Variational Approaches to Lindbladian Evolution

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Overview

1. Why? What is the need?

2. Overview of different ansatz
   Area-law/volume-law, and some lore

3. A closer look at algorithms for
   neural networks approach to Lindbladian dynamics

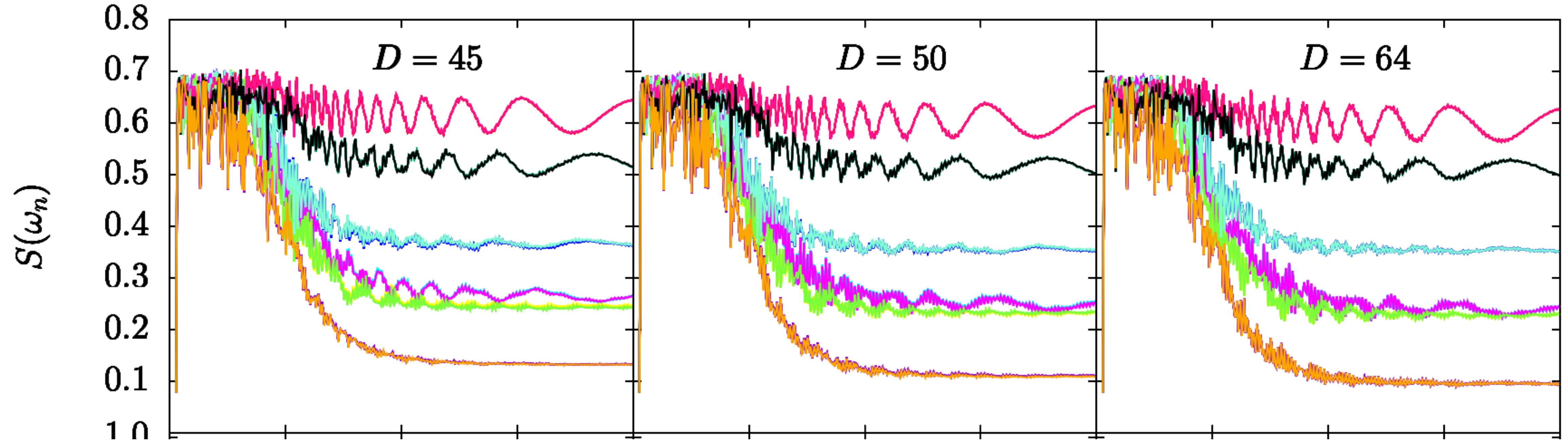
4. Investigations I've been involved in
   - Schwinger Model [JL, Di Luo, Xiaojun Yao, Phiala Shanahan, 2402.06607]
   - Caldeira-Legget (WIP w/ Tom Magorsch, Nora Brambilla, Phiala Shanahan)
   - Extensions to nonrelativistic, multiparticle (≥ 3 particle) setting?

Main problem: Hilbert Spaces can get very large, to the point that *exact* classical simulations become impossible!

Examples from this week:

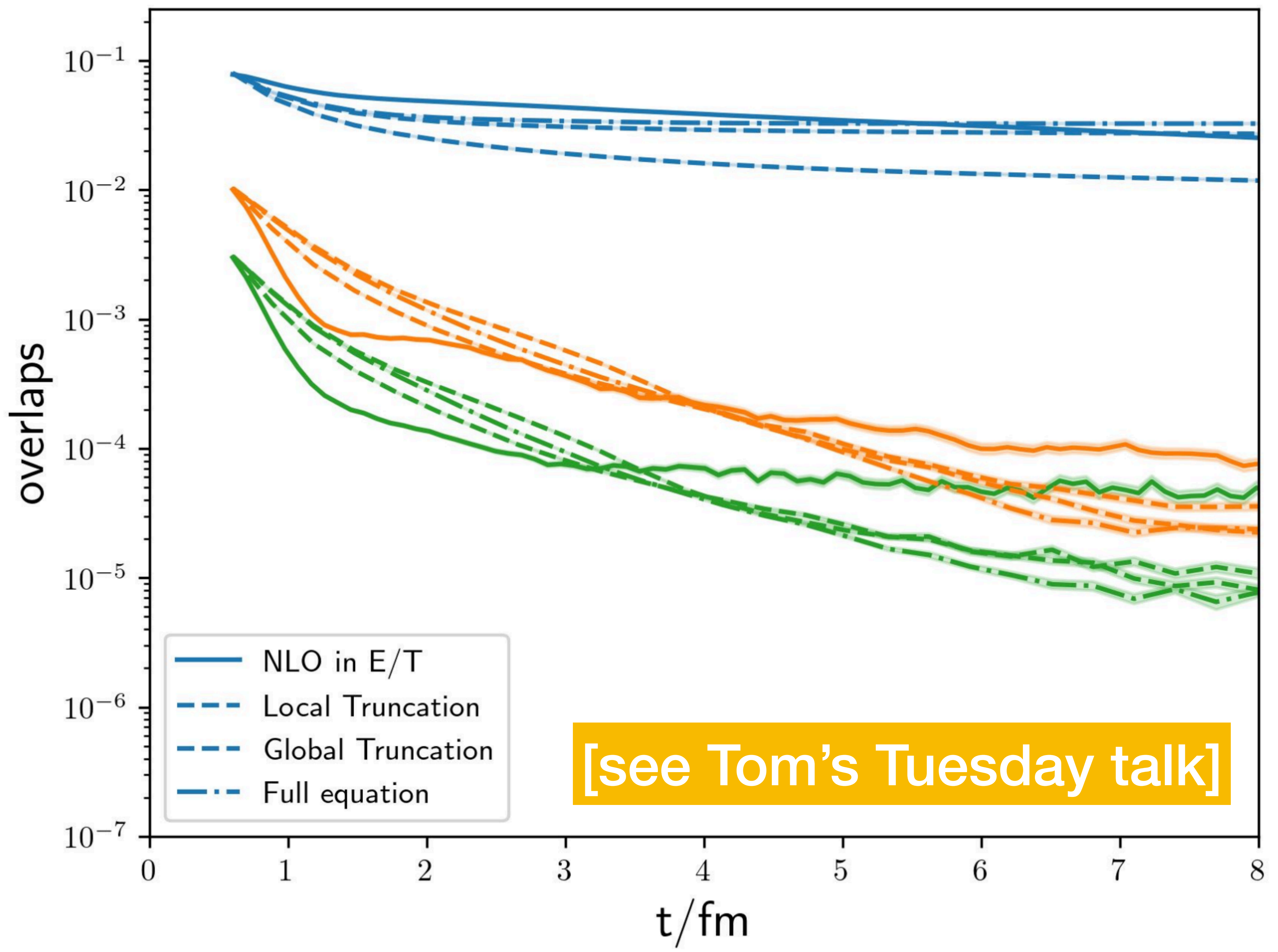
$$H(t) = -\sum_{\omega} \omega J^z_\omega + \mu(t) \sum_{\substack{\omega,\omega' \\ \omega' \neq \omega}} \vec{J}_\omega \cdot \vec{J}_{\omega'},$$

