7 XTRG

The Exponential Tensor Renormalization Group (XTRG) [1] is a powerful numerical method for computing the thermal density matrix $\rho = e^{-\beta H}$ of finite-size quantum systems, where β is the inverse temperature and H is the many-body Hamiltonian. In this problem, you will implement the XTRG algorithm and use it to compute the partition function of a one-dimensional (1D) XY model from high temperatures ($\beta \sim 10^{-6}$) down to low temperatures ($\beta \sim 1$).

(a) Initialize the thermal density matrix as a matrix product operator (MPO) using linear initialization, $\rho(\beta_0) \approx 1 - \beta_0 H$, as described in Appendix C.2 of Ref. [1]. Use $\beta_0 = 10^{-6}$ as the initial inverse temperature.

(b) Implement the XTRG algorithm following the strategy in Sec. II of Ref.[1]. The key idea is to iteratively double the inverse temperature, $\rho(2\beta) = \rho(\beta) \times \rho(\beta)$, by contracting the MPO with itself. After each multiplication, the MPO bond dimension increases and must be truncated. This can be done variationally using DMRG-type sweeping, as detailed in Appendix D of Ref. [1].

(c) Apply your XTRG implementation to the 1D XY model of length $L = 10$. Perform 20 XTRG steps starting from $\beta_0 = 10^{-6}$, so that the final inverse temperature is $\beta = 2^{20}\beta_0$. At each step, compute the partition function $Z = \mathrm{Tr}(\rho(\beta))$. Compare your numerical results with the analytical solution provided in Appendix F of Ref. [1] over the full temperature range.

*Bibliography

[1] B.-B. Chen, L. Chen, Z. Chen, W. Li, and A. Weichselbaum, Phys. Rev. X **8**, 031082 (2018).