SFB 1143

Tensor Networks (SS2021)

Lecture 13: Real and imaginary-time evolutions

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§ 3.5 Real-time evolution

- The idea of TEBD has been used in developing time-evolution methods.

Time-dependent DMRG (t-DMRG):

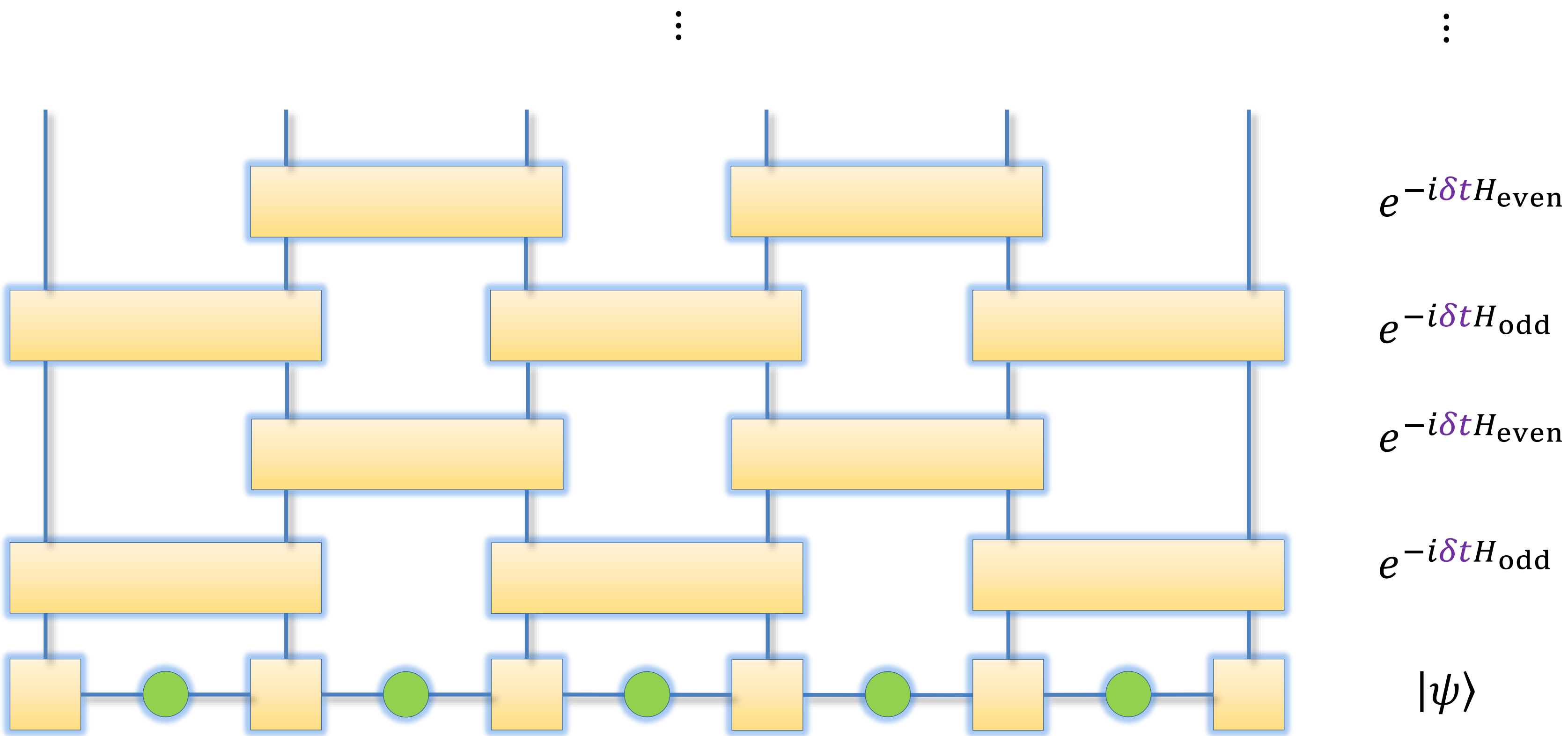
$$
\begin{aligned}
|\psi(t)\rangle &= e^{-iHt}|\psi\rangle \\
&= \left(e^{-i\delta t H}\right)^M |\psi\rangle \\
&= \left[e^{-i\delta t H_{\mathrm{even}}} e^{-i\delta t H_{\mathrm{odd}}} + O(\delta t^2)\right]^M |\psi\rangle
\end{aligned}
$$

A. J. Daley, C. Kollath, U. Schollwöck & G. Vidal, J. Stat. Mech. (2004) P04005;
S. R. White & A. E. Feiguin, Phys. Rev. Lett. 93, 076401 (2004).

§ 3.5 Real-time evolution

$$e^{-iHt}|\psi\rangle \approx \left(e^{-i\delta t H_{\text{even}}} e^{-i\delta t H_{\text{odd}}}\right)^M |\psi\rangle$$