(closed system example)



(N = 12 neutrinos, MPS+TDVP)

[Michael J. Cervia, Pooja Siwach, Amol V. Patwardhan, A. B. Balantekin, S. N. Coppersmith, Calvin W. Johnson, 2022]



[Nora Brambilla, Arthur Lin, Tom Magorsch, Antonio Vairo]

(*Difficulty in this system is more associated with larger sample sizes required to deal with heavy-tailed distributions at larger system sizes, see Tom Magorsch's Tuesday talk)

Idea: find a variational map that represents density matrices with a small number of parameters

$$\psi : \mathbb{R}^N \to \mathscr{H} \qquad\qquad \rho : \mathbb{R}^N \to \mathscr{H} \otimes \mathscr{H}^*$$

(closed) (open quantum system)

[for some $N \ll \dim(\mathscr{H})$]

Original uses include ground state energy approximation:

$$\langle \psi(\alpha) | H | \psi(\alpha) \rangle \geq E_{\text{ground}}$$

Systematic uncertainties arising in real-time/lindbladian evolution are more difficult to quantify!

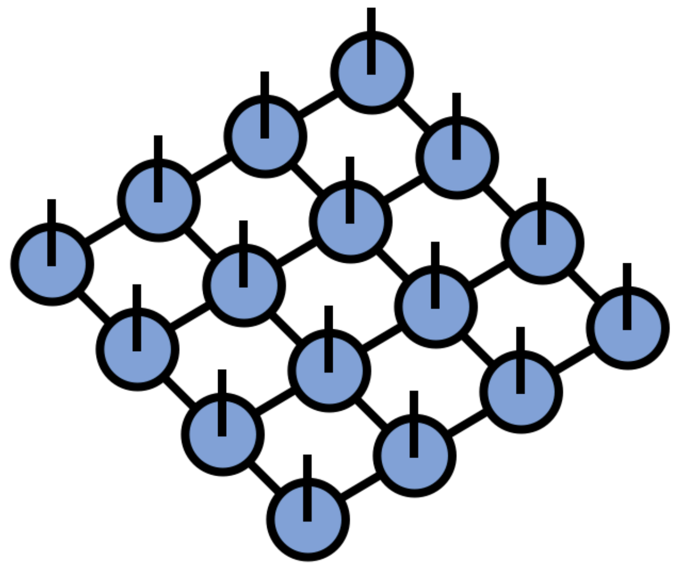
Variational Methods

"Interpretability" "Representation Power"

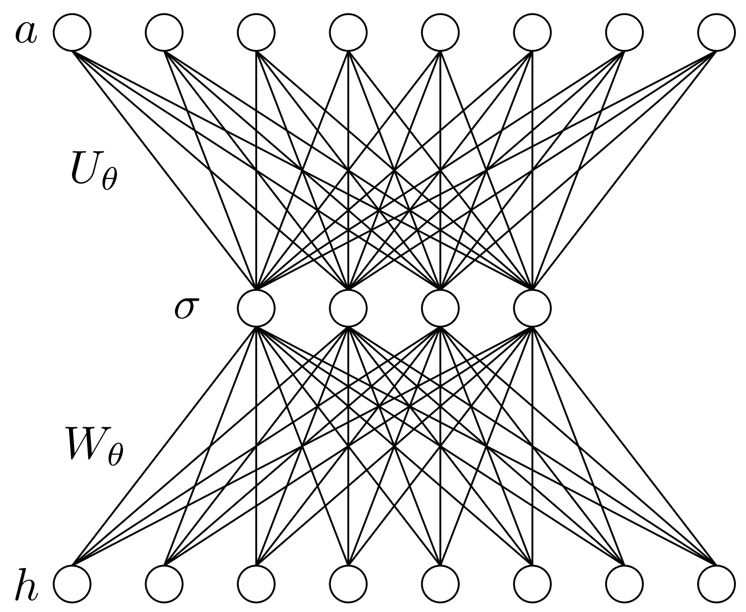
$$\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \cdots & \phi_N(\mathbf{x}_N) \end{vmatrix}$$

