MPO representation of time evolution operators

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In the tutorial for tDMRG, we have time-evolved MPSs by applying rows of two-site gates. Often, it is useful to represent a time evolution operator for a time step as an MPO.

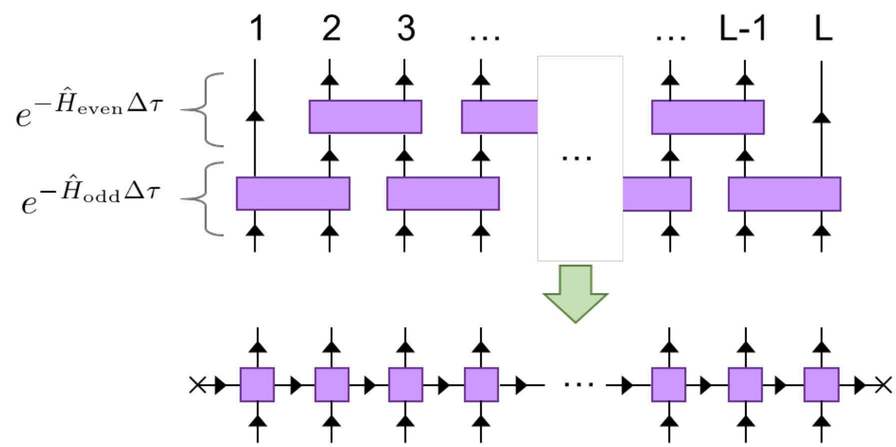
In this tutorial, we use two different approaches for constructing MPOs that represent time evolution operators. As a concrete example, we consider the XY spin-1/2 chain of even length L,

$$\hat{H}_{\mathrm{XY}} = -\sum_{\ell=1}^{L-1} (\hat{S}_{\ell,x}\hat{S}_{\ell+1,x} + \hat{S}_{\ell,y}\hat{S}_{\ell+1,y}) = -\frac{1}{2}\sum_{\ell=1}^{L-1} (\hat{S}_{\ell,+}\hat{S}_{\ell+1,-} + \hat{S}_{\ell,-}\hat{S}_{\ell+1,+}),$$

and a time step $\Delta t = 0.01$.

Exercise (a): MPO for the first-order Trotterization

In the first-order Trotter decomposition, the time evolution operator for time step Δt is split into $\exp(-\mathrm{i}\hat{H}_{\mathrm{odd}}\Delta t)\exp(-\mathrm{i}\hat{H}_{\mathrm{even}}\Delta t)$, which has an error of the order of $O(\Delta t^2)$. The decomposition is represented by two rows of time evolution gates, as depicted in the upper part of the figure below:



We can decompose each two-site gate into two single-site tensors at different sites, and contract the single-site tensors from different rows, to obtain an MPO shown in the lower part of the figure above. Write a script that constructs such an MPO for general even L. Verify your result by explicitly computing $\exp(-\mathrm{i}\hat{H}_{\mathrm{odd}}\Delta t)\exp(-\mathrm{i}\hat{H}_{\mathrm{even}}\Delta t)$ for a small system, say $L = 6$.

Exercise (b): MPO for the first-order Taylor expansion

On the other hand, we can make another first-order approximation of $\exp(-\mathrm{i}\hat{H}_{\mathrm{XY}}\Delta t)$, which as an error of the order of $O(\Delta t^2)$, by using the Taylor expansion: namely, $\exp(-\mathrm{i}\hat{H}_{\mathrm{XY}}\Delta t) \approx \hat{I} - \mathrm{i}\hat{H}_{\mathrm{XY}}\Delta t$. Write a script that constructs such an MPO for general even L. Verify your result by explicitly computing $\hat{I} - \mathrm{i}\hat{H}_{\mathrm{XY}}\Delta t$ for a small system, say $L = 6$.

(*Hint*: Refer to Sec. 5.2 of Schollwoeck2011 [U. Schollwöck, Ann. Phys. **326**, 96 (2011)].)