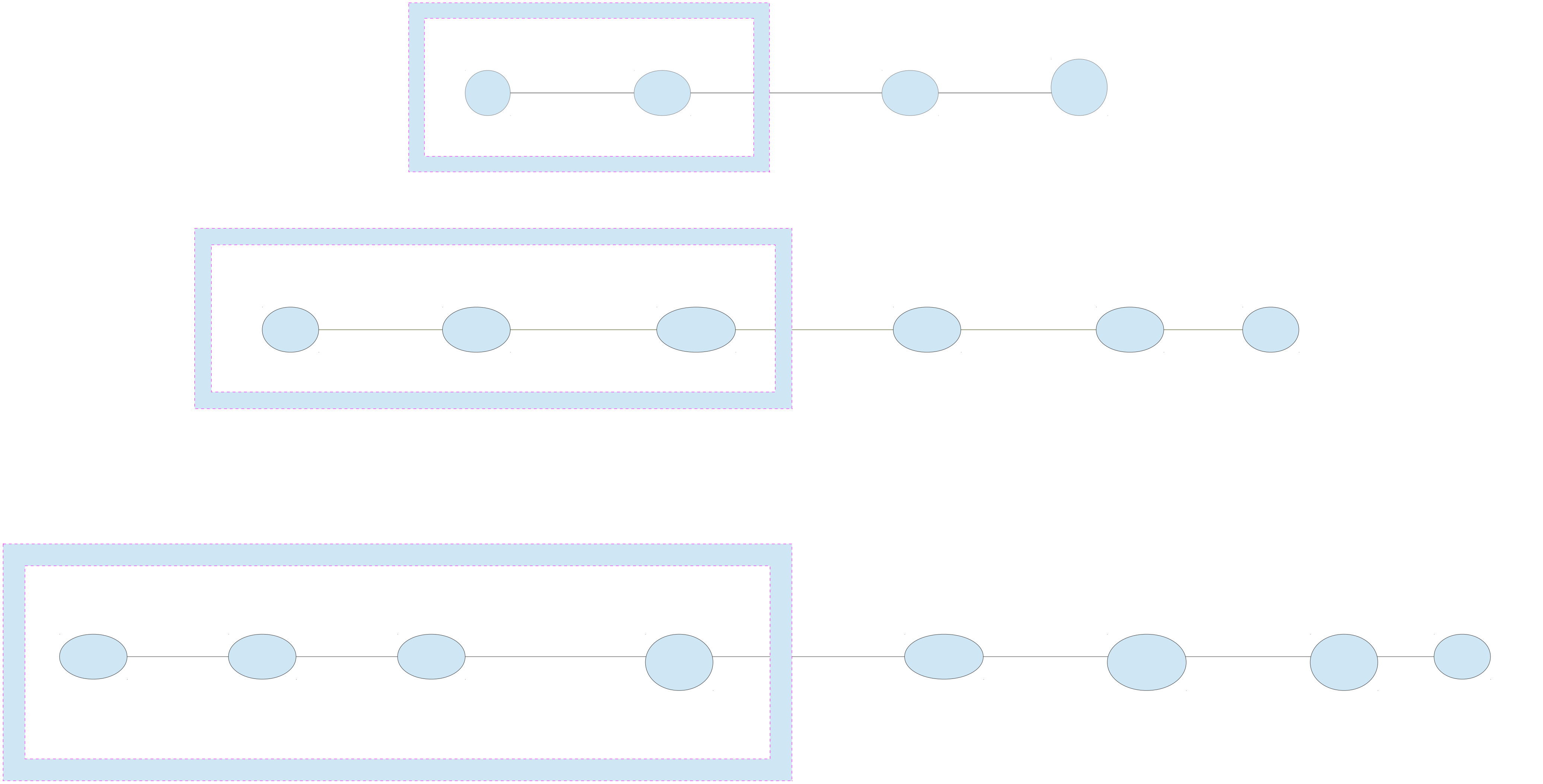
$$w_0 \geqslant w_1 \geqslant w_2 \geqslant \cdots$$



