

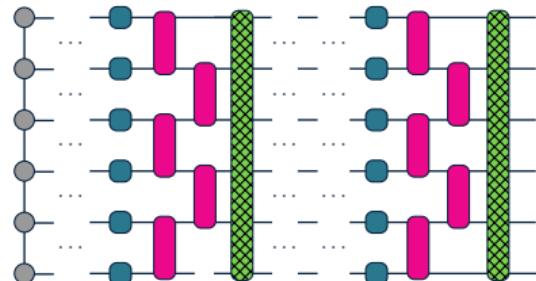
Simulation of Noisy Quantum Systems with POVM-MPS

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Noisy Quantum Simulations

- Simulations of channels vs. unitaries are *higher dimensional* and *constrained*

$$\underbrace{U|\psi\rangle \in \mathbb{C}^{D^N}}_{\text{Arbitrary Normalized Vector}} \rightarrow \underbrace{\Lambda(\rho) \in \mathbb{C}^{D^N \times D^N}}_{\text{Positive-Semidefinite, Hermitian Matrix}} \quad (1)$$

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- How to differentiate between “quantum” correlations in *pure* states versus “classical” correlations in *mixed* states?
- Does *noise* make simulations *easier* [1] ?

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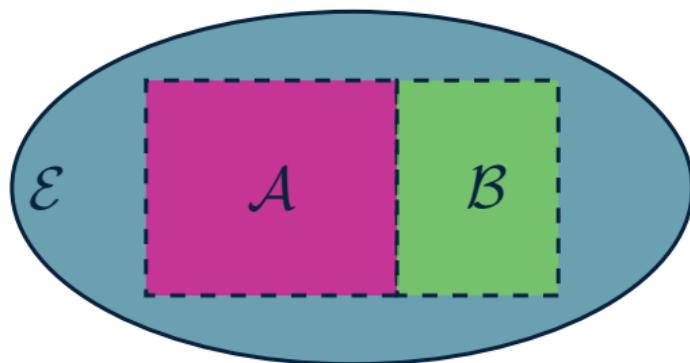
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- How to differentiate between “quantum” correlations in *pure* states versus “classical” correlations in *mixed* states?
- Does *noise* make simulations *easier* ?
- Is there an *area law* for noise/classical correlations?
 - i.e) How does simulation complexity depend on system size, Kraus rank [2] ?

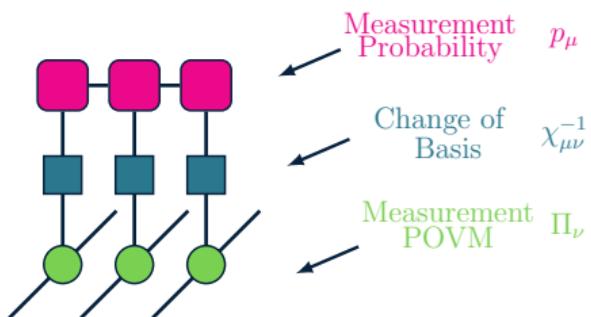
Noisy Quantum Simulations

What if we want to assess *capabilities* of capturing correlations in systems *strictly* between \mathcal{A}, \mathcal{B} , excluding correlations with environments \mathcal{E} ?



POVM-MPS for Quantum Simulations

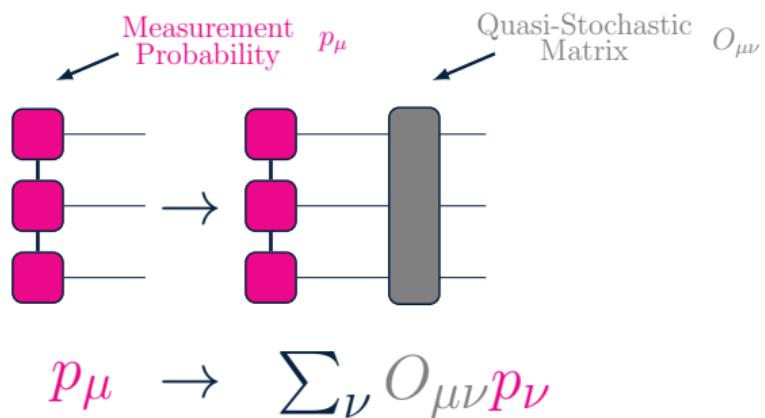
Suppose we model states in terms of measurement *probabilities* $\rho \cong \textcolor{magenta}{p}$



$$\rho_{\sigma\sigma'} = \sum_{\mu\nu} \textcolor{magenta}{p}_\mu \chi_{\mu\nu}^{-1} \Pi_{\nu\sigma\sigma'}$$

POVM-MPS for Quantum Simulations

Suppose we model dynamics in terms of *(quasi-)stochastic matrices* $\Lambda \cong O$



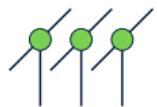
POVM-MPS for Quantum Simulations

To ensure *efficient* classical simulations:

POVM-MPS for Quantum Simulations

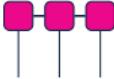
To ensure *efficient* classical simulations:

- Measurements $\Pi = \otimes_i^N \Pi_i$ are *local, informationally complete* (POVM) [3]



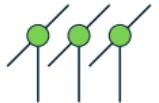
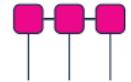
POVM-MPS for Quantum Simulations

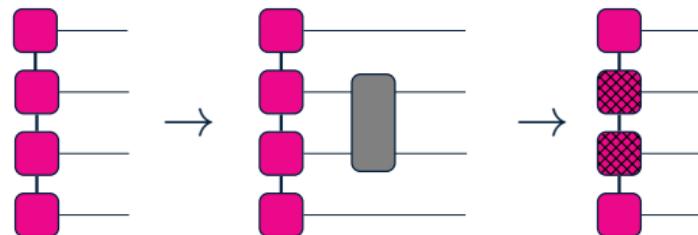
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- Measurements $\Pi = \otimes_i^N \Pi_i$ are *local, informationally complete* (POVM) 
- Probabilities $p \approx p_\chi = \prod_i^N A_i$ are *tensor trains* (pMPS) 

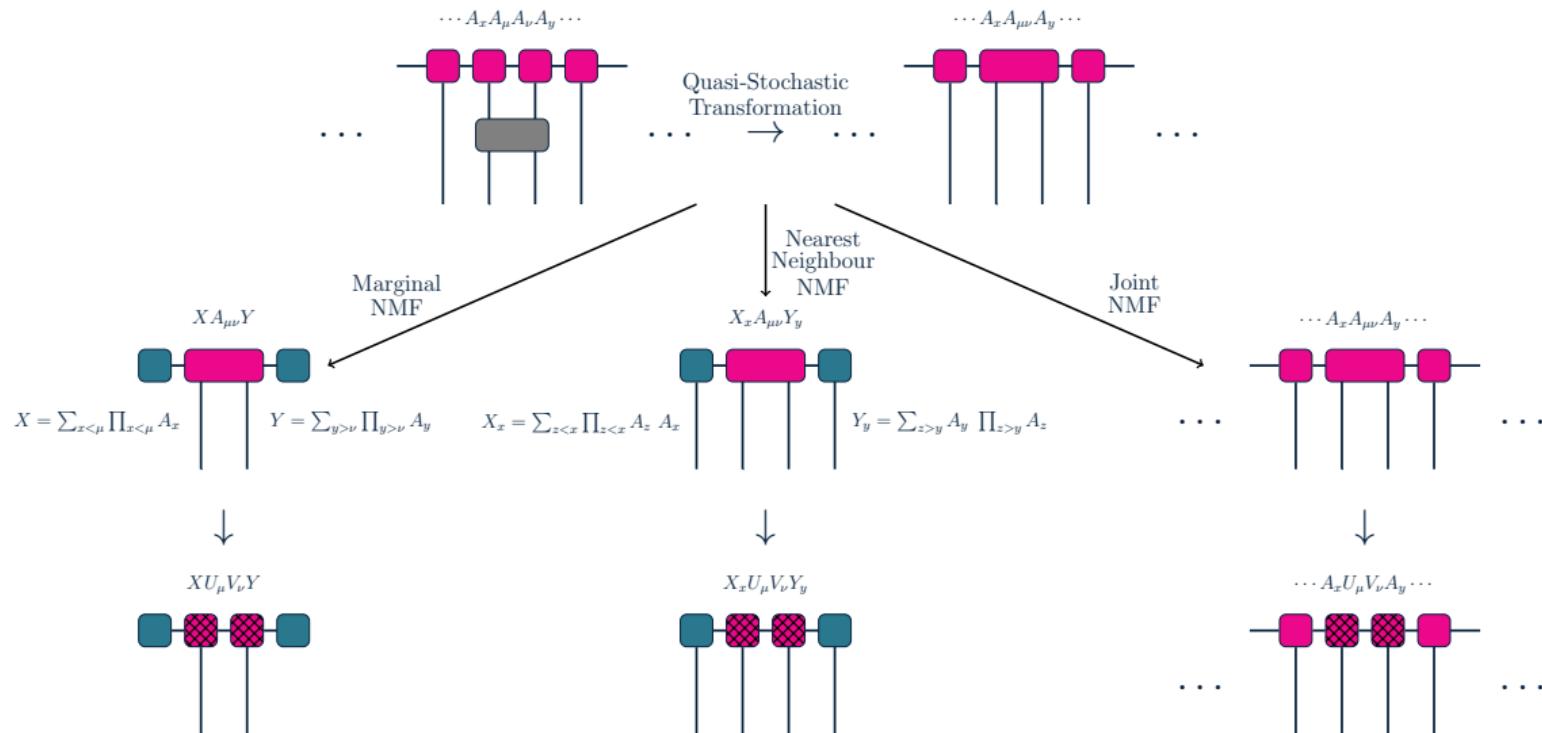
POVM-MPS for Quantum Simulations

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- Measurements $\Pi = \otimes_i^N \Pi_i$ are *local, informationally complete* (POVM) 
- Probabilities $p \approx p_\chi = \prod_i^N A_i$ are *tensor trains* (pMPS) [4] 
- How may we *normalize and truncate* updates $p \rightarrow O p \rightarrow p'_\chi$?