+correlations

Hartree-Fock



Tensor Networks

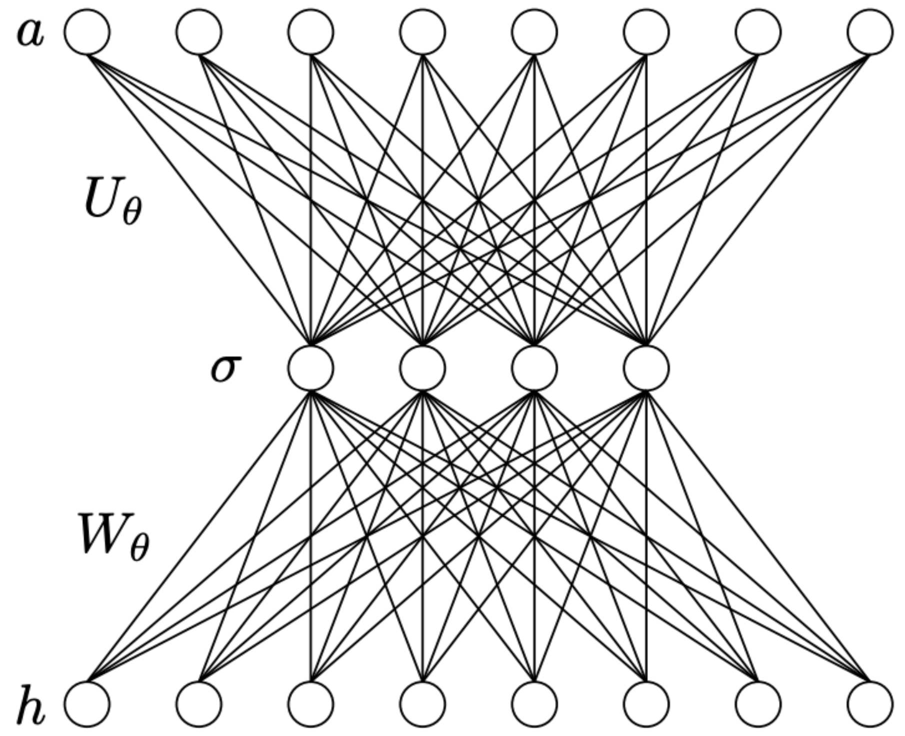


Neural Networks

- Control over systematics errors?
- Scaling of cost with system size?

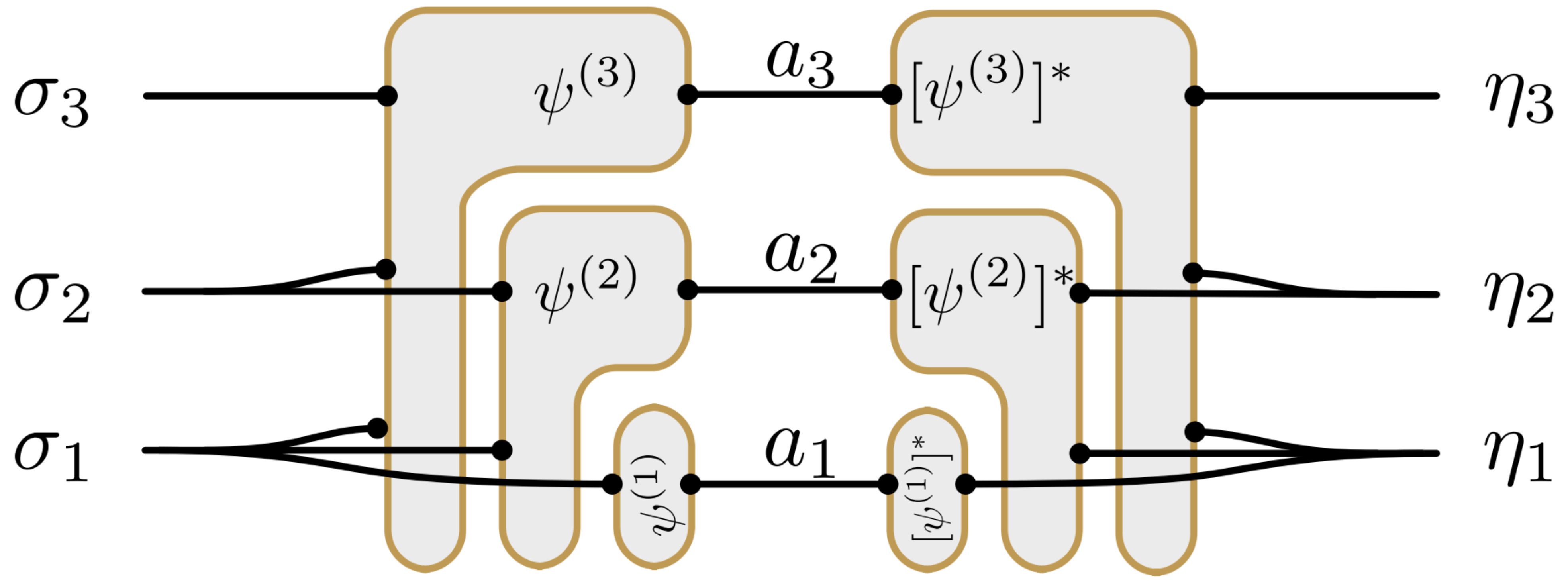
A tour of some variational approaches to Open Quantum Systems