Finite-size system



§ 3.5 Real-time evolution

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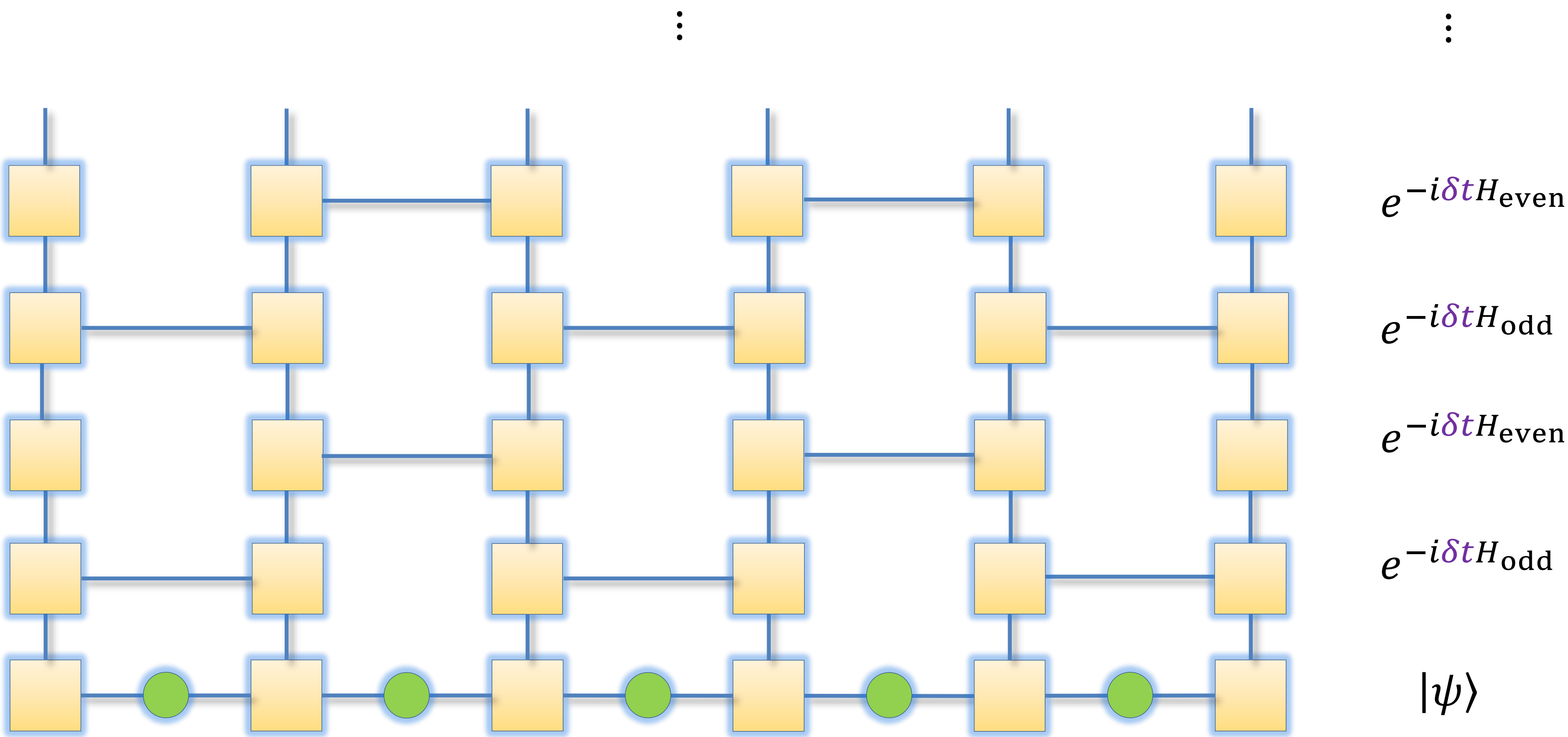

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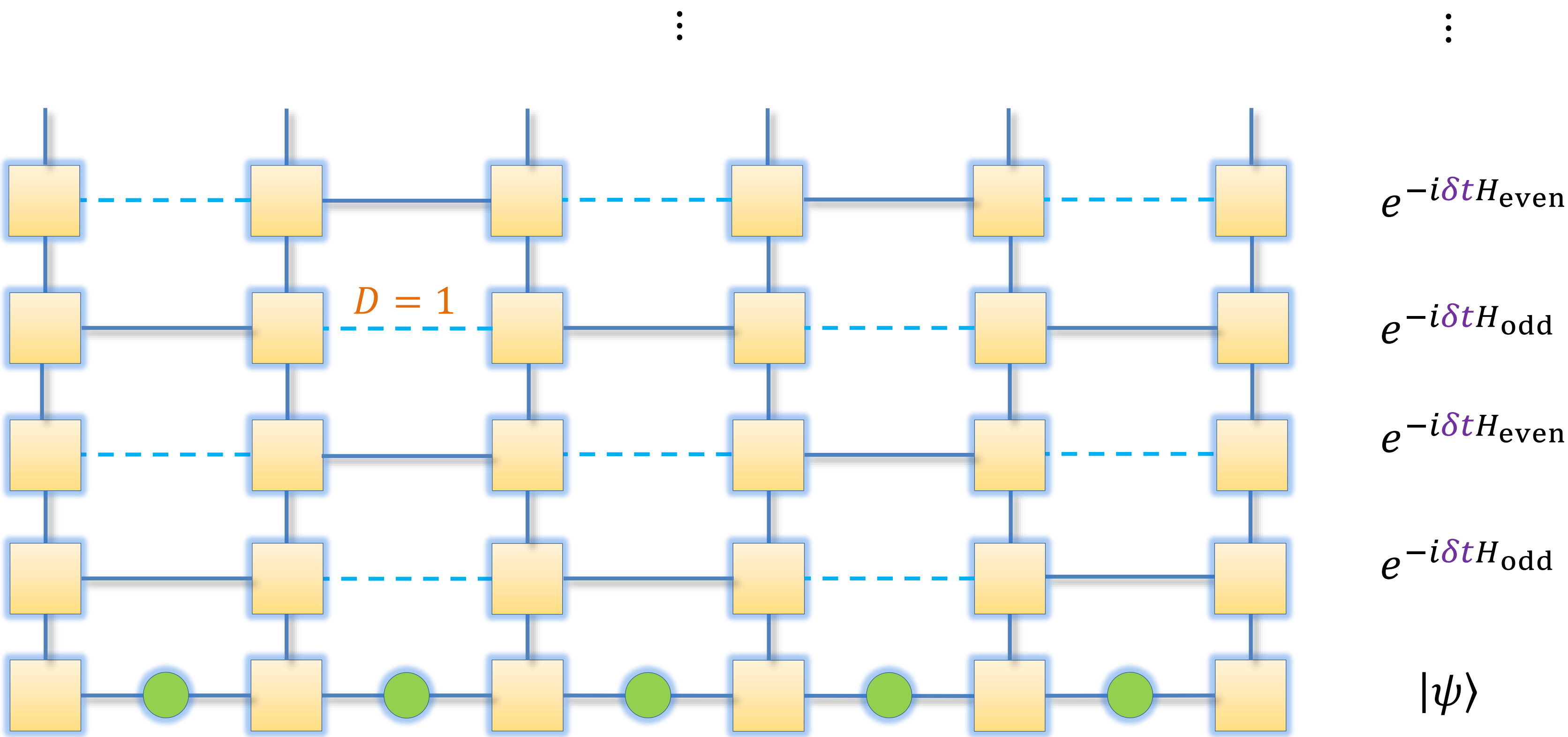