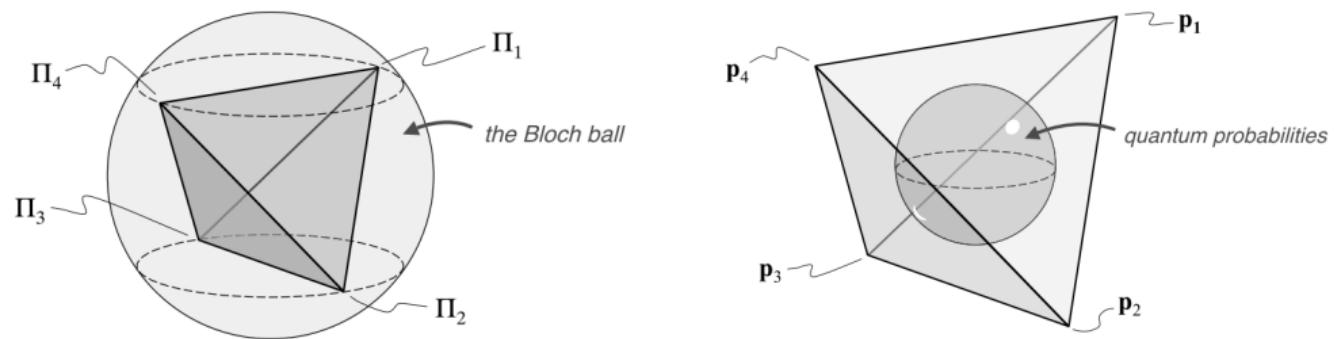


Tensor Factorizations and Truncations

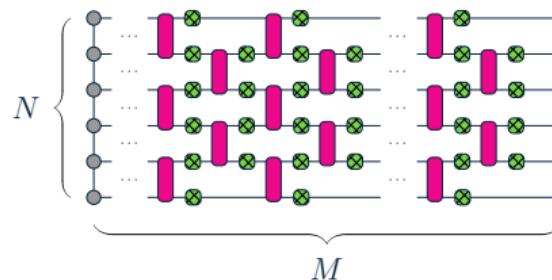


Quantum Probability Simplexes

Not only do POVM-MPS updates $p \rightarrow p_\chi$ have to be *non-negative*, but they must obey non-trivial quantum probability simplex *constraints* [5]



Random Noisy Quantum Circuits



M layers of Random *2-local* Unitaries (Pink) + Noise (Green) with *Product* Initial States

1. Convert states to probabilities and channels to quasi-stochastic matrices

$$\rho \rightarrow p \quad , \quad \Lambda \rightarrow O$$

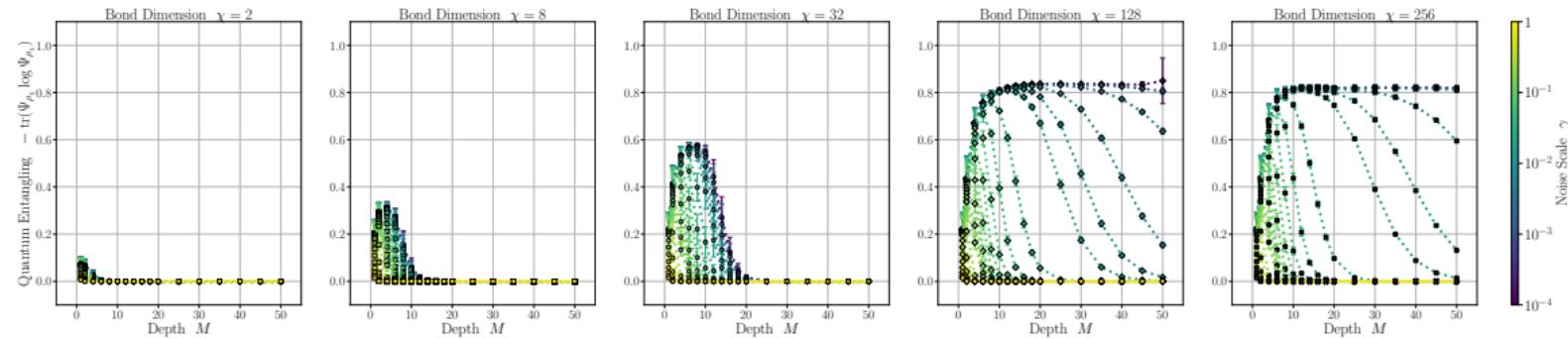
2. Apply channels and truncate bond-dimension to χ (SVD-based truncation)

$$p \rightarrow p' = Op \approx p'_\chi$$

3. Convert evolved probabilities to states ρ'_χ and compute quantities

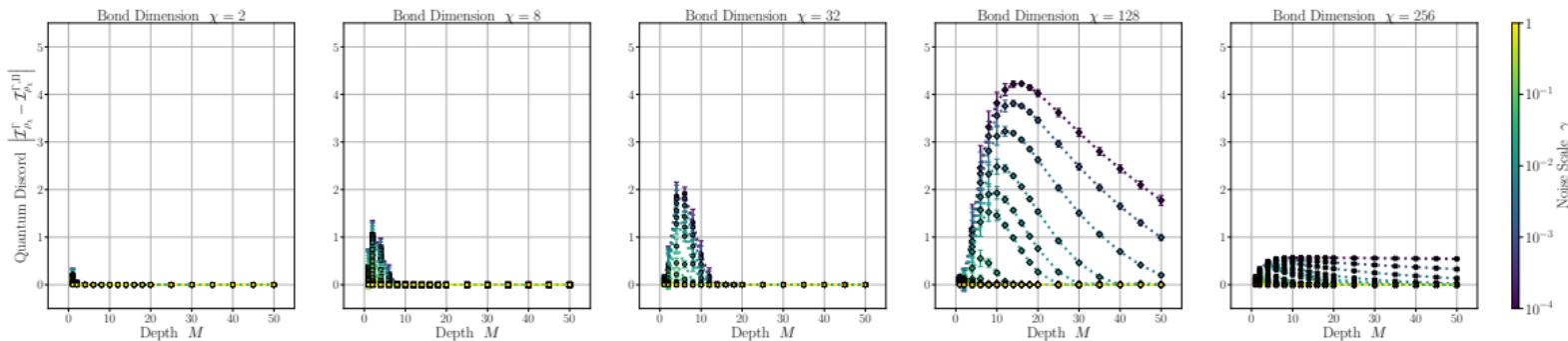
$$\mathcal{L}_{\rho_\chi \rho} \in \{\text{tr}(\sqrt{\rho \rho_\chi}) \ , \ \sqrt{p} \cdot \sqrt{p_\chi} \ , \ \text{tr}(\rho \rho_\chi)\} \quad , \quad \mathcal{S}_{\rho_\chi}^A$$

POVM-MPS Operator Entanglement



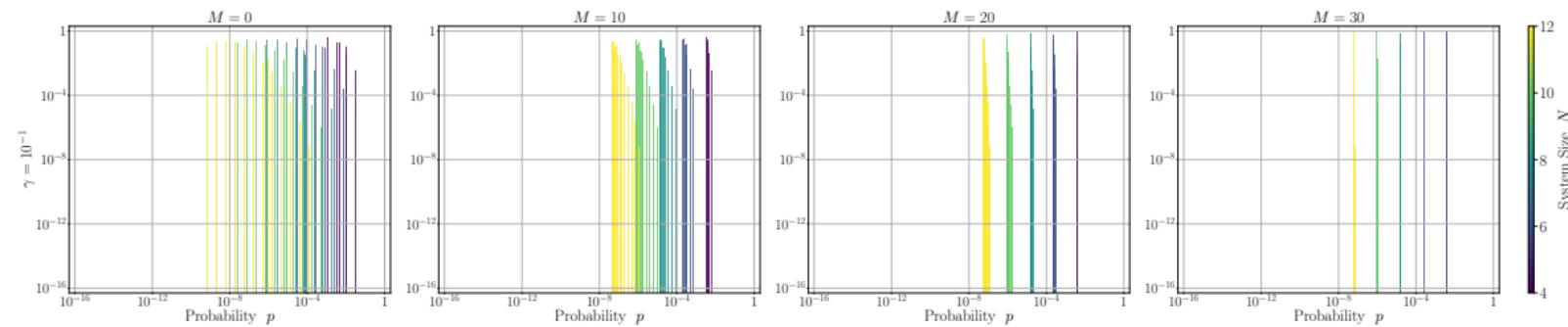
(a) Quantum Operator Entanglement of SVD-POVM-MPS ρ_χ for $N = 8$ qubits.

POVM-MPS Quantum Discord



(b) Quantum Discord of SVD-POVM-MPS ρ_χ for $N = 8$ qubits.

Distribution of POVM-MPS Probabilities



(c) POVM Probability Counts of Exact POVM-MPS ρ for N qubits.

Advantages and Disadvantages of POVM-MPS

- Pro: Dynamics are represented as single *matrix multiplications*
- Con: Channels must be converted to matrices at runtime
 - i.e) Single qubit channels are "free" - No increase in bond dimension χ

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Are physical mixed states *always* inherently harder to simulate *precisely*?

Appendix

Benchmarks for Noisy Quantum Simulations

Accuracy of simulations is characterized by *infidelity* and *entanglement*

Infidelity: Similarity of states $\rho \approx \sigma$ or distributions $p \approx s$

- Quantum

$$\mathcal{L}_{\rho\sigma}^Q = 1 - \text{tr}(\sqrt{\rho\sigma}) \quad (1)$$

- Classical

$$\mathcal{L}_{\rho\sigma}^C = 1 - \sqrt{p} \cdot \sqrt{s} \quad (2)$$

- Pure

$$\mathcal{L}_{\rho\sigma}^P = 1 - \sqrt{\text{tr}(\rho\sigma)} \quad (3)$$

Benchmarks for Noisy Quantum Simulations

Accuracy of simulations is characterized by *infidelity* and *entanglement*

Entanglement: Entropy of states $\rho_{\mathcal{A}} = \text{tr}_{\mathcal{B}}(\rho)$, $p_{\mathcal{A}} = \sum_{\mathcal{B}} p$, for partitions \mathcal{A}

- Quantum

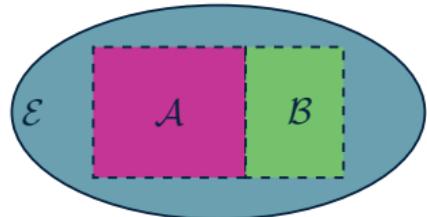
$$\mathcal{S}_{\rho}^{Q\mathcal{A}} = -\text{tr}(\rho_{\mathcal{A}} \log \rho_{\mathcal{A}}) \quad (4)$$

- Classical

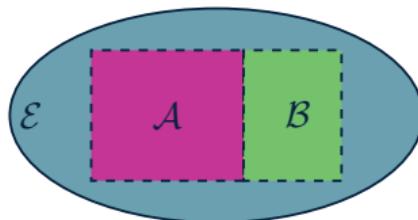
$$\mathcal{S}_{\rho}^{C\mathcal{A}} = -p_{\mathcal{A}} \cdot \log p_{\mathcal{A}} \quad (5)$$

- Renyi

$$\mathcal{S}_{\rho}^{R\mathcal{A}} = 1 - \text{tr}(\rho_{\mathcal{A}}^2) \quad (6)$$



State versus Operator Entanglement



- *State Entanglement*

$$\rho \rightarrow \rho_{\mathcal{A}} \rightarrow S_{\rho}^{\mathcal{A}} = -\text{tr}(\rho_{\mathcal{A}} \log \rho_{\mathcal{A}}) \quad (7)$$

- Captures entropy of reduced state within \mathcal{A} , which can be due to correlations with *any* other partition (\mathcal{B} , environment, ancilla etc.)