Latent space purification



[Giacomo Torlai and Roger G. Melko 1801.09684]
[Michael J. Hartmann, Giuseppe Carleo 1902.05131]

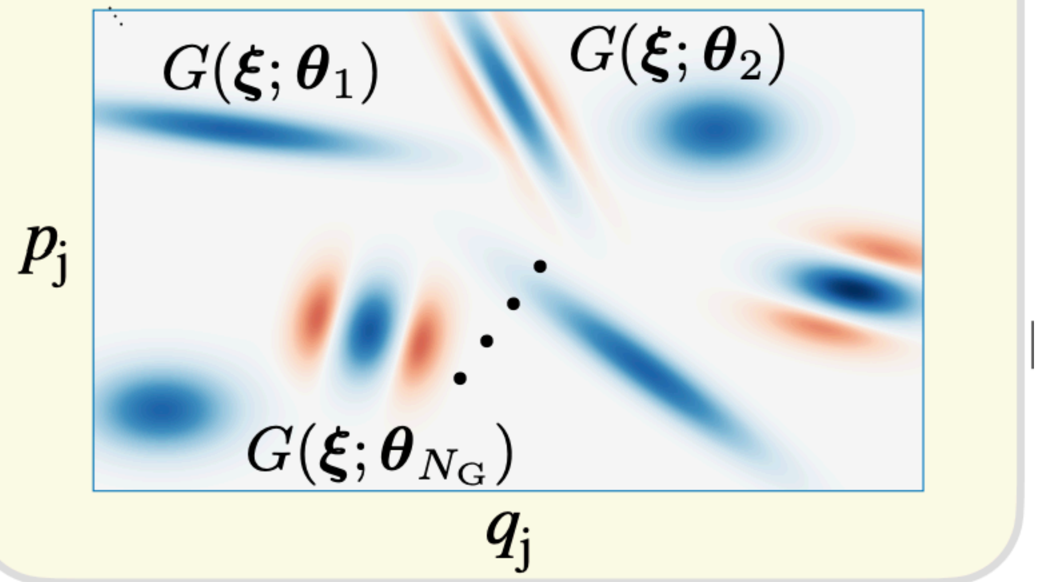
Autoregressive Gram-Hadamard Density Operator



[Filippo Vicentini, Riccardo Rossi, and Giuseppe Carleo 2206.13488]

Gaussian Ensembles

$$W_{\boldsymbol{\theta}}(\boldsymbol{\xi}) = \frac{1}{2}\left[\sum_{i=1}^{N_G} G(\boldsymbol{\xi};\boldsymbol{\theta}_i(t)) + c.c.\right]$$

