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Computational Quantum Many-Body Physics

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NumeriQS Retreat



#### TNs as MB States and Operators

- TN compact representation of states and operators for many-body (MB) systems П
- L-body system: reduce complexity

$$
\sim O(2^L) \implies \sim poly(L)
$$

- efficient approximation states/operators with low entanglement
- TN based algorithms: unitary dynamics at long time scales; ○ system-size larger than ED





Operator acting on L-body system  $\hat{O}: \mathcal{H} \to \mathcal{H}$ 

 $\circ$   $\circ$  $\circ$  $\overline{O}$  $\overline{O}$  $\circ$  $\circ$  $\blacksquare$  1D: matrix-product-operator (MPO),

$$
\hat{O} = \sum_{\sigma_1, \ldots, \sigma_L} \sum_{\sigma'_1, \ldots, \sigma'_L} \hat{O}^{\sigma_1, \sigma'_1} \ldots \hat{O}^{\sigma_L, \sigma'_L} |\sigma_1, \ldots, \sigma_L\rangle \langle \sigma'_1, \ldots, \sigma'_L
$$





complexity: 
$$
\sim L \chi^2 d^2
$$

# U(1) Symmetry

• action of  $U(1)$ :  $\mathbb{V} = \bigoplus_{n} \mathbb{V}_{n}$   $\mathbb{V}_{n}$  sub-space

- quantum charge  $n \in \mathbb{Z}$ ,
- $\circ$  symmetry generator  $\hat{n} = \sum_n n \; \hat{\Pi}$

 $\hat{\Pi}_n$  projector in  $V_n$ 

• 
$$
\hat{O}: \mathbb{V} \to \mathbb{V}
$$
 charge-preserving  $\Leftrightarrow \left[\hat{O}, \hat{n}\right] = 0$   
\n
$$
\hat{O} = \bigoplus_{n} \hat{O}^{[n]} \qquad \hat{O}^{[n]} : \mathbb{V}_{n} \to \mathbb{V}_{n}
$$
\n*e.g. spin L-body lattice with total magnetization conserved*

 $\hat{S}^{\textsf{z\_tot}} = \sum_{j=1}^L \hat{s}^{\textsf{z}}_j \qquad [\hat{H},\hat{S}^{\textsf{z\_tot}}] = 0$ 

 $\sqrt{2}$  $\overline{\phantom{a}}$  $\begin{array}{c|ccccc}\hat{O}^{[1]} & 0 & \cdots & 0 \ \hline 0 & & \cdots & 0 \end{array}$  $\begin{array}{ccc} \vdots & \vdots & \vdots \\ 0 & 0 & \cdots \end{array}$ . . . . .  $\setminus$  $\cdot$ 



#### Operator Charge

 $\hat{\mathcal{O}}: \mathcal{H} \to \mathcal{H}$  maps states with charge  $\emph{n}$  into states with  $\emph{n}'$ 

$$
\hat{\mathcal{O}} = \sum_{i,j} O_{ij} |i,n\rangle \langle j,n'
$$

|

- *vectorized* operator  $|\hat{O}\rangle\!\rangle = \sum_{i,j} O_{ij}|i,n\rangle|j,n'\rangle$
- superoperator  $\hat{\mathcal{Q}}: \mathcal{H} \otimes \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}$

$$
\hat{\mathcal{Q}}\,\ket{\hat{\mathcal{O}}}_{\hat{\mathbf{z}}}=q_{\hat{\mathcal{O}}}\,\ket{\hat{\mathcal{O}}}_{\hat{\mathbf{z}}},
$$



#### Operator Charge

 $\hat{\mathcal{O}}: \mathcal{H} \to \mathcal{H}$  maps states with charge  $\emph{n}$  into states with  $\emph{n}'$ 

$$
\hat{\mathcal{O}} = \sum_{i,j} O_{ij} |i,n\rangle \langle j,n'
$$

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*vectorized* operator  $|\hat{O}\rangle\!\rangle = \sum_{i,j} O_{ij}|i,n\rangle|j,n'\rangle$ 

■ superoperator  $\hat{\mathcal{Q}}: \mathcal{H} \otimes \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}$ 



operator

\n
$$
\hat{Q} \mid \hat{O} \rangle = q_{\hat{O}} \mid \hat{O} \rangle,
$$
\ncharge

\n
$$
Q = \hat{n} \otimes 1 + \alpha \cdot 1 \otimes \hat{n}^T
$$
\n
$$
\underline{q_{\hat{O}} = n + \alpha n'}
$$



#### Sector Resolution



 $\Box$   $\alpha = -1$  $\Box$   $\alpha = (L+1)$  $\Box$   $\alpha = +1$ 

block-diagonal operator

unique charge for each block, i.e.  $q_{\hat{\mathcal{O}}} = n + (L+1)$  n'; blocks anti-diagonal operators.



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## Invariance of TNs under U(1) symmetry

#### charge or flow of conserved quantity

$$
|\sigma_i\rangle \rightarrow |\sigma_i, m_i\rangle
$$
\n
$$
|\sigma'_i\rangle \rightarrow |\sigma'_i, m'_i\rangle
$$
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$$
|\sigma'_i\rangle \rightarrow |\sigma'_i, m'_i\rangle
$$
\n
$$
|\sigma'_i\rangle \rightarrow |\sigma_i, q_i\rangle
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- local charge conservation:  $q^{}_i = \sum_{j=1}^{i} m^{}_j + \alpha \,$  m $'_j$
- boundary conditions:  $q_0 = 0$ ,  $q_L = q_{\hat{\mathcal{O}}}$ ,

$$
\implies \text{operator charge conservation:} \ \ q_{\hat{\mathcal{O}}} = \sum_{i=1}^{L} m_i + \alpha \ m'_i
$$