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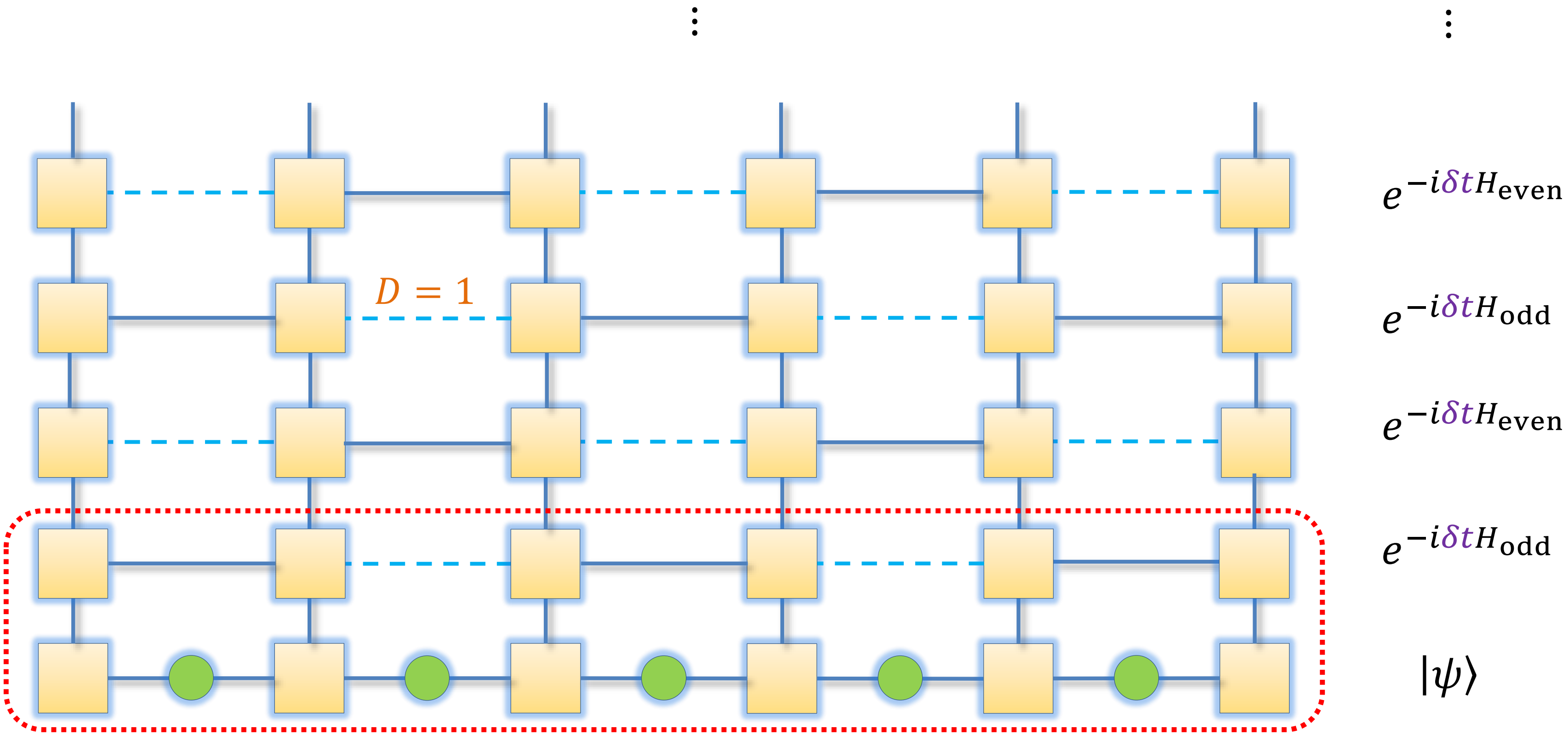
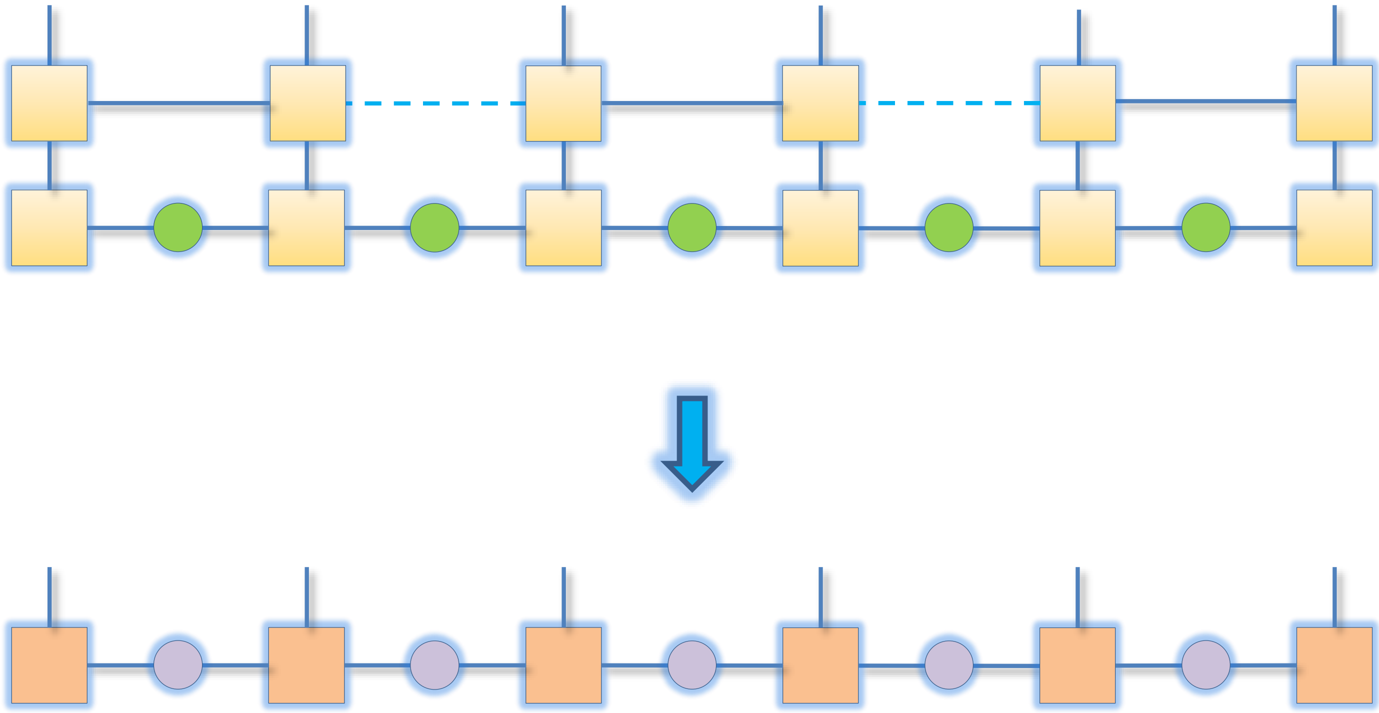