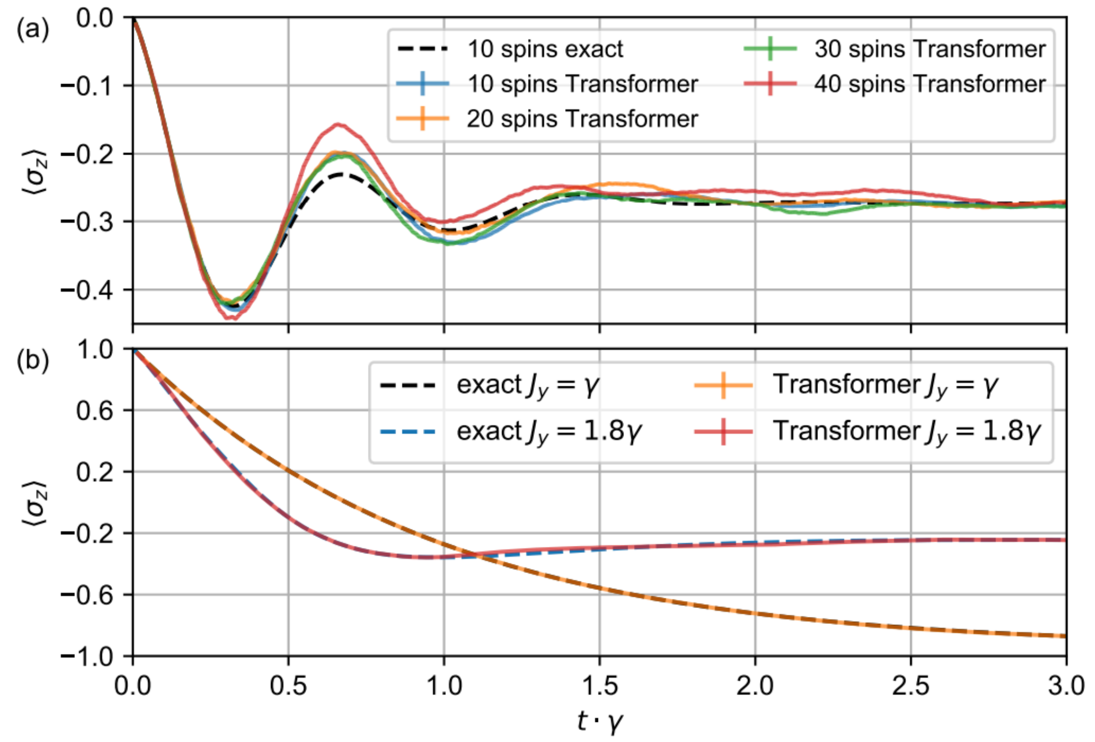


[Jacopo Tosca, Francesco Carnazza, Luca Giacomelli, and Cristiano Ciuti 2507.14076]

POVM methods

[Juan Carrasquilla, Giacomo Torlai, Roger G. Melko, Leandro Aolita, 1810.10584]

[Di Luo, Zhuo Chen, Juan Carrasquilla, and Bryan K. Clark 2009.05580]



Tensor Networks

[F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, 0406426]
[Michael Zwolak, Guifr´e Vidal, 0406440]

$$|\psi_{\text{mps}}\rangle = \sum_{s_1,\ldots,s_N=1}^{d} \mathrm{Tr}(A_1^{s_1}\ldots A_N^{s_N})|s_1,\ldots,s_N\rangle.$$

$$\downarrow$$

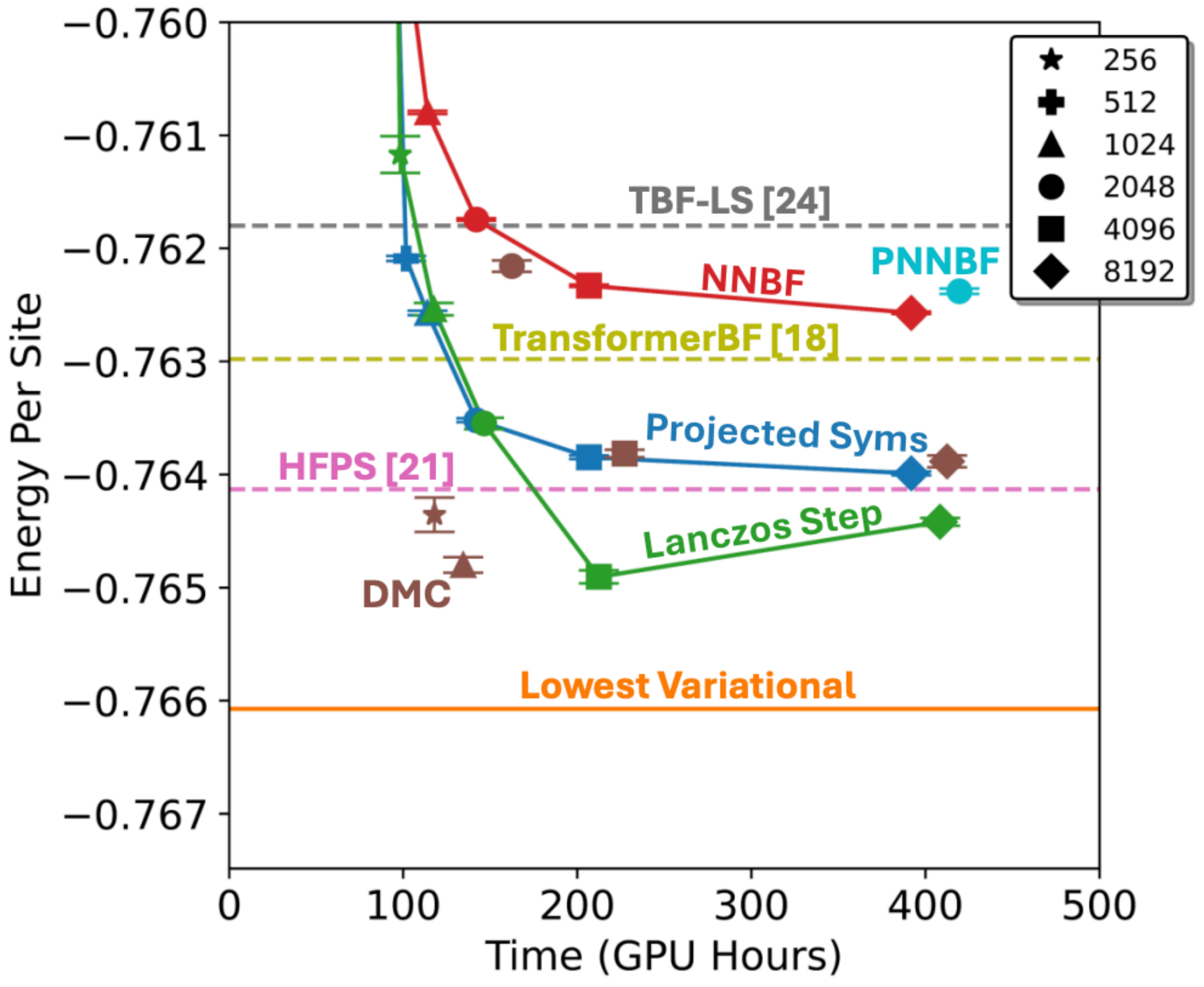
$$\rho = \sum_{s_1,s_1',\ldots,s_N,s_N'=1}^{d} \mathrm{Tr}(M_1^{s_1,s_1'}\ldots M_N^{s_N,s_N'}) \times |s_1,\ldots,s_N\rangle\langle s_1',\ldots,s_N'|,$$

and others!