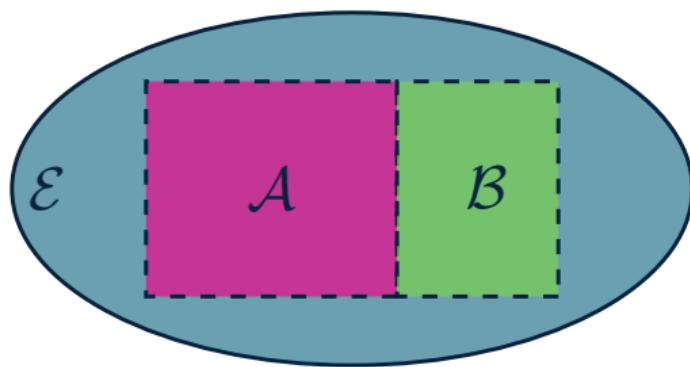
i.e) Maximum entanglement of \mathcal{A} with environment

→ Maximally mixed $\rho_{\mathcal{A}} = I$, even if no correlations with \mathcal{B}

→ Maximum state entanglement $S_{\rho}^{\mathcal{A}} = \log d_{\mathcal{A}}$, even though classical

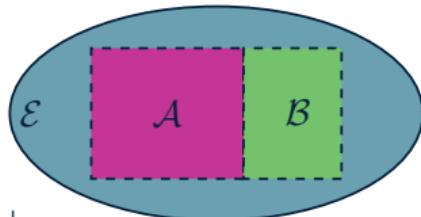
State versus Operator Entanglement

- What if we just want to capture correlations *strictly* between \mathcal{A}, \mathcal{B} ?



State versus Operator Entanglement

- *Operator Entanglement*



$$\rho \rightarrow |\rho\rangle\langle\rho| = \rho \otimes I|\Omega\rangle \rightarrow \Psi_\rho = \frac{|\rho\rangle\langle\rho|}{\langle\langle\rho|\rho\rangle\rangle} \rightarrow \Psi_{\rho_{\mathcal{A}}} \quad (8)$$

$$Q_\rho^{\mathcal{A}} = S_{\Psi_\rho}^{\mathcal{A}} = S_{|\rho\rangle\langle\rho|}^{\mathcal{A}} = -\text{tr}(\Psi_{\rho_{\mathcal{A}}} \log \Psi_{\rho_{\mathcal{A}}}) \quad (9)$$

- Captures entropy of reduced vectorized states within \mathcal{A}

i.e) Pure States: $|\psi\rangle \rightarrow |\psi\rangle\langle\psi| \rightarrow |\psi\psi\rangle \rightarrow |\psi\psi\rangle\langle\psi\psi|$

i.e) Mixed States: $\sum_\lambda p_\lambda \rho_\lambda \rightarrow \sum_\lambda p_\lambda |\rho_\lambda\rangle\langle\rho_\lambda| \rightarrow \sum_{\lambda\kappa} p_\lambda p_\kappa |\rho_\lambda\rangle\langle\rho_\kappa|$

State versus Operator Entanglement

- Pure states: $\rho = |\psi\rangle\langle\psi| \rightarrow |\rho\rangle\rangle = |\psi\psi\rangle \rightarrow \Psi_\rho = \rho \otimes \rho$

$$\mathcal{Q}_{|\psi\rangle}^{\mathcal{A}} = 2\mathcal{S}_{|\psi\rangle}^{\mathcal{A}} \quad (10)$$

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- Maximum entanglement with environment:

$$\rho = I_{\mathcal{A}} \otimes \rho_{\mathcal{B}} \rightarrow \Psi_\rho = |\Omega_{\mathcal{A}}\rangle\langle\Omega_{\mathcal{A}}| \otimes \Psi_{\mathcal{B}}$$

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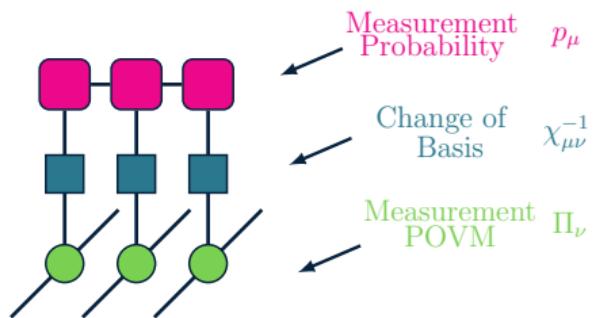
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- Local operations: $\rho = \sum_{\lambda} p_{\lambda} \rho_{\lambda_{\mathcal{A}}} \otimes \rho_{\lambda_{\mathcal{B}}} \rightarrow \Psi_\rho = \sum_{\lambda_{\kappa}} p_{\lambda} p_{\kappa} |\rho_{\lambda_{\mathcal{A}}}\rangle\rangle\langle\langle\rho_{\kappa_{\mathcal{A}}}| \otimes |\rho_{\lambda_{\mathcal{B}}}\rangle\rangle\langle\langle\rho_{\kappa_{\mathcal{B}}}|$

$$\mathcal{Q}_{\sum_{\lambda} p_{\lambda} \rho_{\lambda_{\mathcal{A}}} \otimes \rho_{\lambda_{\mathcal{B}}}}^{\mathcal{A}} \geq 0 \quad (14)$$

POVM-MPS for Quantum Simulations

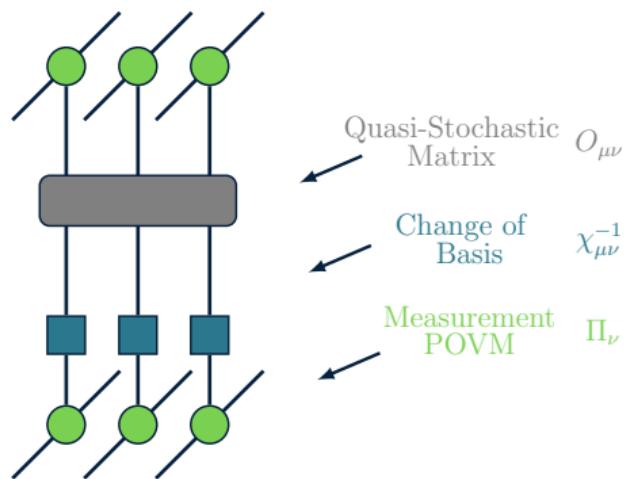
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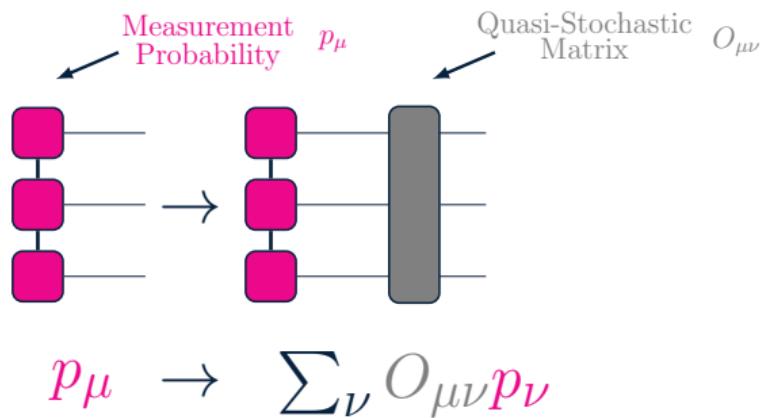
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$$\Lambda_{\sigma\sigma' \pi\pi'} = \sum_{\mu\nu \eta\kappa} O_{\mu\nu} \chi_{\mu\eta}^{-1} \Pi_{\eta\sigma\sigma'} \Pi_{\nu\pi\pi'}$$

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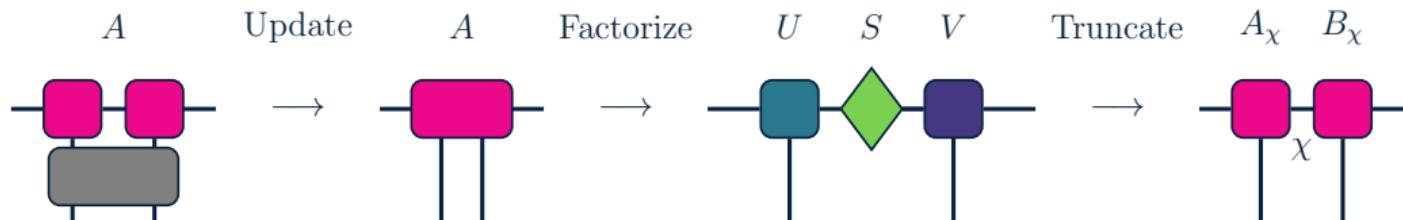
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Tensor Factorizations and Truncations

Factorize tensors $A_{\sigma\pi\alpha\beta}$  , via decompositions/conditional-independence

Truncate virtual bonds to dimension $\chi \ll O(D^N)$



Retain largest singular-values/probabilities $S_\chi = \{\lambda_\alpha : \alpha < \chi\}$, with error [4]

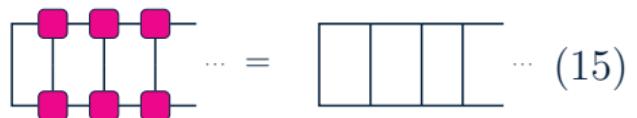
$$\epsilon_\chi^2 = 1 - \sum_{\alpha < \chi} \lambda_\alpha^2 \quad , \quad \epsilon_\chi = 1 - \sum_{\alpha < \chi} \lambda_\alpha . \quad (15)$$

Tensor Factorizations and Truncations

- Tensor Network States

- i.e) MPS: Amplitudes - Singular Value Decomposition (SVD)

$$\psi_\sigma = \prod_i A_{\sigma_i} \quad : \quad |\psi|^2 = \sum_\sigma |\psi_\sigma|^2 = 1$$



- Tensor Network Probabilities

- i.e) pMPS: Probabilities - Non-Negative Matrix Factorization (NMF)

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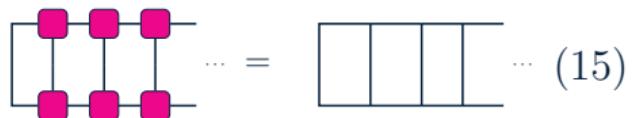


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Tensor SVD versus NMF Updates

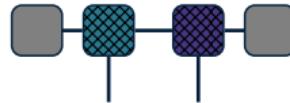
- SVD algorithms $A \rightarrow USV : 0 \leq A, U, V \leq 1$