§ 3.5 Real-time evolution

- Each small time step: MPO-MPS evolution (c.f. Lecture 10)

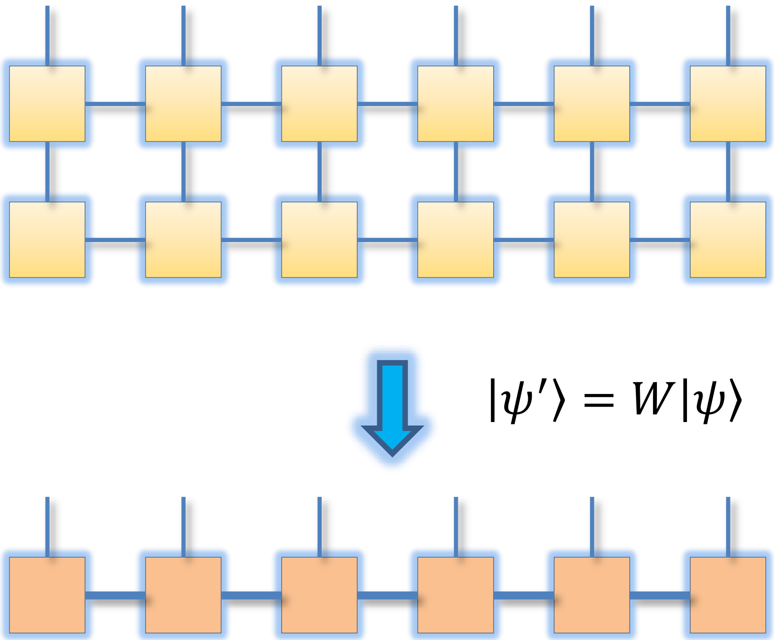


§ 3.5 Real-time evolution

- Reminder: Use DMRG to compress bond dimensions (as compression with bond canonical form is generally not optimal).

$$\min_{|\tilde{\psi}(D)\rangle} \left\| |\psi'\rangle - |\tilde{\psi}(D)\rangle \right\|_2$$

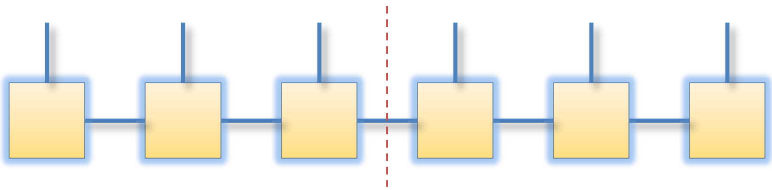
$$\max_{|\tilde{\psi}(D)\rangle} \left|\langle\psi'|\tilde{\psi}(D)\rangle\right|^2 = \max_{|\tilde{\psi}(D)\rangle} \langle\tilde{\psi}(D)|\psi'\rangle\langle\psi'|\tilde{\psi}(D)\rangle$$



$$|\psi'\rangle = W|\psi\rangle$$

§ 3.5 Real-time evolution

- Caution: The entanglement entropy of a time-evolved state $e^{-iHt}|\psi\rangle$ can grow linearly with time!



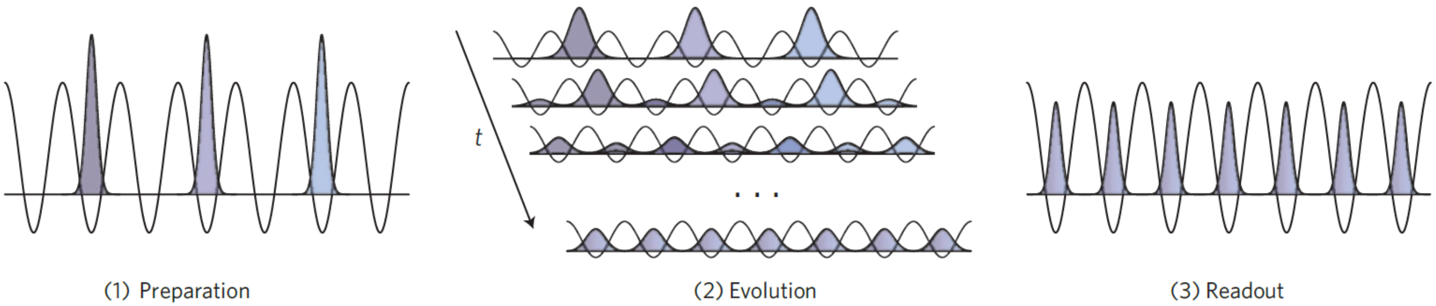
$S(t) \sim \alpha t \quad \Rightarrow \quad D_{\max} \sim e^{S(t)} \sim e^{\alpha t}$

Exponential wall!

See, e.g., N. Schuch, M.M. Wolf, K.G.H. Vollbrecht & J. I. Cirac, New J. Phys. 10 033032 (2008).

§ 3.5 Real-time evolution

Example: Non-equilibrium dynamics of ultracold bosonic atoms in an optical lattice



$$\hat{H} = \sum_j \left[-J\left(\hat{a}_j^\dagger \hat{a}_{j+1} + \mathrm{h.c.}\right) + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) + \frac{K}{2}\hat{n}_j j^2 \right]$$