Expressivity of the ansatz?

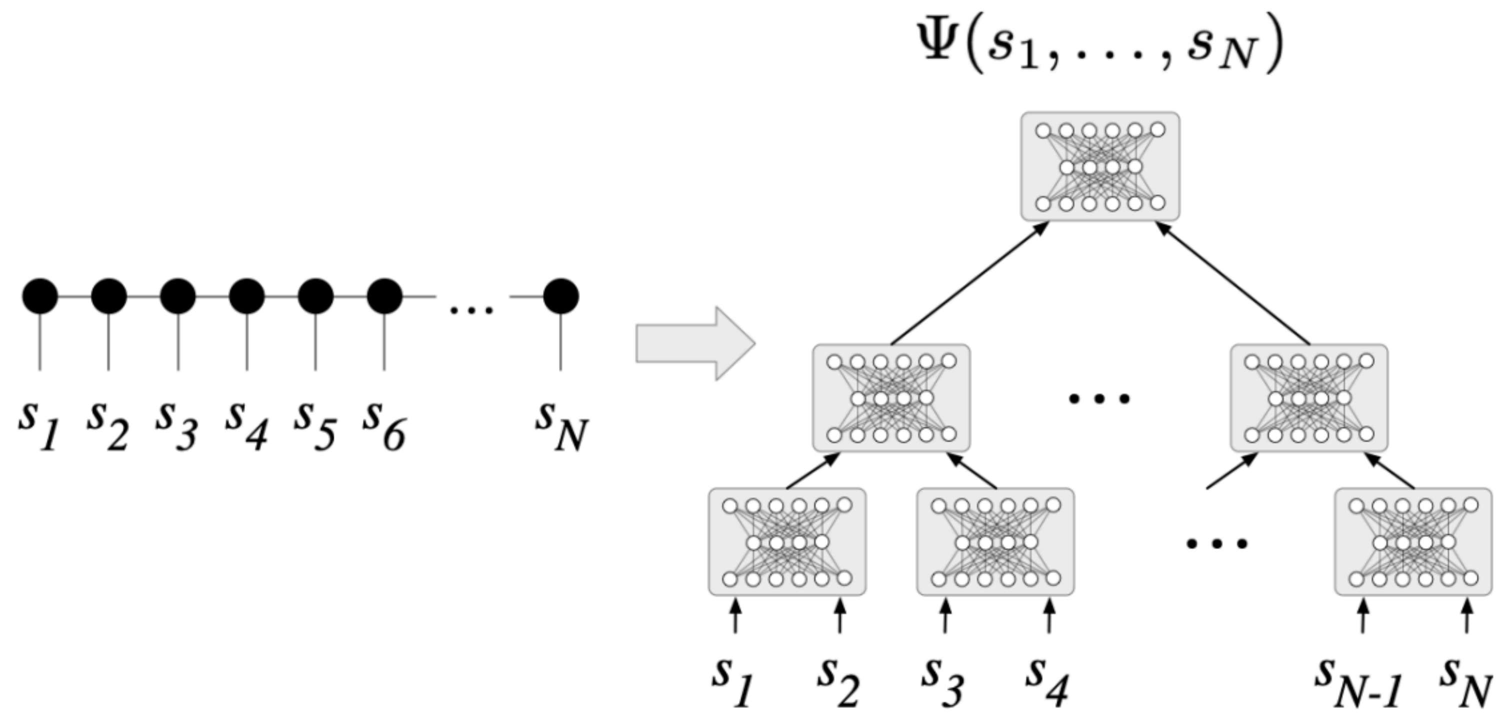
[Approximation by Superpositions of
a Sigmoidal Function, G. Cybenko]