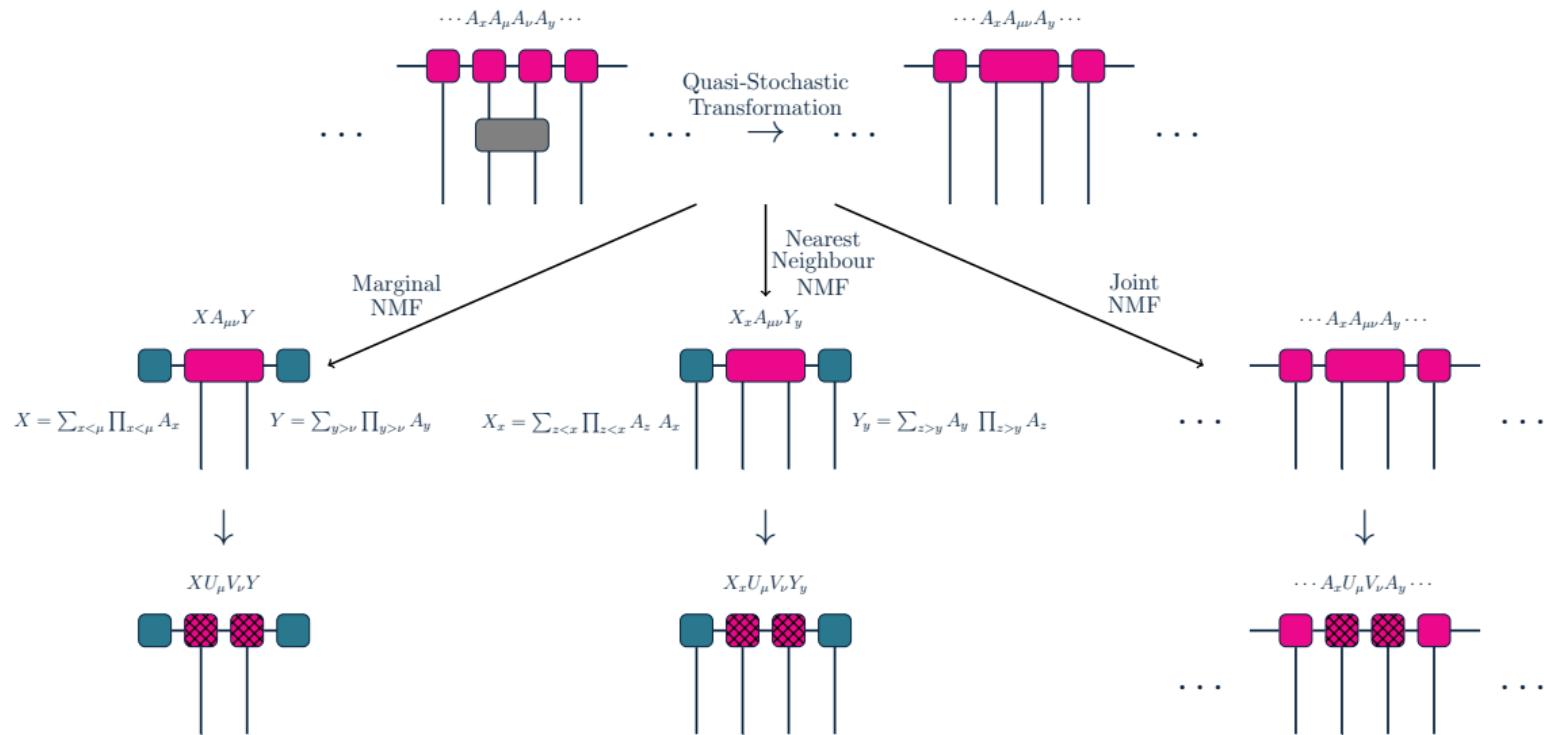
- i.e) *Boundaries* may be arbitrary
- i.e) *Closed forms, Convergence guarantees, Local unitary gauge freedom* [6]
- i.e) Power methods, or Arnoldi or Krylov iterations

Tensor SVD versus NMF Updates

- SVD algorithms $A \rightarrow USV : 0 \not\leq A, U, V \not\leq 1$
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 - i.e) *Closed forms, Convergence guarantees, Local unitary gauge freedom*
 - i.e) Power methods, or Arnoldi or Krylov iterations
- NMF algorithms $A \rightarrow UV : 0 \leq A, U, V \leq 1$
 - i.e) *Boundaries* must enforce non-negativity
 - i.e) *No closed forms, No convergence guarantees, Inverse gauge freedom [7]*
 - i.e) Multiplicative updates, Alternating least squares, Gradient methods



Tensor SVD versus NMF Updates



Tensor SVD versus NMF Updates

$$A = A_{x\mu\nu y} = X_{x\alpha} Z_{\alpha\mu\nu\beta} Y_{\beta z} \approx X_{x\alpha} U_{\alpha\mu\gamma} V_{\gamma\nu\beta} Y_{\beta z} + E_{x\mu\nu y} = XUVY + E$$

Frobenius Norm - Multiplicative Updates

$$\|A - XUVY\| \rightarrow \begin{cases} U \rightarrow \frac{A \cdot X V Y}{X U V Y \cdot X V Y} \odot U \\ V \rightarrow \frac{A \cdot X U Y}{X U V Y \cdot X U Y} \odot V \end{cases} \quad (17)$$

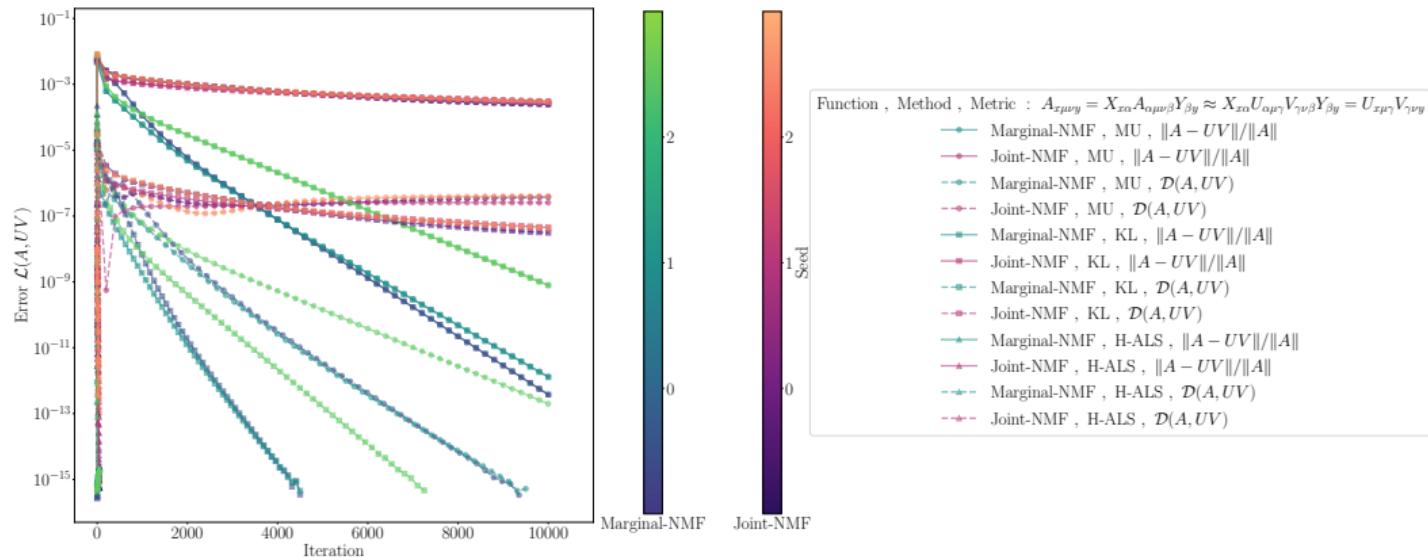
KL Divergence - Multiplicative Updates

$$-A \cdot \log \frac{XUVY}{A} \rightarrow \begin{cases} U \rightarrow \frac{\frac{A}{U V} \cdot V}{\frac{1}{U} \cdot V} \odot U \\ V \rightarrow \frac{\frac{A}{U V} \cdot U}{\frac{1}{V} \cdot U} \odot V \end{cases} \quad (18)$$

Least Squares - Local Updates

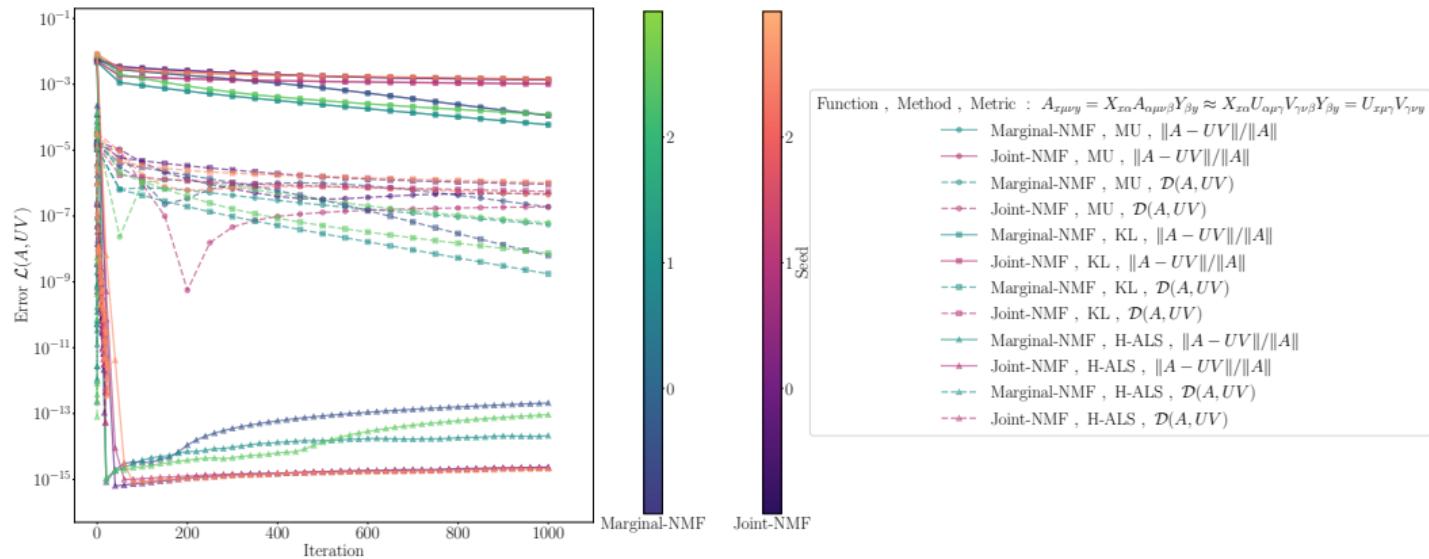
$$\|A - XUVY + X_i U_i V_i Y_i - X_i U_i V_i Y_i\| \rightarrow \begin{cases} U_i \rightarrow \left[\frac{E_i \cdot X_i V_i Y_i}{X_i V_i Y_i \cdot X_i V_i Y_i} \right]_{+\epsilon} \\ V_i \rightarrow \left[\frac{E_i \cdot X_i U_i Y_i}{X_i U_i Y_i \cdot X_i U_i Y_i} \right]_{+\epsilon} \end{cases} \quad (19)$$

Tensor SVD versus NMF Updates



- (d) NMF Convergence for Multiplicative, and Hierarchical Least Squares Updates, for Random Tensor Trains of size $D^{N-2} \times D^2 \times D^N$, for $D = 2$, $N = 6$.

