2 Infinite-size DMRG

The goal of this problem is to implement the infinite-size DMRG (iDMRG) for the anti-ferromagnetic $S = 1/2$ Heisenberg chain with open boundary conditions,

$$\hat{H}_{\text{Heisenberg}} = \sum_{\langle ij \rangle} \left[\hat{S}_i^z \hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) \right],$$

and the Ising model in a transverse field with open boundary conditions,

$$\hat{H}_{\text{Ising}} = \sum_{\langle ij \rangle} \hat{S}_i^z \hat{S}_j^z + \lambda \sum_i \hat{S}_i^x,$$

where $\hat{S}_i^\alpha$ are local spin-1/2 operators on site i. Here we refer to the figures and equations of Ref. 1.

(a) Implement the iDMRG for translation invariant systems of a two-site unit cell. The procedure is summarized in Fig. 1.

(b) Benchmark your implementation by computing the ground state energy per site for the Heisenberg model and compare with the exact result for an infinite chain $e_0 = (1/4) - \ln(2)$ [2]. The energy per site e_0 can be extracted from the difference between total energies E_0 for two consecutive iDMRG iteration, $e_0(N) = [E_0(N) - E_0(N-2)]/2$. Check your results with different bond dimensions $D = 20, 30, 40, 50$. (With $D = 20$ or 50, you would be able to achieve decent accuracy in energy $\approx 10^{-4}$ or 10^{-5}, respectively.)

(c) Verify the claim in Ref. 1 that the trial wave function used in the step 4 of Fig. 1 is a good choice, by computing the fidelity $1 - \langle \Psi_n^{\text{trial}} | \Psi_n \rangle$. Make a plot similar to Fig. 2 for the Heisenberg model.

(d) Analyze the behavior of iDMRG for the Ising model at the critical point $\lambda = 1/2$ by studying the spectrum of the transfer operator [see Eq. (28)]. Make a plot similar to Fig. 4.

References

[1] I. P. McCulloch, arXiv:0804.2509 (2008).

[2] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).