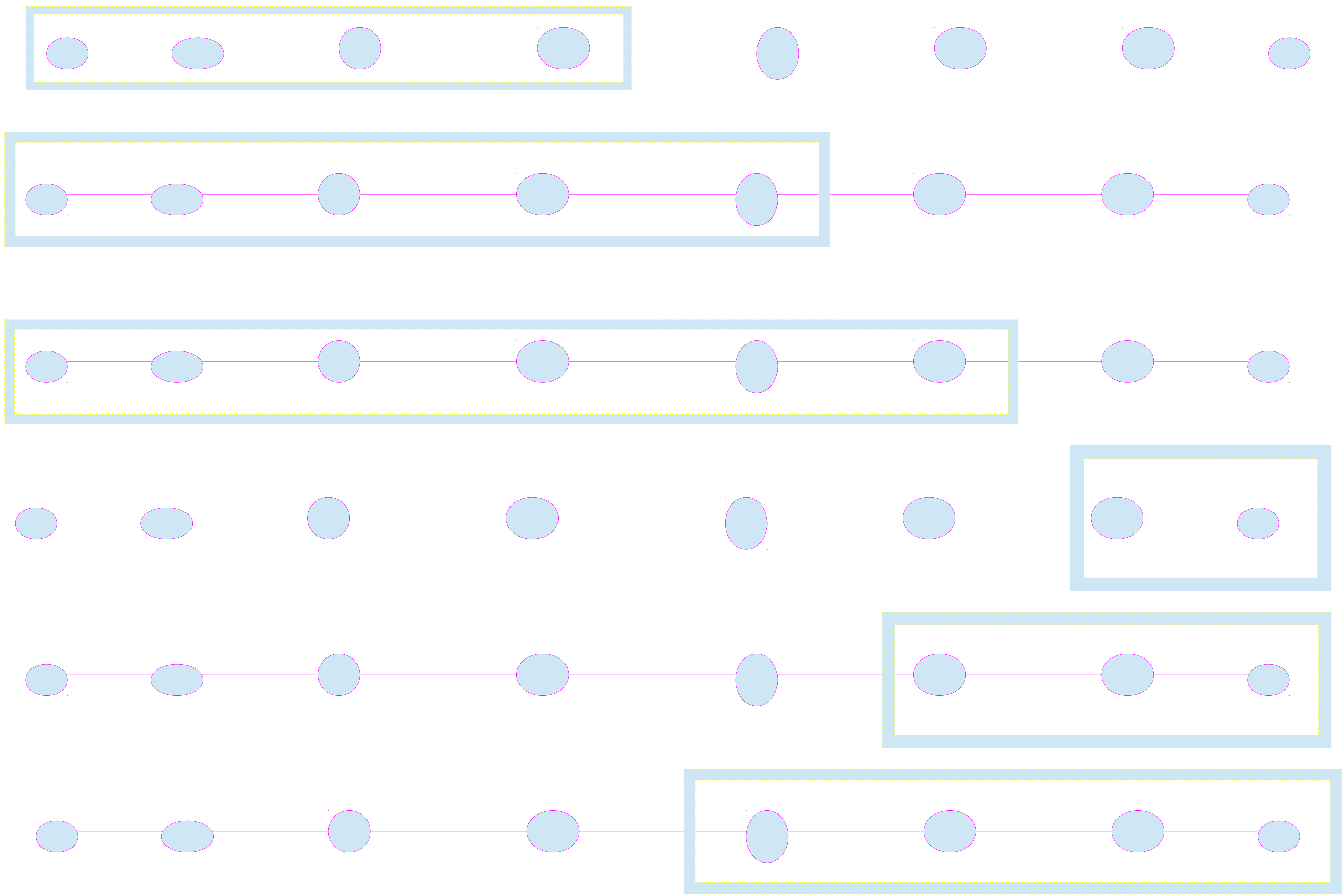
$$\langle \hat{A} \rangle = \sum_{\alpha=1}^{N^s} w_\alpha \langle w_\alpha | \hat{A} | w_\alpha \rangle \simeq \sum_{\alpha=1}^{M^s} w_\alpha \langle w_\alpha | \hat{A} | w_\alpha \rangle$$