S. Trotzky, Y.-A. Chen, A. Flesch, I. P. McCulloch, U. Schollwöck, J. Eisert & I. Bloch, Nat. Phys. 8, 325 (2012).

§ 3.5 Real-time evolution

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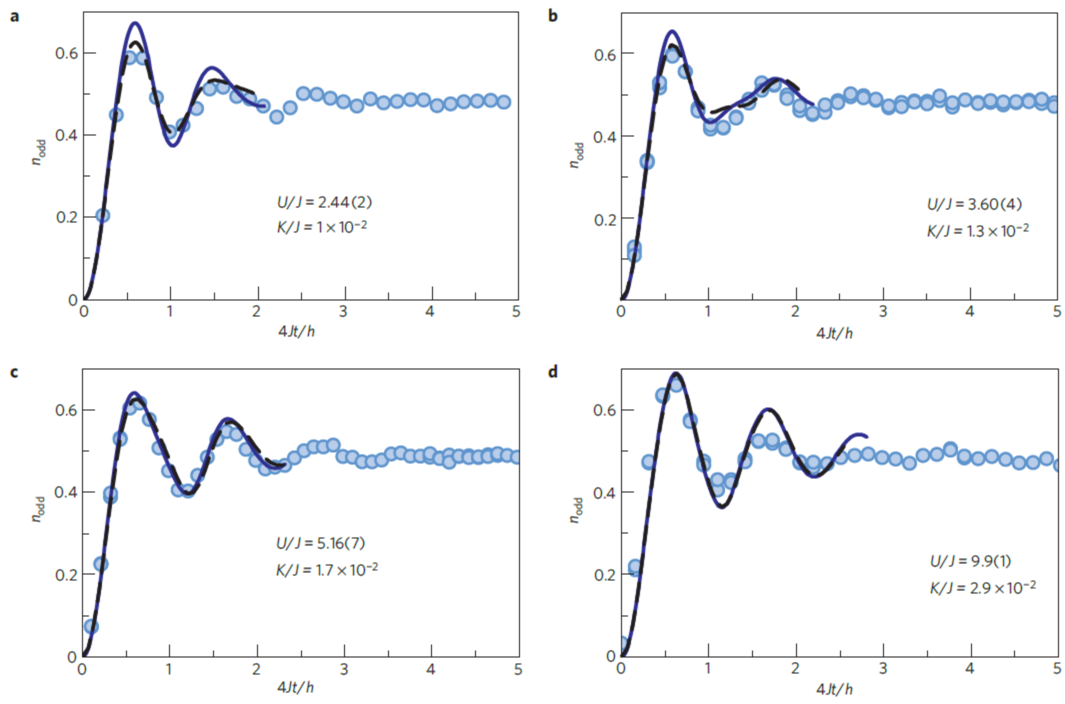

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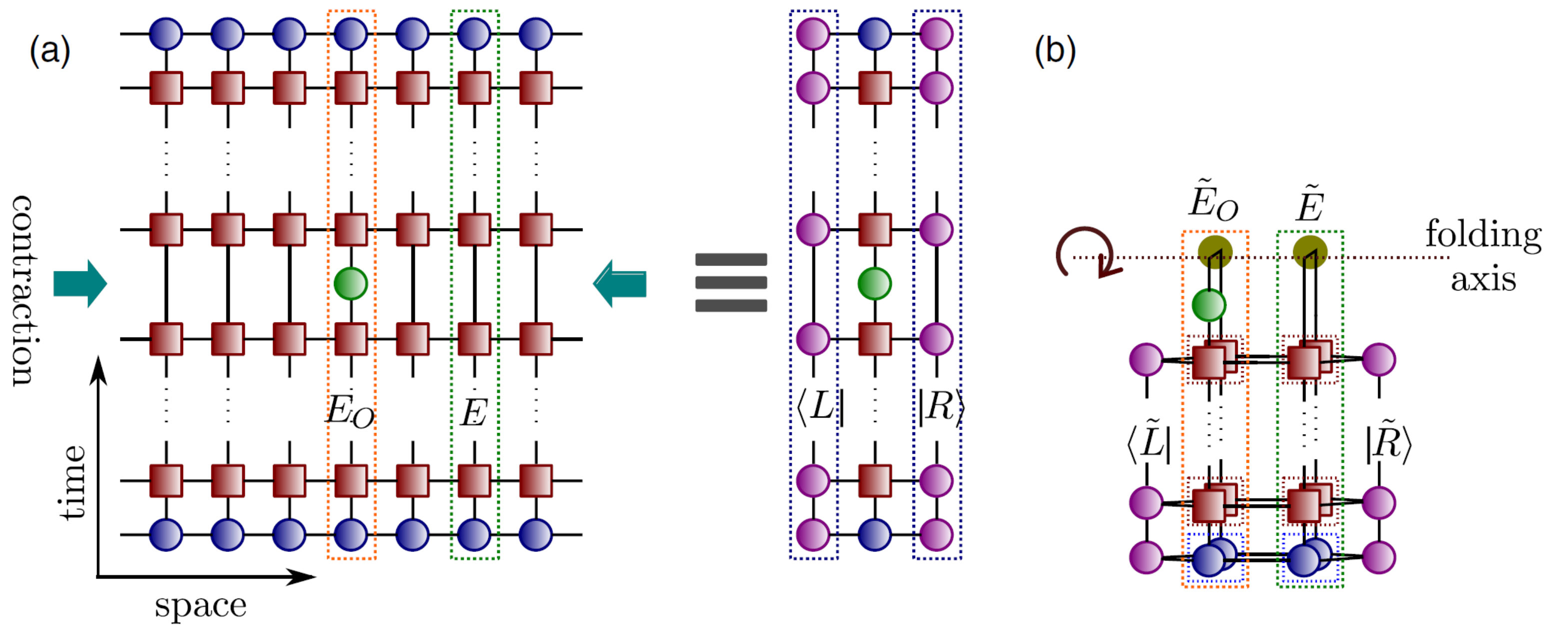
§ 3.5 Real-time evolution

- The exponential growth of entanglement in time-evolved states is a big challenge for MPS-based methods!

Review: S. Paeckel, T. Köhler, A. Swoboda, S. R. Manmana, U. Schollwöck & C. Hubig, Ann. Phys. 411, 167998 (2019).