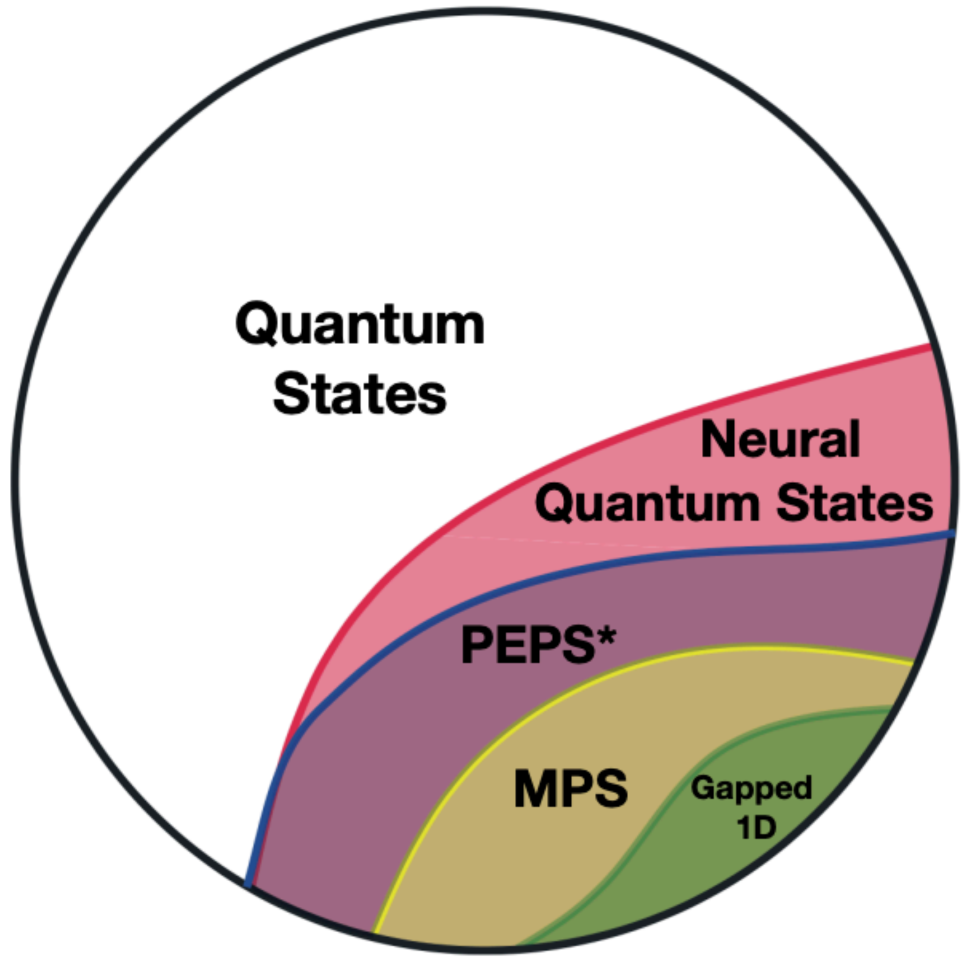
“Any multidimensional function can be written as the sum of smoothened step functions”



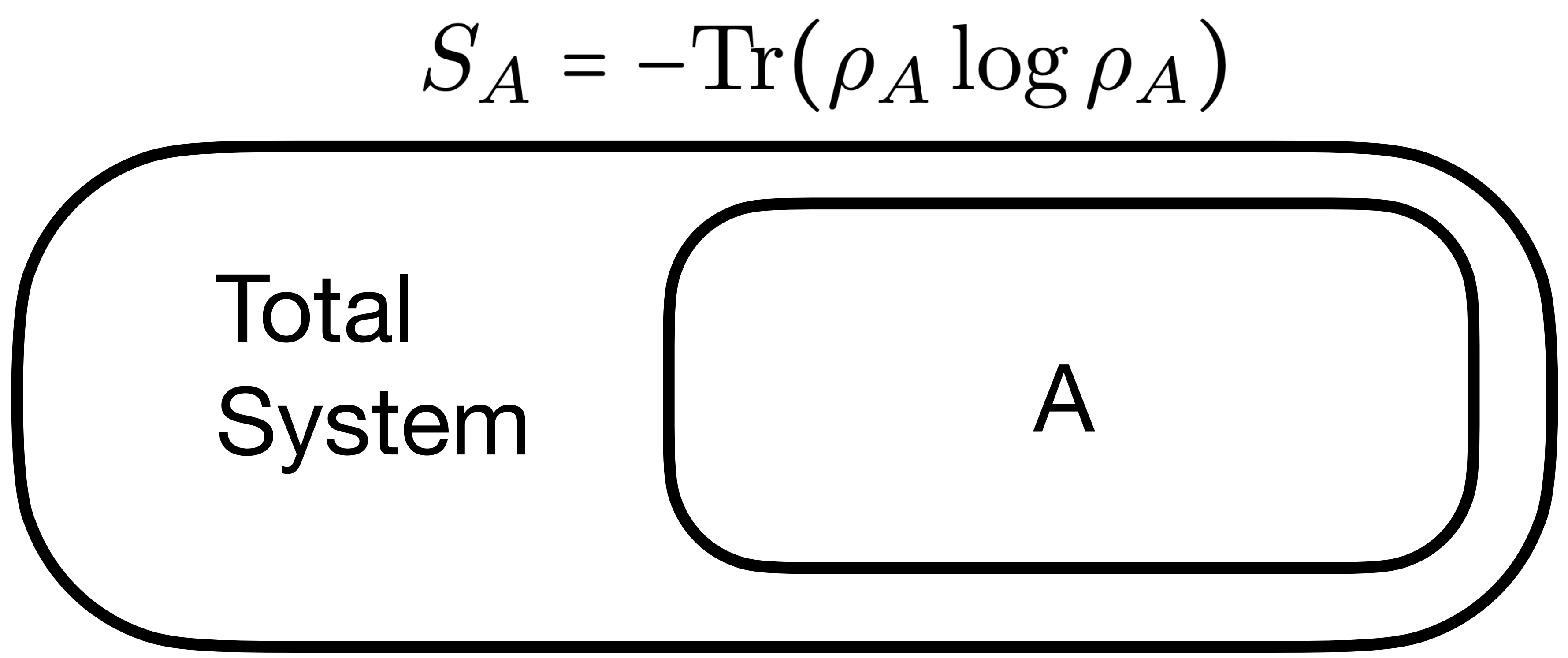
[Kieran Loehr and Bryan K. Clark, 2510.26906]

“Although NNBF is theoretically universal in the limit of large networks, we find that practical gains saturate with increasing network size.”