$$\hat{H}_{l+1}^{tr} = T^\dagger \hat{H}_{l+1} T$$

Infinite System DMRG

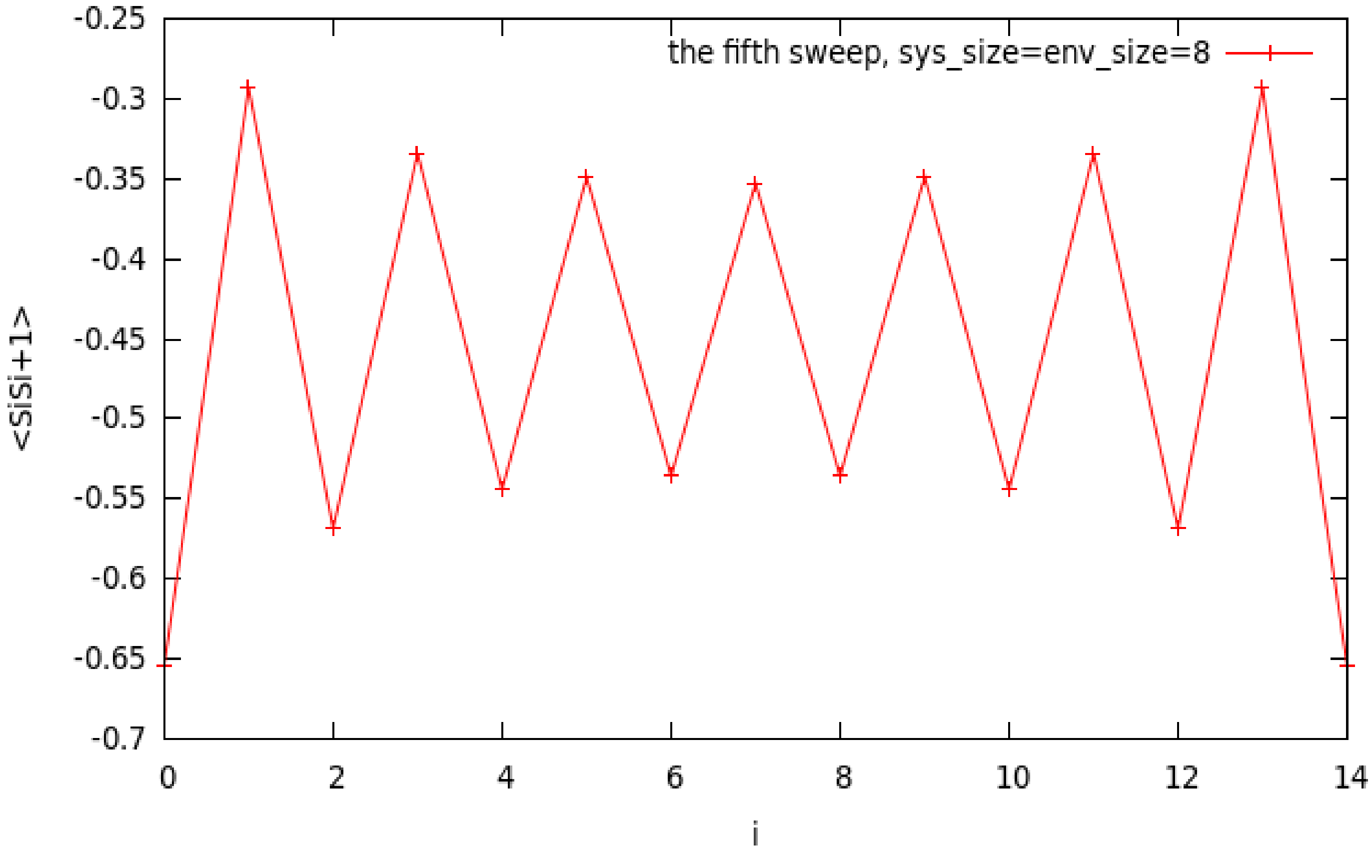


Finite System DMRG

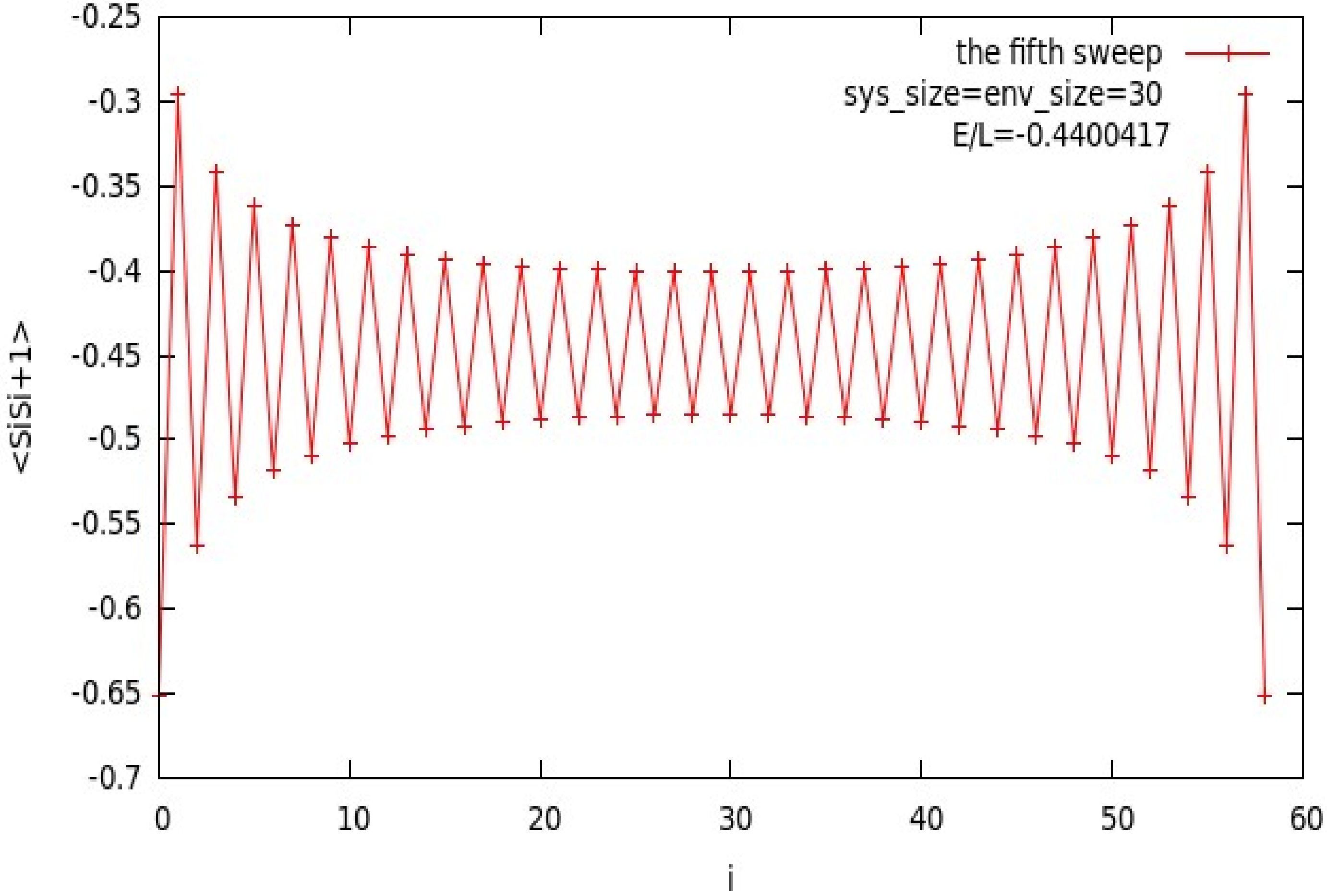


Results for L=16 (16 states to keep, 5 sweeps are finished, OBC)

The exact result for E/L from Bethe Ansatz	The converged result for E/L from DMRG
-0.4319357	-0.4319835



Results for L=60 (16 states to keep, 5 sweeps are finished, OBC)



More Applications of DMRG

1. Systems with periodic boundary conditions

2. T=0 dynamical properties of one-dimensional systems

3. Two-dimensional systems

4. Momentum-space DMRG

5. Transfer-matrix DMRG

6. Time-dependent DMRG

7. Applications to other areas: quantum chemistry, small grains, nuclear physics

Thank You for Listening!

Does it make sense?