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Computational Quantum Many-Body Physics

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TNs as MB States and Operators

- TN compact representation of states and operators for many-body (MB) systems
- 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 $\hat{O}: \mathcal{H} \rightarrow \mathcal{H}$
- 1D: matrix-product-operator (*MPO*), OOOOOOO

$$\hat{O} = \sum_{\sigma_1,...,\sigma_L} \sum_{\sigma_1',...,\sigma_L'} \hat{O}^{\sigma_1,\sigma_1'} \dots \hat{O}^{\sigma_L,\sigma_L'} \ket{\sigma_1,\dots,\sigma_L} raket{\sigma_1',\dots,\sigma_L'}$$





• 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 $n\in\mathbb{Z}$,
- symmetry generator $\hat{n} = \sum_n n \, \hat{\Pi}_n$,



•
$$\hat{O} : \mathbb{V} \to \mathbb{V}$$
 charge-preserving $\Leftrightarrow \qquad \left[\hat{O}, \hat{n}\right] = 0$
 $\hat{O} = \bigoplus_{n} \hat{O}^{[n]} \qquad \hat{O}^{[n]} : \mathbb{V}_{n} \to \mathbb{V}_{n}$

e.g. spin *L*-body lattice with **total magnetization** conserved $\hat{S}^{z \text{ tot}} = \sum_{j=1}^{L} \hat{s}_{j}^{z}$ $[\hat{H}, \hat{S}^{z \text{ tot}}] = 0$





Operator Charge

• $\hat{\mathcal{O}}: \mathcal{H}
ightarrow \mathcal{H}$ maps states with charge *n* into states with *n'*

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

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

$$\hat{\mathcal{Q}} \; | \hat{\mathcal{O}}
angle = q_{\hat{\mathcal{O}}} \; | \hat{\mathcal{O}}
angle ,$$



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operator
$$\hat{\mathcal{Q}} | \hat{\mathcal{O}} \rangle = q_{\hat{\mathcal{O}}} | \hat{\mathcal{O}} \rangle,$$
charge
$$\mathcal{Q} = \hat{n} \otimes 1 + \alpha \ 1 \otimes \hat{n}^{T}$$

$$\underline{q_{\hat{\mathcal{O}}} = n + \alpha n'}$$



Sector Resolution



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



Invariance of TNs under U(1) symmetry

• *charge* or flow of conserved quantity

$$\begin{aligned} \sigma_i \rangle \to |\sigma_i, m_i\rangle & |\sigma_i'\rangle \to |\sigma_i', m_i'\rangle & |a_i\rangle \to |a_i, q_i\rangle \\ & \begin{array}{c} m_1 \in \{0, 1\} & m_2 \in \{0, 1\} & m_L \in \{0, 1\} \\ & \downarrow \sigma_1 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2 \\ & \downarrow \sigma_1 & \downarrow \sigma_2 \\ & \downarrow \sigma_1 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2 \\ & \downarrow \sigma_1 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2 \\ & \downarrow \sigma_1 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2 \\ & \downarrow \sigma_1 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2 \\ & \downarrow \sigma_2 & \downarrow \sigma_2$$

- local charge conservation: $q_i = \sum_{j=1}^i m_j + \alpha m'_j$
- boundary conditions: $q_0 = 0$, $q_L = q_{\hat{O}}$,

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



ΟΤΟΟ

0 0 0 0 0 0 0

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

$$\mathcal{L}_{j,j'}(t) = rac{ ext{Tr}\left(\left[\hat{O}_{j},\hat{O}_{j'}(t)
ight]^2
ight)}{2 ext{ Tr}\left(\mathbb{I}
ight)}$$

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

$$\mathcal{C}_{j,j'}(t) = 1 - rac{ ext{Tr}\left(\hat{\sigma}^z_{j'}(t) \; \hat{\sigma}^z_{j} \; \hat{\sigma}^z_{j'}(t) \; \hat{\sigma}^z_{j}
ight)}{ ext{Tr}\left(\mathbb{I}
ight)}$$

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



Projected OTOCs in U(1)-Symmetry Sector



Projected OTOC





Projected OTOC



Projected OTOC



NumeriQS Retreat

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Projected OTOC Speed





Summary and Outlook

Implementing symmetry in MPO

Computations of global quatities in symmetry-sector

 reduction of computational cost
 blockwise operations
 dynamics at large times for large system-size



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Outlook

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



Thank you!



Symmetry Resolved OpEE

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, $\hat{Q} = \hat{Q}_A \otimes 1_B + 1_A \otimes \hat{Q}_B$

Schmidt decomposition of operator $\hat{\mathcal{O}}$:

$$\frac{\hat{\mathcal{O}}}{\sqrt{\mathrm{Tr}(\hat{\mathcal{O}}^{\dagger}\hat{\mathcal{O}})}} = \sum_{q_A} \sum_j \lambda_j^{(q_A)} \ \hat{\mathcal{O}}_{A,j}^{(q_A)} \otimes \hat{\mathcal{O}}_{B,j}^{(q_{\bar{\mathcal{O}}}-q_A)}$$
with
$$\begin{bmatrix} \hat{Q}_A, \hat{\mathcal{O}}_{A,j}^{(q_A)} \end{bmatrix}_{\alpha} = q_A \hat{\mathcal{O}}_{A,j}^{(q_A)} \qquad \begin{bmatrix} \hat{Q}_B, \hat{\mathcal{O}}_{B,j}^{(q_B)} \end{bmatrix}_{\alpha} = q_B \ \hat{\mathcal{O}}_{B,j}^{(q_B)} \ \delta_{q_B,(q_{\bar{\mathcal{O}}}-q_A)}.^a$$

^a α -deformed commutator $[\hat{A}, \hat{B}]_{\alpha} = \hat{A} + \alpha \hat{B}$



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

$$egin{aligned} S(\hat{\mathcal{O}}) &= \sum_{q_A} p(q_A) S_{q_A}(\hat{\mathcal{O}}) + \sum_{q_A} - p(q_A) \log{(p(q_A))} \ S_{q_A}(\hat{\mathcal{O}}) &= -\sum_j \left(rac{(\lambda_j^{(q_A)})^2}{p(q_A)}
ight) \log{\left(rac{(\lambda_j^{(q_A)})^2}{p(q_A)}
ight)} \end{aligned}$$

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

interplay between entanglement of a state and symmetries

²Rath 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: theory and resperiment, PRX Quantum 4 010318

Symmetry Resolved OpEE





Heisenberg chain with L = 16 Trotterised (4-th order) time-evolution operator until time t = 20. $S(\hat{U}(t)^{[n]})$ 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 $\epsilon_n = 1 - \text{Tr}\left(\left(U_{\text{exact}}^{(n)}\right)^{\dagger} U_{\text{MPO}}^{(n)}\right) / \mathcal{D}_n$