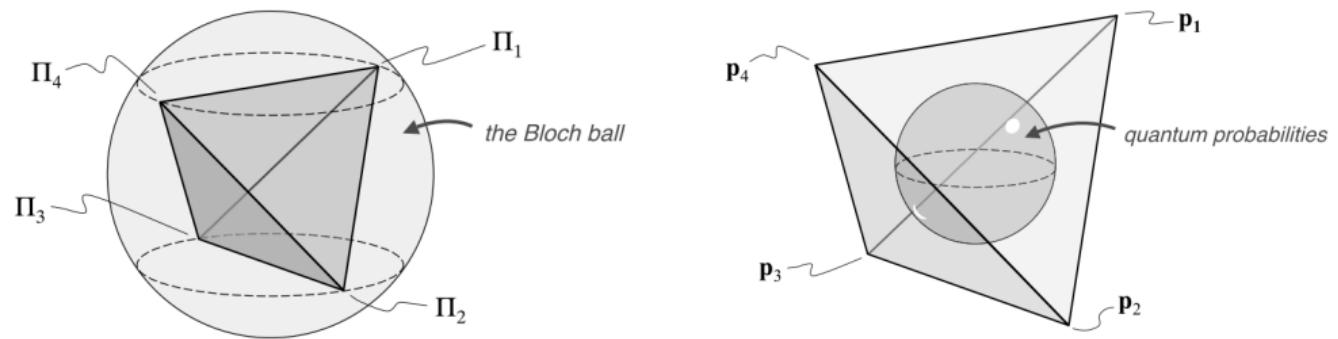
Tensor SVD versus NMF Updates



- (e) NMF Convergence for Multiplicative, and Hierarchical Least Squares Updates, for Random Tensor Trains of size $D^{N-2} \times D^2 \times D^N$, for $D = 2$, $N = 6$.

Quantum Probability Simplexes

Not only do POVM-MPS updates $p \rightarrow p_\chi$ have to be *non-negative*, but they must obey non-trivial quantum probability simplex *constraints* [5]



Quantum Probability Simplexes

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i.e) Symmetric POVM's: $\chi_{\mu\nu}^{-1} = \xi \delta_{\mu\nu} - 1_\mu 1_\nu$: $\xi = D(D + 1)$

$$\sum_\mu p_\mu = 1 \quad , \quad 1 \leq \xi \sum_\mu p_\mu^2 \leq 2 \quad , \quad 1 \leq \xi^2 \sum_{\mu\nu} \chi_{\mu\nu} p_\mu p_\nu p_\nu \leq 4 \quad (20)$$

i.e) Tensor Products of N SIC-POVM's: $\Pi_\mu \rightarrow \Pi_{\mu\sigma\omega\dots} = \otimes_i^N \Pi_{\mu_i}$

i.e) Quasi-stochastic transformations $O_{\mu\nu}$ are *stochastic* for *unital* channels

Quantum Probability Simplexes

Tensor Products of N SIC-POVM's: $\Pi_\mu \rightarrow \Pi_{\mu\sigma\omega\dots} = \otimes_i^N \Pi_{\mu_i}$

$N = 1 :$

$$\rho = \xi p_\mu \Pi_\mu - I$$

$$O_{\mu\nu} = \xi \langle\langle \Pi_\mu | \Lambda(\Pi_\nu) \rangle\rangle - \langle\langle \Pi_\mu | \Lambda(I) \rangle\rangle 1_\nu$$

$$1_\mu p_\mu = 1 \tag{21}$$

$$1 \leq \xi p_\mu p_\mu \leq 2$$

$$1 \leq 2\xi p_\mu p_\mu - 1 \leq \xi^2 \chi_{\mu\nu\omega} p_\mu p_\nu p_\omega \leq 3\xi p_\mu p_\mu - 2 \leq 4$$

Quantum Probability Simplexes

Tensor Products of N SIC-POVM's: $\Pi_\mu \rightarrow \Pi_{\mu\sigma\omega\dots} = \otimes_i^N \Pi_{\mu_i}$

$N = 2 :$

$$\rho = \xi^2 p_{\mu\sigma} \Pi_{\mu\sigma} - \xi p_\mu \Pi_\mu - \xi p_\sigma \Pi_\sigma + I$$

$$O_{\mu\sigma\nu\pi} = \xi^2 \langle\langle \Pi_{\mu\sigma} | \Lambda(\Pi_{\nu\pi}) \rangle\rangle - \xi \langle\langle \Pi_{\mu\sigma} | \Lambda(\Pi_\nu) \rangle\rangle 1_\pi - \xi \langle\langle \Pi_{\mu\sigma} | \Lambda(\Pi_\pi) \rangle\rangle 1_\nu + \langle\langle \Pi_{\mu\sigma} | \Lambda(I) \rangle\rangle 1_{\nu\pi}$$

$$1_{\mu\sigma} p_{\mu\sigma} = 1 \tag{22}$$

$$1 \leq \xi(p_\mu p_\mu + p_\sigma p_\sigma) - 1 \leq \xi^2 p_{\mu\sigma} p_{\mu\sigma} \leq \xi(p_\mu p_\mu + p_\sigma p_\sigma) \leq 4$$

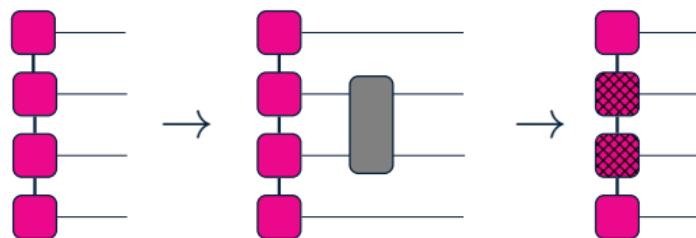
$$2 - 5\xi(p_\mu p_\mu + p_\sigma p_\sigma) \leq \xi^4 \chi_{\mu\nu\tau} \chi_{\sigma\pi\tau} p_{\mu\sigma} p_{\nu\pi} p_{\nu\tau} - 2\xi^3 (\chi_{\mu\nu\tau} p_{\mu\sigma} p_{\nu\sigma} p_\nu + \chi_{\sigma\pi\tau} p_{\mu\sigma} p_{\mu\pi} p_\tau)$$

$$5 - 6\xi(p_\mu p_\mu + p_\sigma p_\sigma) \geq$$

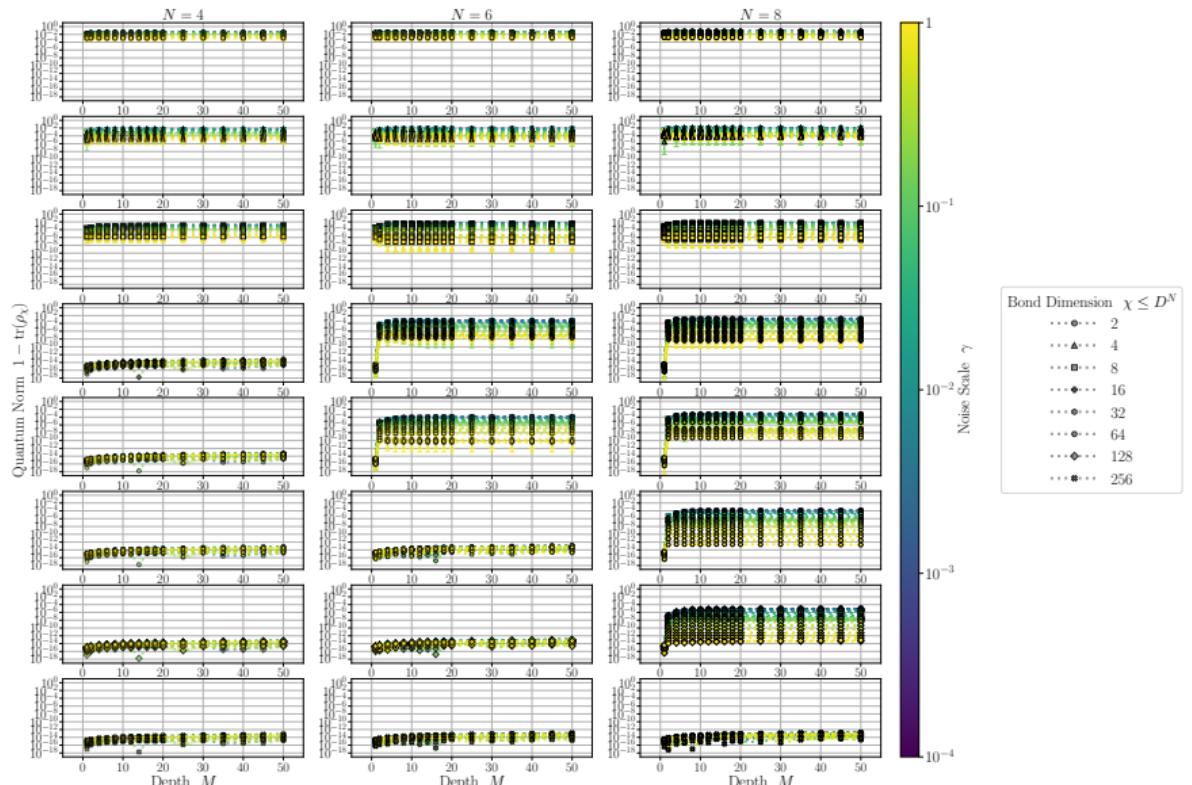
Quantum Probability Simplexes

Not only do POVM-MPS updates $p \rightarrow p_\chi$ have to be *non-negative*, but they must obey non-trivial quantum probability simplex *constraints*

What other structure does $O_{\mu\nu}$ have i.e) for 2-local unitaries
that allows for *efficient, convergent* updates?