### OTOC

#### $\circ$  $\circ$  $\overline{O}$  $\Omega$  $\circ$  $\overline{O}$  $\circ$

■ Out-of-time-ordered correlator (OTOC): standard detector of quantum chaos

$$
\mathcal{C}_{j,j'}(t) = \frac{\text{Tr}\left(\left[\hat{O}_{j},\hat{O}_{j'}(t)\right]^{2}\right)}{2\text{ Tr}\left(\mathbb{I}\right)}
$$

spin $-1/2$  system:  $\hat{\sigma}_j^z(t) = \hat{U}(t)^\dagger \hat{\sigma}_j^z \hat{U}(t)$ ,

$$
C_{j,j'}(t) = 1 - \frac{\text{Tr}\left(\hat{\sigma}^z_{j'}(t)\ \hat{\sigma}^z_j\ \hat{\sigma}^z_{j'}(t)\ \hat{\sigma}^z_j\right)}{\text{Tr}\left(\mathbb{I}\right)}
$$

 $\blacksquare$  U(1) symmetric systems:  $\hat{\sigma}_i(t)$  is charge-preserving



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# Projected OTOCs in U(1)-Symmetry Sector



#### Projected OTOC





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t

### Projected OTOC

#### $C_{j,j'}(t)$   $^{[n]}=1-\text{Tr}\left(\left(\hat{\sigma}_{15}^{z}(t)^{[n]}\hat{\sigma}_{j}^{z}[n]\right)^{2}\right)/\mathcal{D}_{n}$



### Projected OTOC

 $C_{j,j'}(t)$   $^{[n]}=1-\text{Tr}\left(\left(\hat{\sigma}_{15}^{z}(t)^{[n]}\hat{\sigma}_{j}^{z}[n]\right)^{2}\right)/\mathcal{D}_{n}$ 



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#### Projected OTOC Speed





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### Summary and Outlook

**Implementing symmetry in MPO** 

Computations of global quatities in symmetry-sector П ◦ reduction of computational cost −→ blockwise operations ◦ dynamics at large times for large system-size



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■ OTOC projected in sectors



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**Implementing symmetry in MPO** 

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■ OTOC projected in sectors

**Outlook** 

- study operator entanglement entropy with symmetry-resolution
- **implement symmetry in higher D lattice**



#### Thank you!



■ Bipartition of the system into A and B, i.e.  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$  $\hat{Q}$ : generator of  $U(1)$  symmetry,  $\;\hat{Q}=\hat{Q}_A\otimes\mathbb{1}_B+\; \mathbb{1}_A\otimes\hat{Q}_B$ Schmidt decomposition of operator  $\hat{O}$ :

$$
\frac{\hat{\mathcal{O}}}{\sqrt{\text{Tr}(\hat{\mathcal{O}}^{\dagger}\hat{\mathcal{O}})}} = \sum_{q_A} \sum_{j} \lambda_j^{(q_A)} \hat{\mathcal{O}}_{A,j}^{(q_A)} \otimes \hat{\mathcal{O}}_{B,j}^{(q_{\hat{\mathcal{O}}}-q_A)}
$$
\nwith\n
$$
\left[\hat{Q}_A, \hat{\mathcal{O}}_{A,j}^{(q_A)}\right]_{\alpha} = q_A \hat{\mathcal{O}}_{A,j}^{(q_A)} \qquad \left[\hat{Q}_B, \hat{\mathcal{O}}_{B,j}^{(q_B)}\right]_{\alpha} = q_B \hat{\mathcal{O}}_{B,j}^{(q_B)} \delta_{q_B, (q_{\hat{\mathcal{O}}}-q_A)}.
$$

<sup>a</sup>α-deformed commutator  $[\hat{A}, \hat{B}]_{\alpha} = \hat{A} + \alpha \hat{B}$ 



Operator Entanglement Entropy (OpEE) : indicator of the operator complexity

$$
S(\hat{\mathcal{O}}) = \sum_{q_A} p(q_A) S_{q_A}(\hat{\mathcal{O}}) + \sum_{q_A} -p(q_A) \log (p(q_A))
$$
  

$$
S_{q_A}(\hat{\mathcal{O}}) = -\sum_{j} \left( \frac{(\lambda_j^{(q_A)})^2}{p(q_A)} \right) \log \left( \frac{(\lambda_j^{(q_A)})^2}{p(q_A)} \right)
$$

$$
p(q_A) = \sum_j (\lambda_j^{(q_A)})^2
$$

interplay between entanglement of a state and symmetries

 $^{2}$ Rath A, Vitale V, Murciano S, Votto M, Dubail J, Kueng R, Branciard C, Calabrese P and Vermersch B 2023,  $16/Entanglement barrier and its symmetry resolution: the <sub>QdWeffed</sub> experiment, PRX Quantum 4 010318$ UNIVERSITÄT BONN

### Symmetry Resolved OpEE





Heisenberg chain with  $L = 16$  Trotterised (4-th order) time-evolution operator until time  $t=20$ .  $\quad S(\hat{U}(t)^{[n]})$  for the sectors  $n = 1, 2, 4, 8$ .

Heisenberg chain with  $L = 10$  and  $L = 16$  Trotterised (4-th order) time-evolution operator until time  $t = 20$ .  $S(\hat{U}(t)^{[n]})$  for the biggest sector  $n=5$  and  $n=8$ .



#### Reduction of the computational cost

Projected OTOCs in U(1)-Symmetry Sector  $\epsilon_n = 1 - \text{Tr}\left(\left(U^{(n)}_{\text{exact}}\right)^{\dagger} U^{(n)}_{\text{MPO}}\right) / \mathcal{D}_n$ 







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