§ 3.5 Real-time evolution

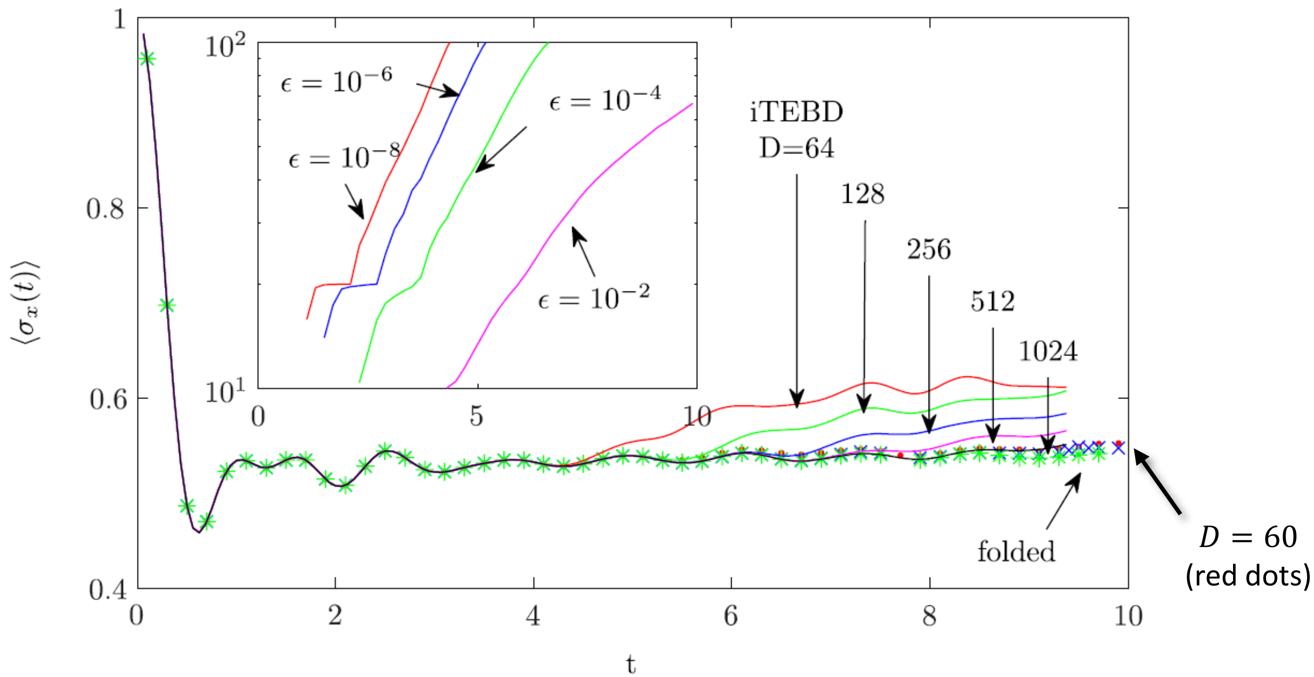
- Folding approach: $\langle O(t)\rangle = \dfrac{\langle\Psi(t)|O|\Psi(t)\rangle}{\langle\Psi(t)|\Psi(t)\rangle} = \dfrac{\langle L|E_O|R\rangle}{\langle L|E|R\rangle}$



M. C. Bañuls, M. B. Hastings, F. Verstraete & J. I. Cirac, Phys. Rev. Lett. 102, 240603 (2009).

§ 3.5 Real-time evolution

- Folding approach: $|\Psi_0\rangle = \otimes_i \frac{1}{\sqrt{2}}(|0\rangle_i + |1\rangle_i)$ $\quad H = -(\sum_i \sigma_z^i \sigma_z^{i+1} + g\sigma_x^i + h\sigma_z^i)$



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§ 3.6 Finite temperature

- The imaginary-time evolution is naturally related to the partition function of quantum systems at finite temprature.

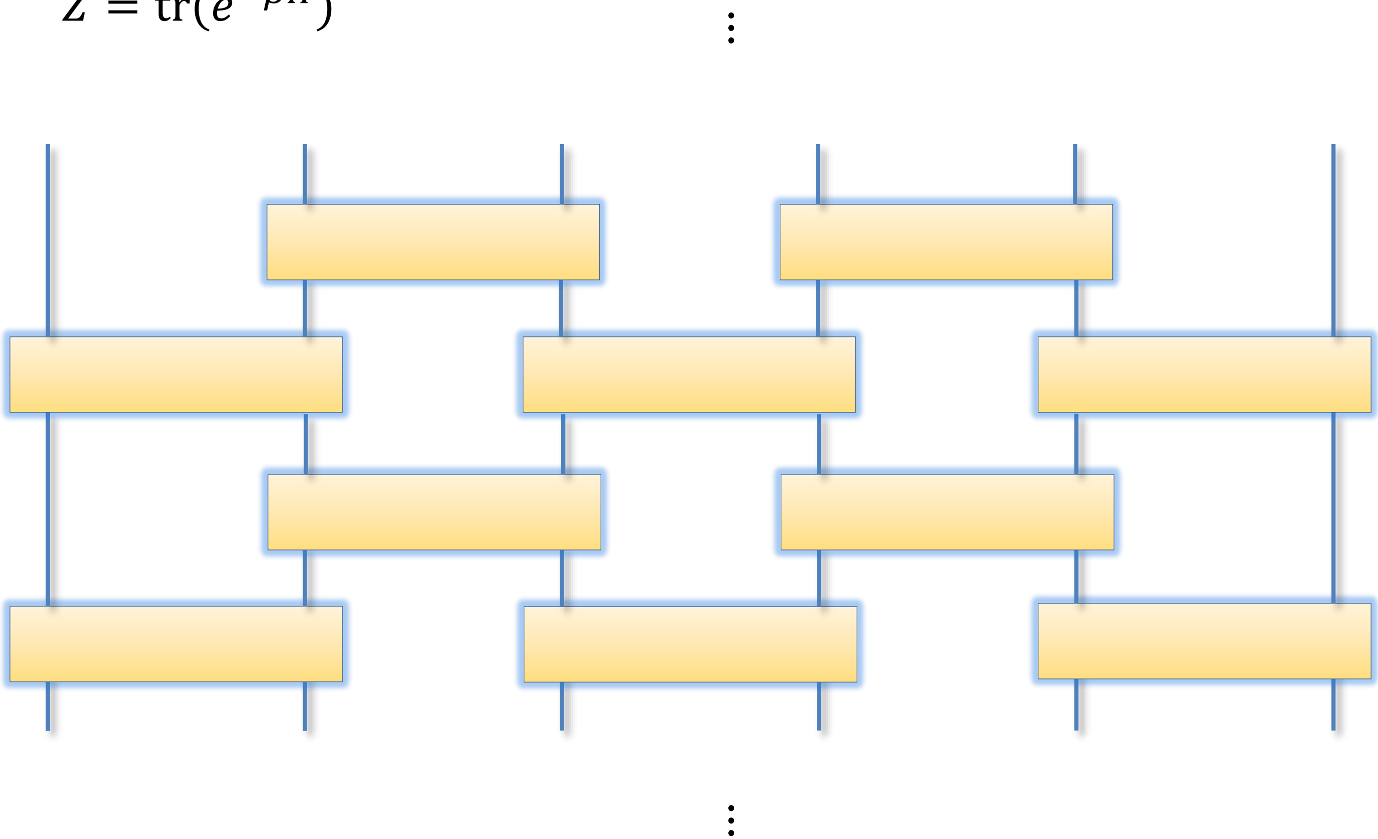
$$Z = \mathrm{tr}(e^{-\beta H}) \qquad \beta = 1/T$$

sum over all states in the physical Hilbert space

§ 3.6 Finite temperature

- 1D quantum system with nearest-neighbor interactions:

$Z = \mathrm{tr}(e^{-\beta H})$



$e^{-\delta\tau H_{\mathrm{even}}}$

$e^{-\delta\tau H_{\mathrm{odd}}}$

$e^{-\delta\tau H_{\mathrm{even}}}$

$e^{-\delta\tau H_{\mathrm{odd}}}$

⋮

⋮

§ 3.6 Finite temperature

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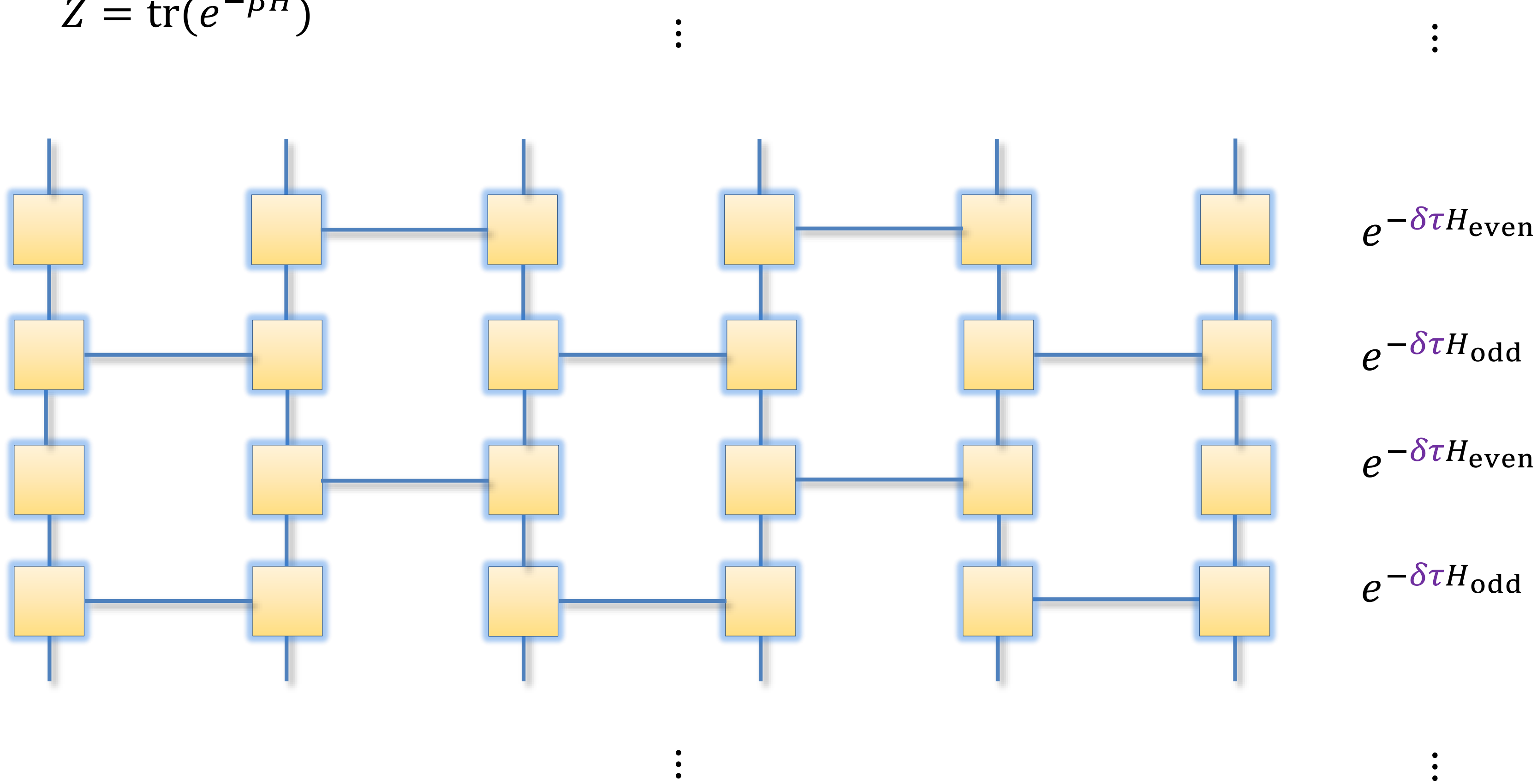

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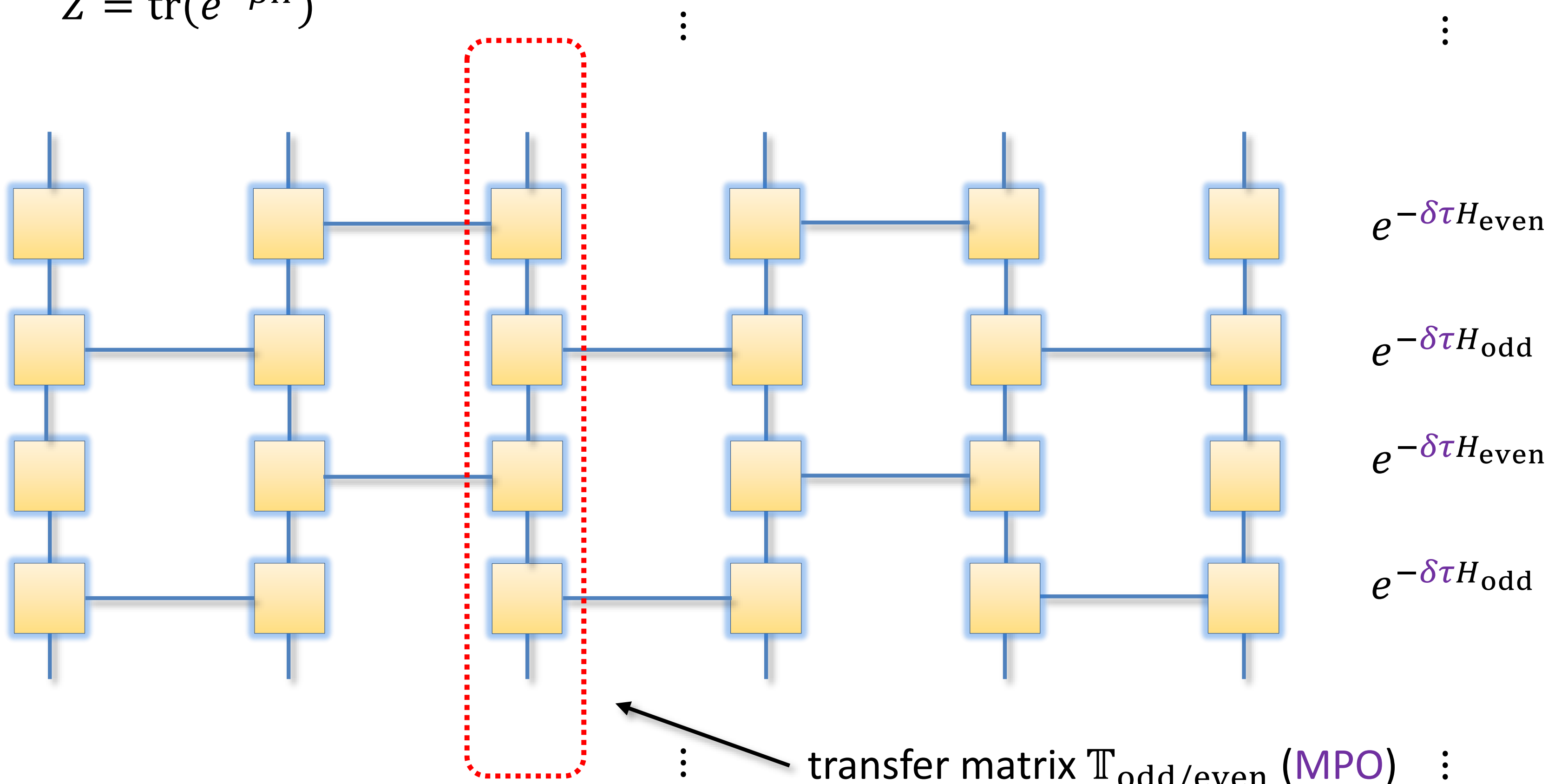