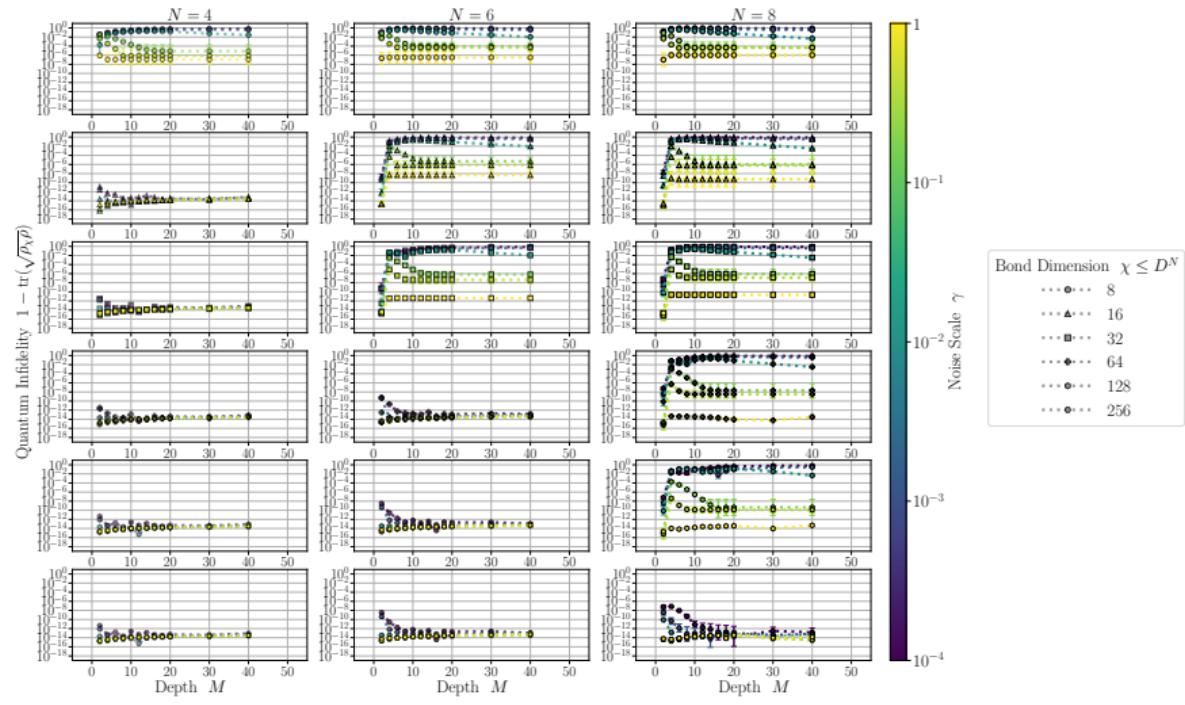


POVM-MPS Norm



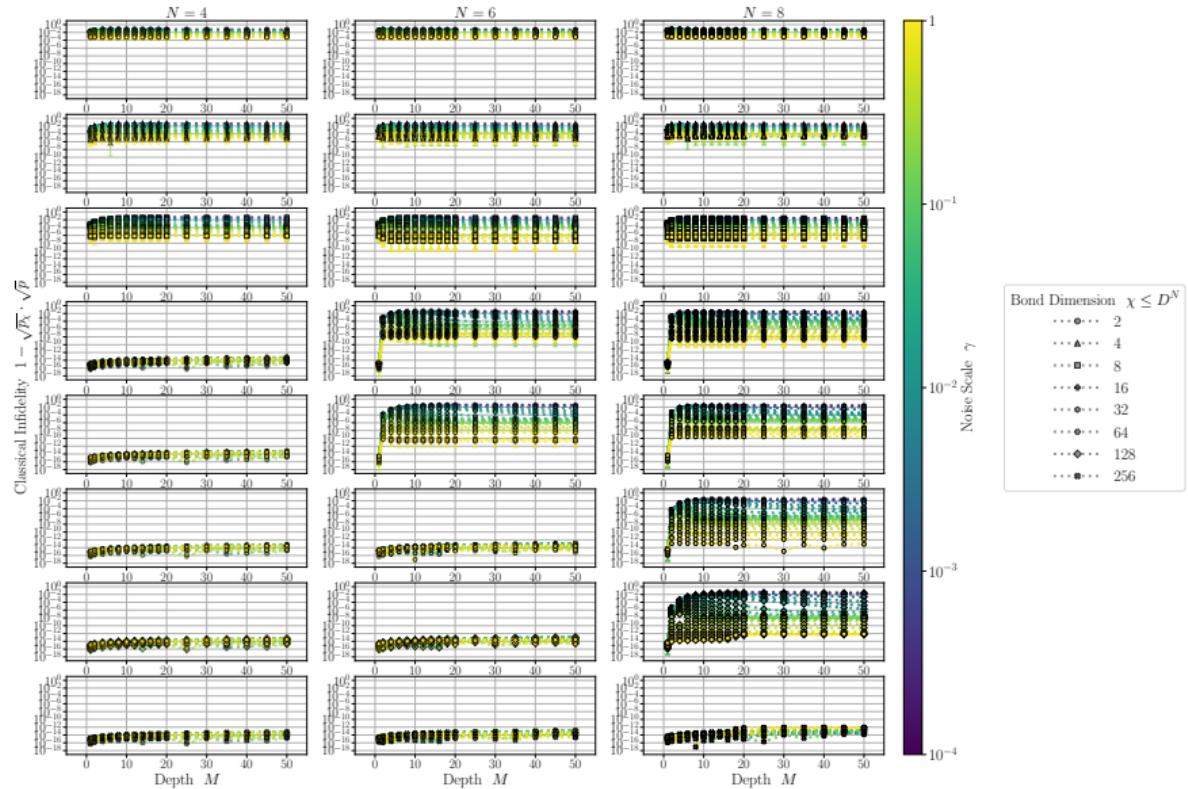
(f) Trace of SVD-POVM-MPS ρ_χ for N qubits.

POVM-MPS Infidelity

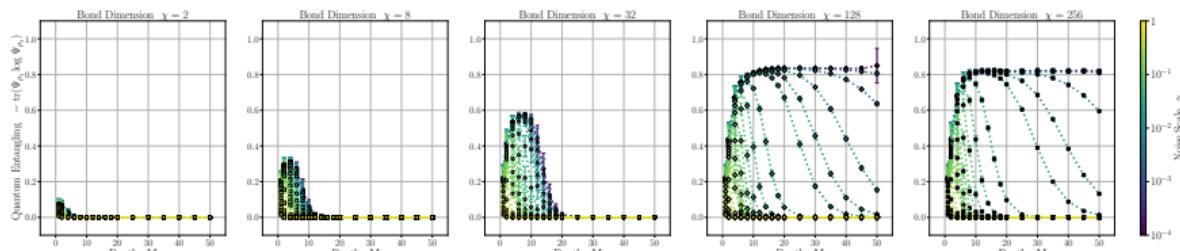


(g) Quantum Infidelity of POVM-MPS $\rho_\chi \approx \rho$ for N qubits.

POVM-MPS Infidelity

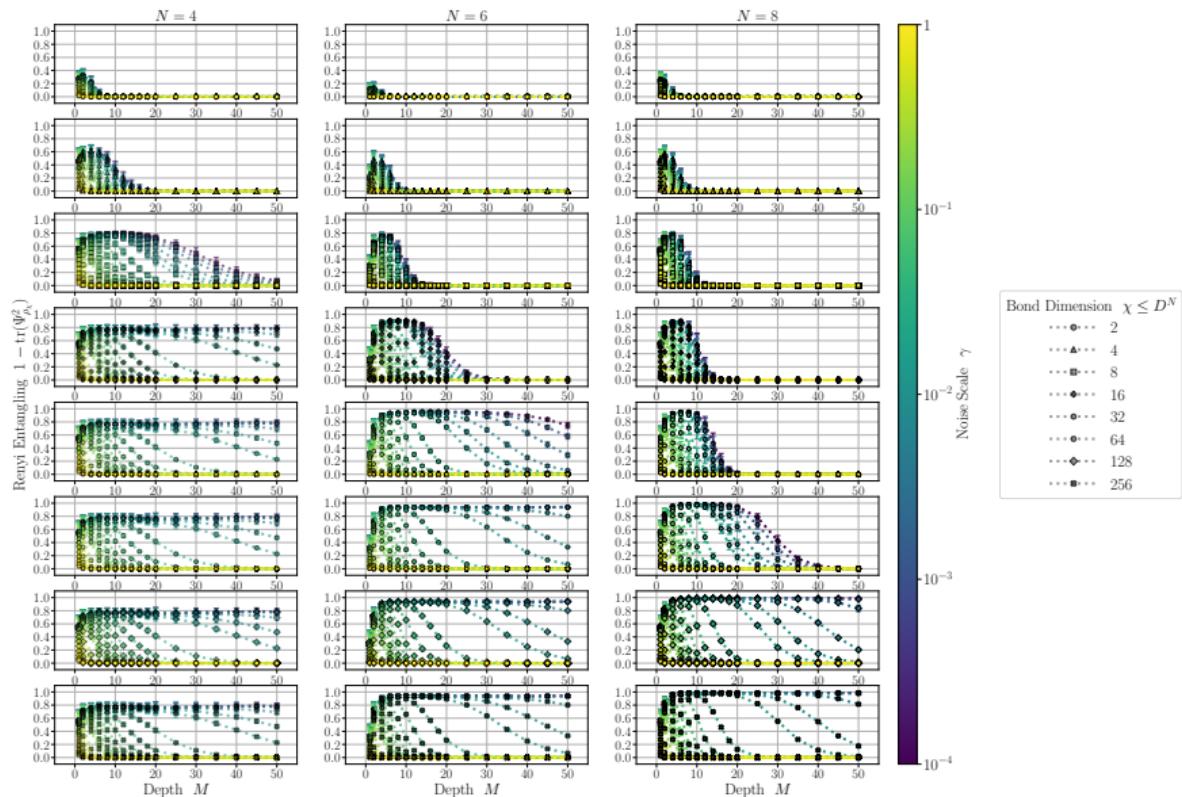


POVM-MPS Operator Entanglement



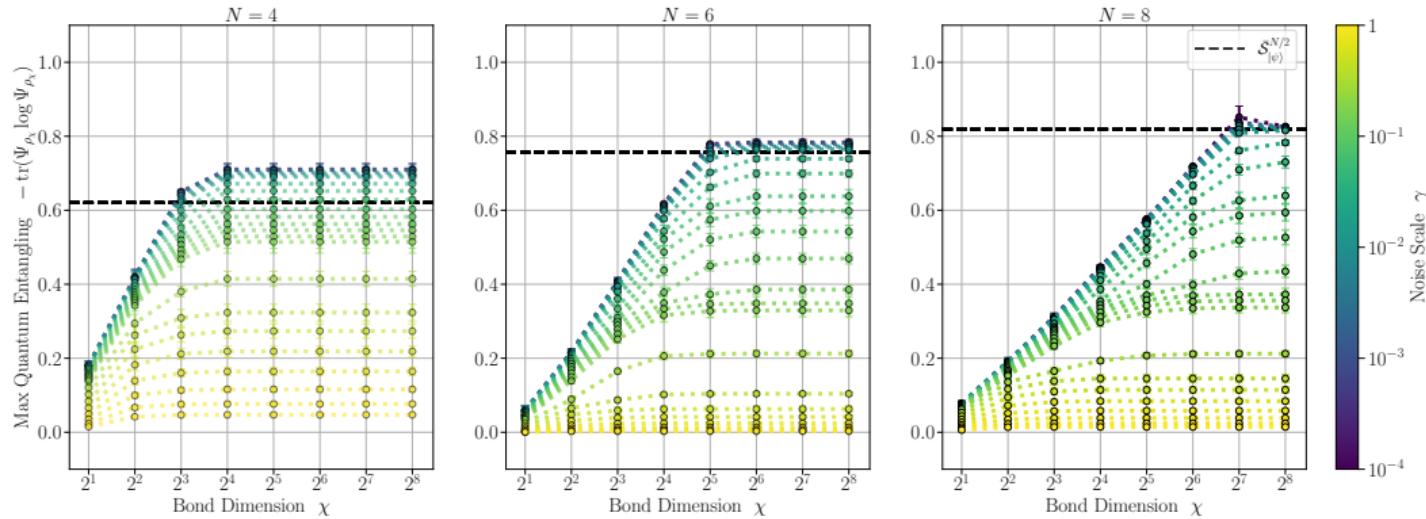
(i) Quantum Operator Entanglement of SVD-POVM-MPS ρ_χ for N qubits.

POVM-MPS Operator Entanglement



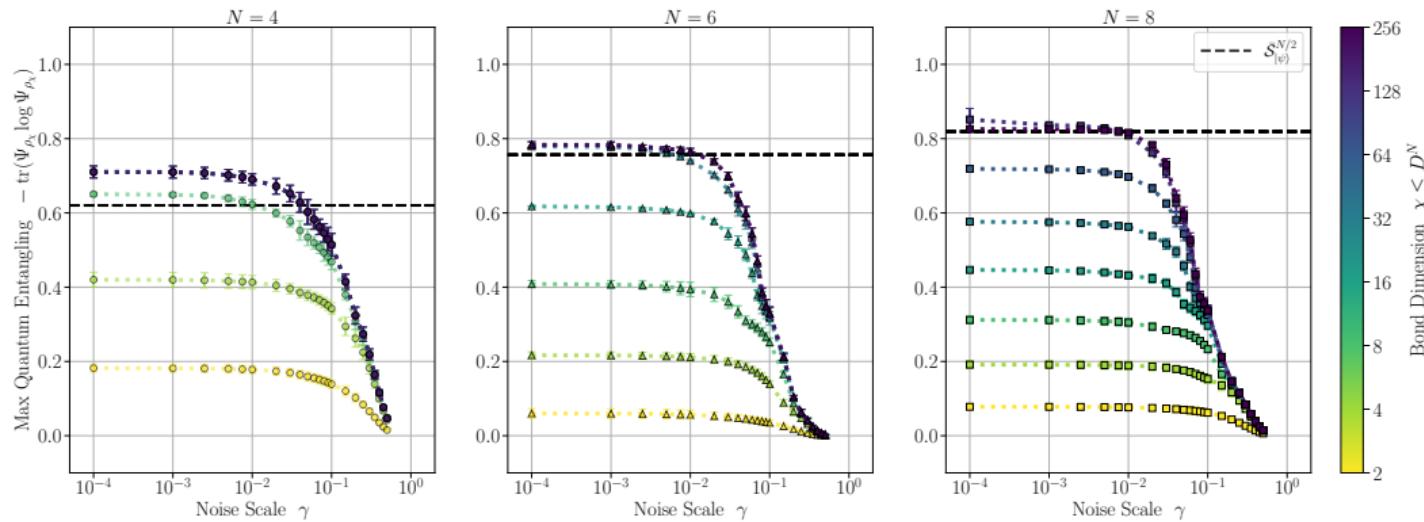
(j) Renyi Operator Entanglement of SVD-POVM-MPS ρ_χ for N qubits.

POVM-MPS Operator Entanglement Scaling



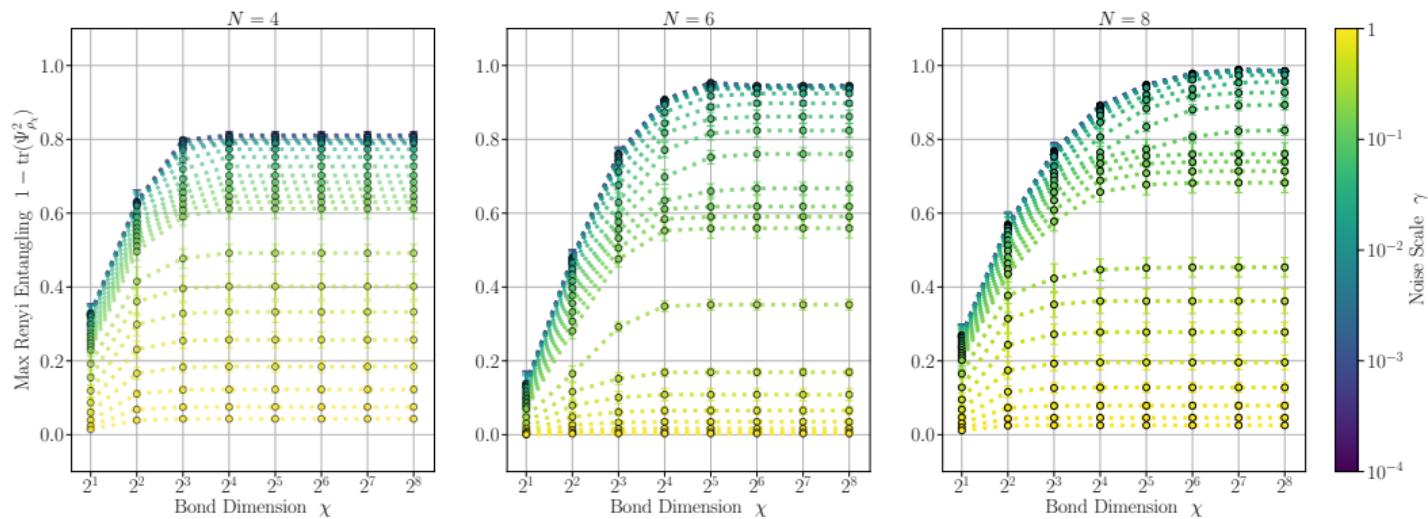
(k) Quantum Operator Entanglement of SVD-POVM-MPS ρ_χ with bond dimension χ , for N qubits.

POVM-MPS Operator Entanglement Scaling



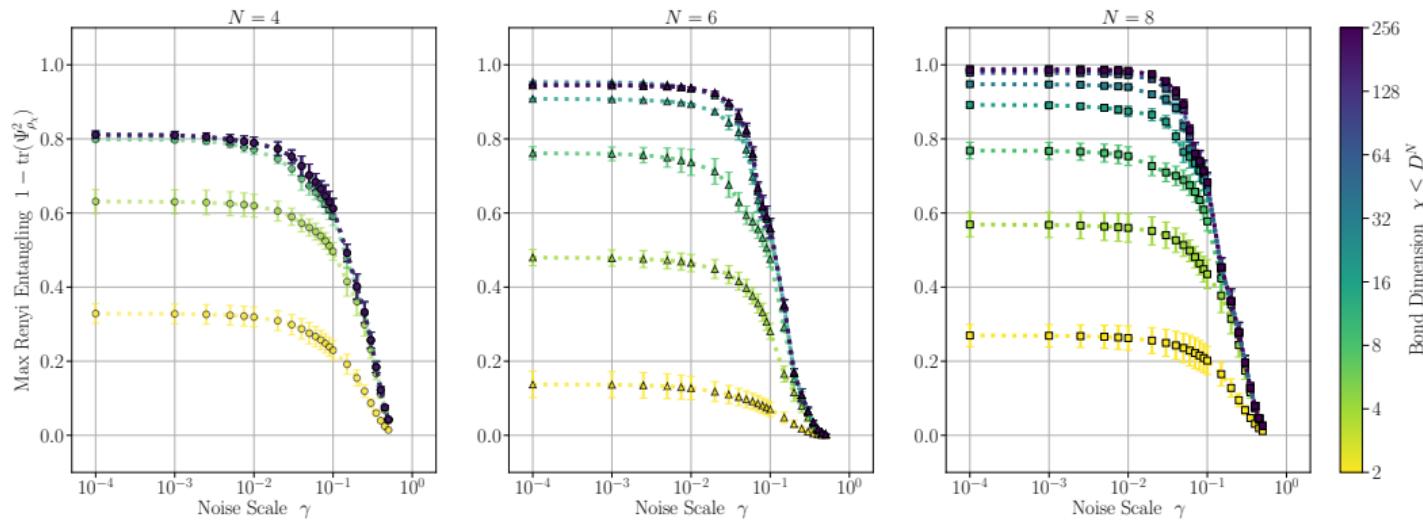
(1) Quantum Operator Entanglement of SVD-POVM-MPS ρ_χ with noise scale γ , for N qubits.

POVM-MPS Operator Entanglement Scaling



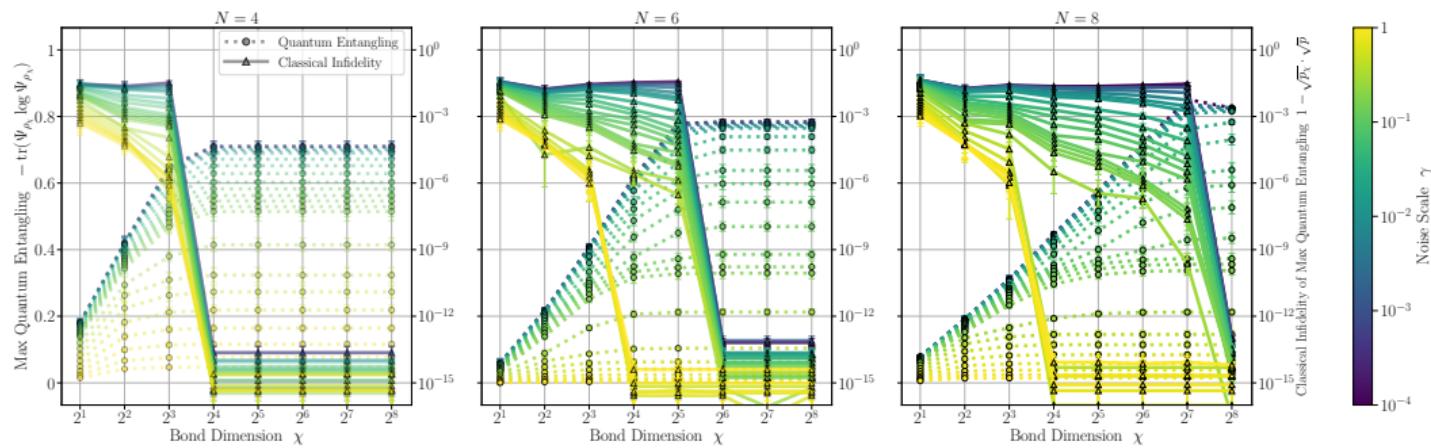
(m) Renyi Operator Entanglement of SVD-POVM-MPS ρ_χ with bond dimension χ , for N qubits.

POVM-MPS Operator Entanglement Scaling



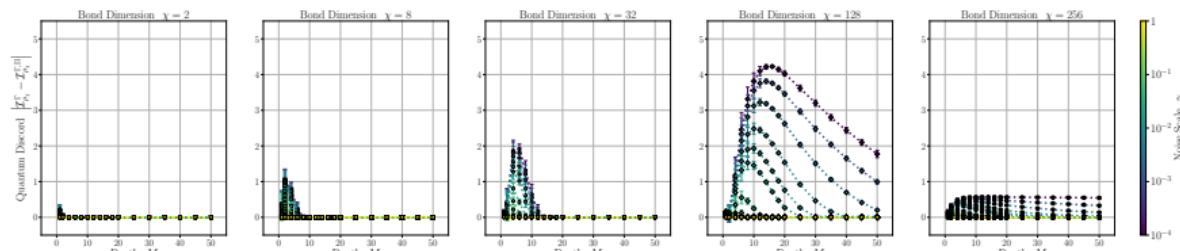
(n) Renyi Operator Entanglement of SVD-POVM-MPS ρ_χ with noise scale γ , for N qubits.