§ 3.6 Finite temperature

- 1D quantum system with nearest-neighbor interactions:

$$Z = \mathrm{tr}(e^{-\beta H})$$

$$= \mathrm{tr}\left[(\mathbb{T}_{\mathrm{odd}}\mathbb{T}_{\mathrm{even}})^{N/2}\right]$$

$$\to \lambda_{\mathrm{max}}^{N/2} \quad \text{for } N \to \infty$$

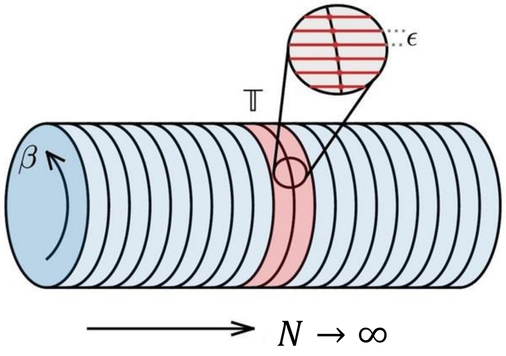

Figure from PRL 125, 170604 (2020)

leading eigenvalue of $\mathbb{T} = \mathbb{T}_{\mathrm{odd}}\mathbb{T}_{\mathrm{even}}$

X.-Q. Wang and T. Xiang, Phys. Rev. B 56, 5061 (1997); T. Xiang, Phys. Rev. B 58, 9142 (1998).

§ 3.6 Finite temperature

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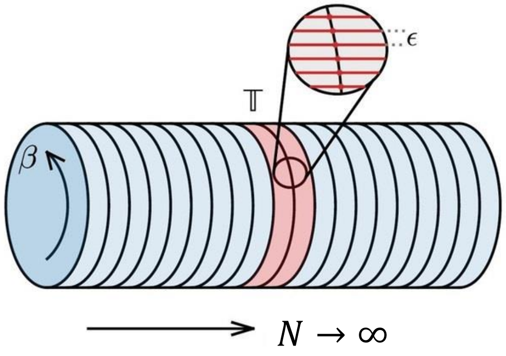
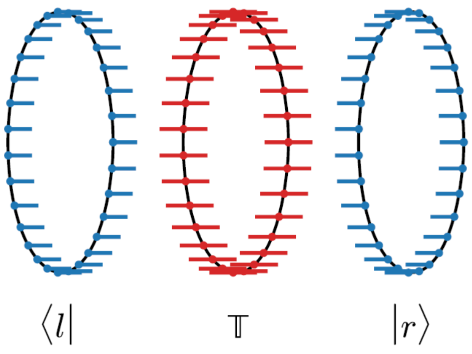


Figure from PRL 125, 170604 (2020)

How to obtain $\lambda_{\max}$ (and associated eigenvectors)?

- DMRG (if $\mathbb{T}$ is Hermitian)
- Power method



§ 3.6 Finite temperature

- 1D quantum system with nearest-neighbor interactions:

$$Z = \mathrm{tr}(e^{-\beta H})$$

$$= \mathrm{tr}[\mathbb{T}^N]$$

$$\to \lambda_{\max}^N \qquad \text{for } N \to \infty$$

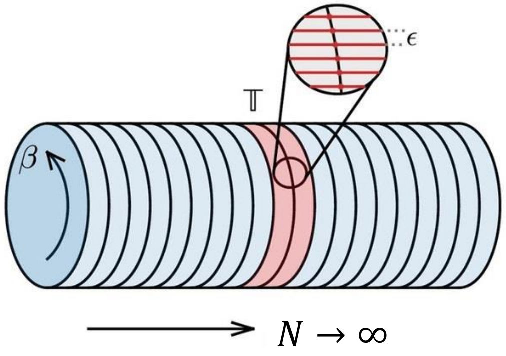
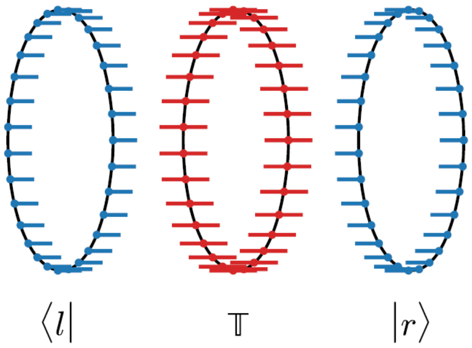


Figure from PRL 125, 170604 (2020)

Recent development:

$\delta\tau \to 0$ can be taken explicitly (i.e., no Trotter error) and long-range Hamiltonians can be treated on equal footing!



W. Tang, HHT, and L. Wang, Phys. Rev. Lett. 125, 170604 (2020).