POVM-MPS Operator Entanglement Scaling



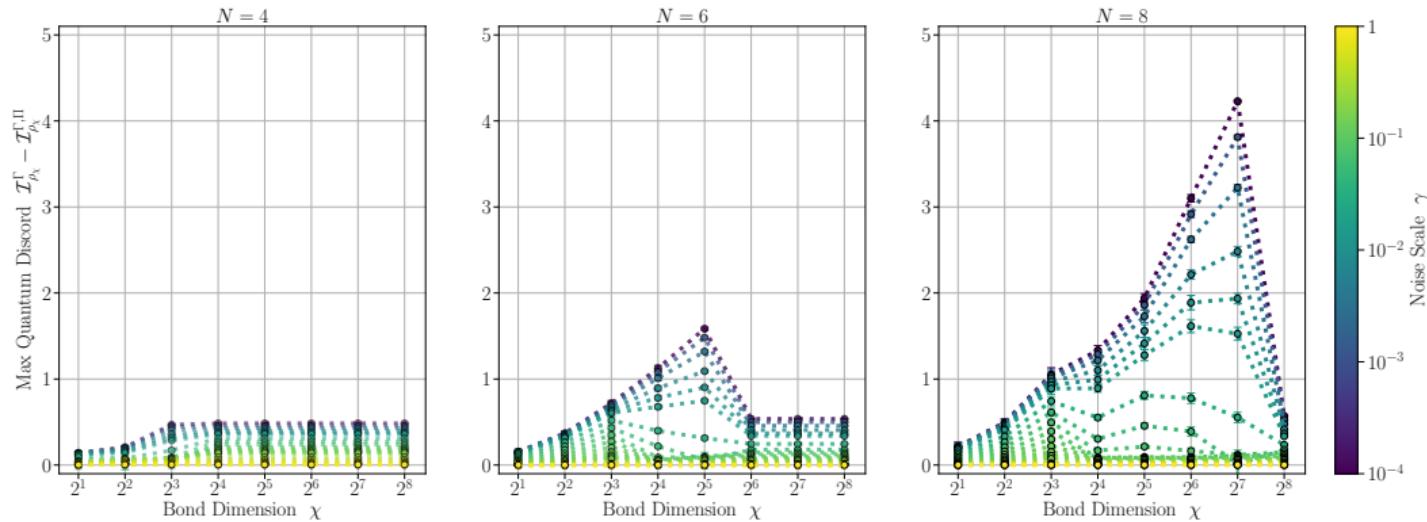
(o) Quantum Operator Entanglement and Classical Infidelity of SVD-POVM-MPS ρ_{χ} with bond dimension χ , for N qubits.

POVM-MPS Quantum Discord



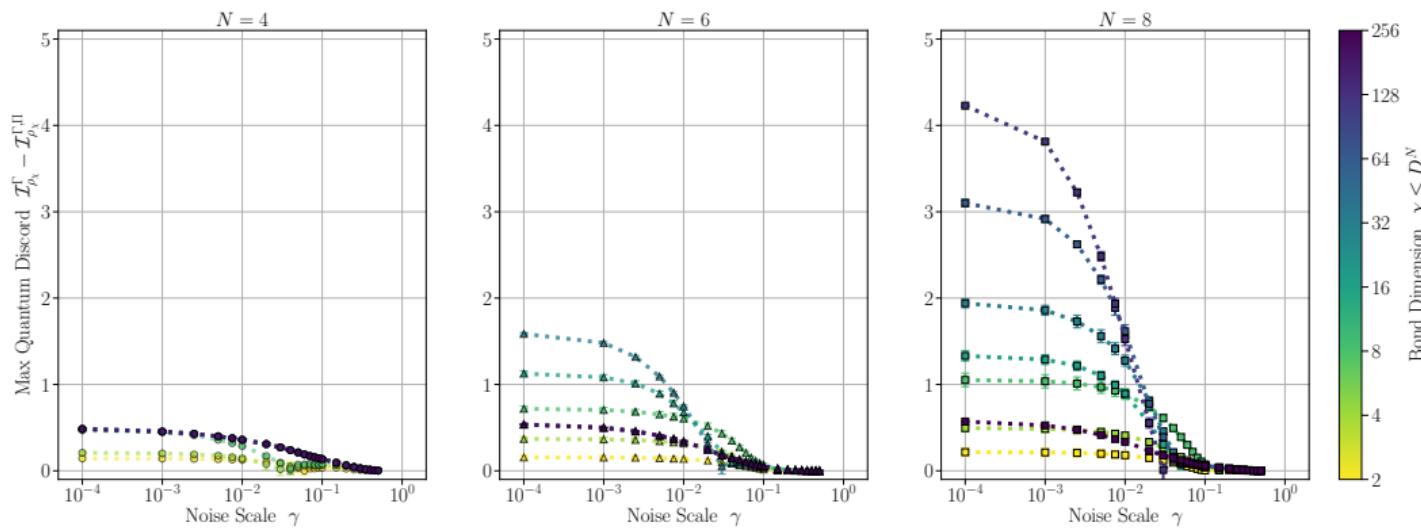
(p) Quantum Discord of SVD-POVM-MPS ρ_{χ} for N qubits.

POVM-MPS Quantum Discord Scaling



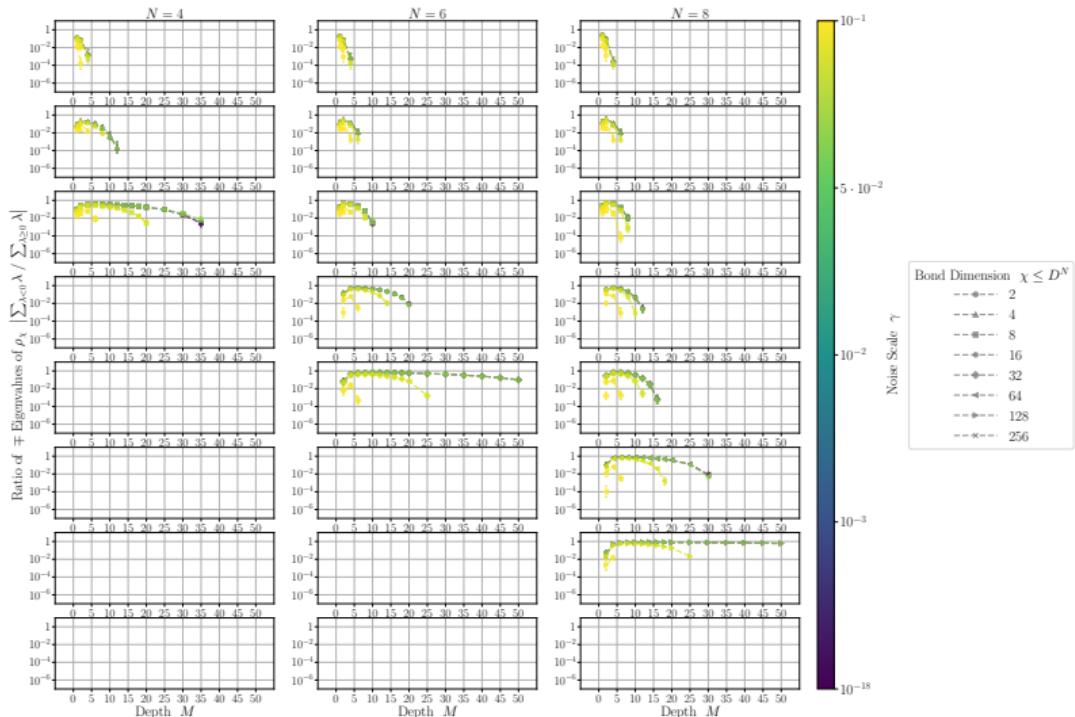
(q) Quantum Discord of SVD-POVM-MPS ρ_χ with bond dimension χ , for N qubits.

POVM-MPS Quantum Discord Scaling



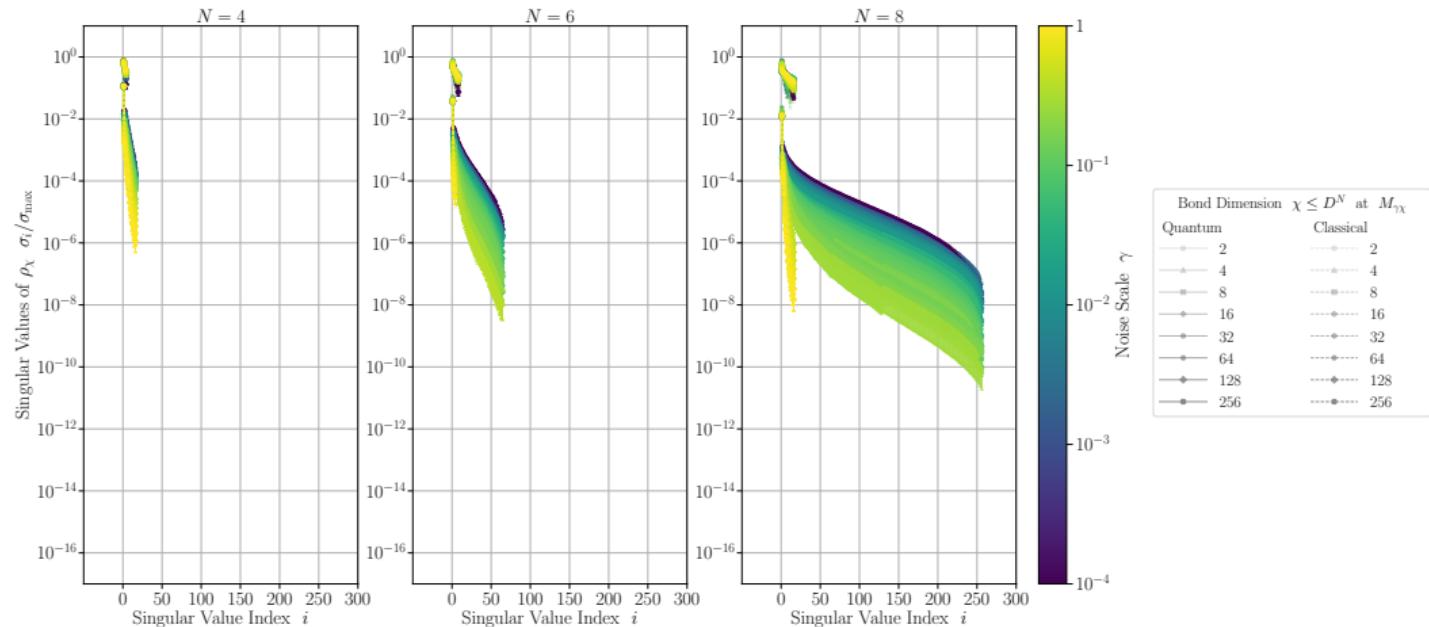
(r) Quantum Discord of SVD-POVM-MPS ρ_χ with noise scale γ , for N qubits.

POVM-MPS Quantum and Classical Spectrum Scaling



(s) Ratio of Negative/Positive Spectrum of SVD-POVM-MPS ρ_χ with noise scale γ , bond dimension χ , as a function of depth M , for N qubits.

POVM-MPS Quantum and Classical Spectrum Scaling



(t) Quantum and Classical Spectrum of SVD-POVM-MPS ρ_χ with noise scale γ , bond dimension χ , for N qubits.