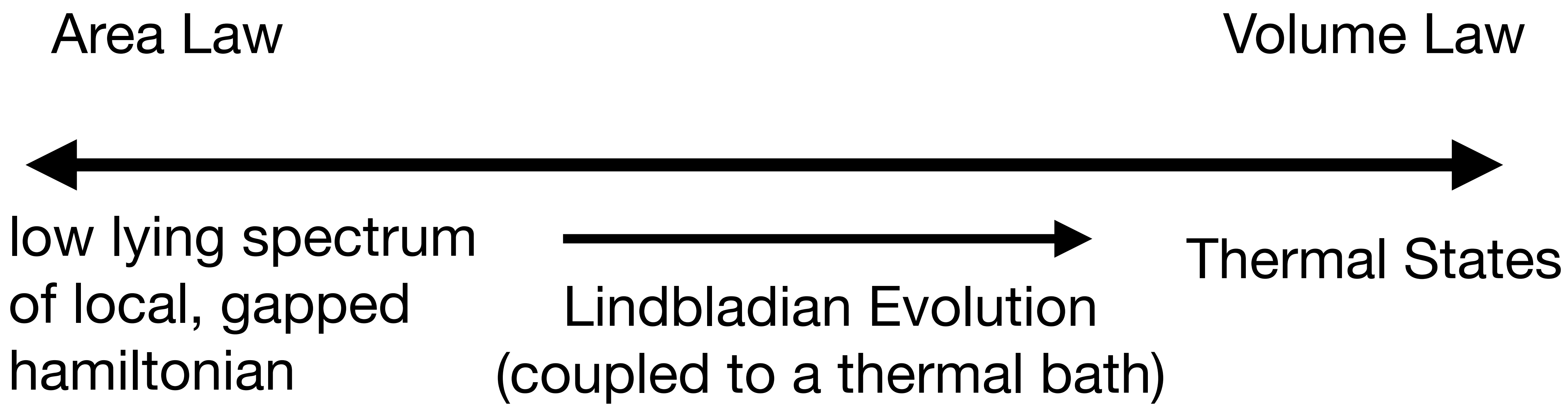




[Or Sharir, Amnon Shashua, Giuseppe Carleo, 2103.10293]



$S_A = -\mathrm{Tr}(\rho_A \log \rho_A)$
Total System
A



Area Law
Volume Law
low lying spectrum of local, gapped hamiltonian
Lindbladian Evolution (coupled to a thermal bath)
Thermal States

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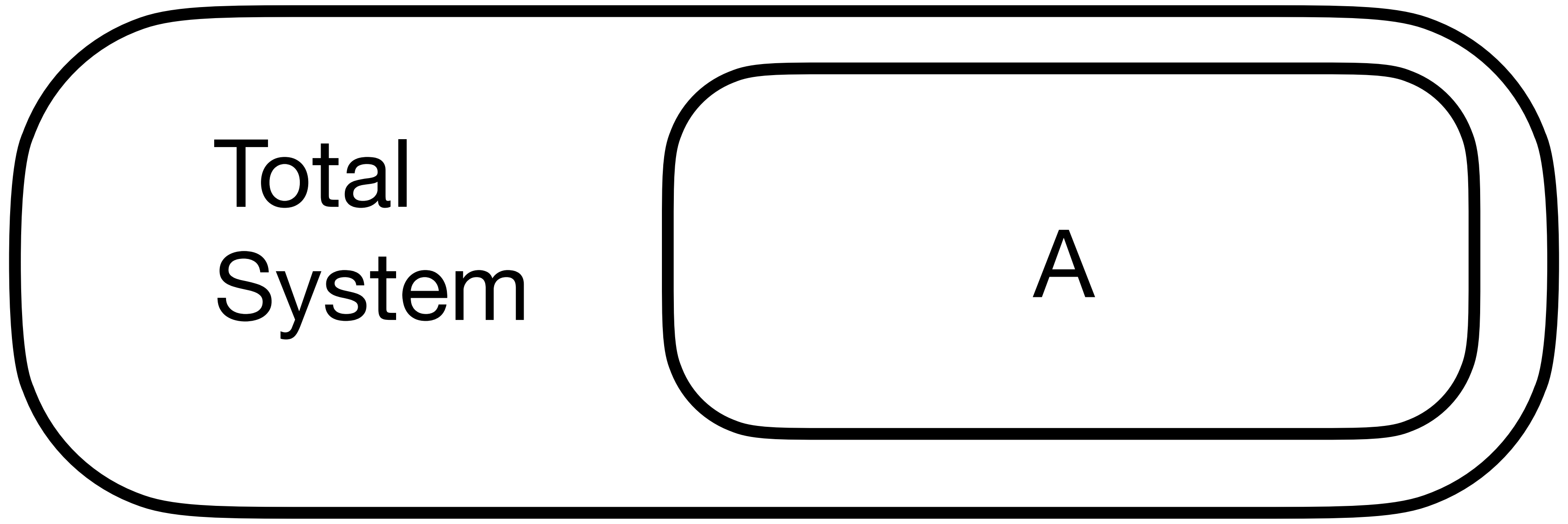

Area Law

Volume Law

low lying spectrum of local, gapped hamiltonian

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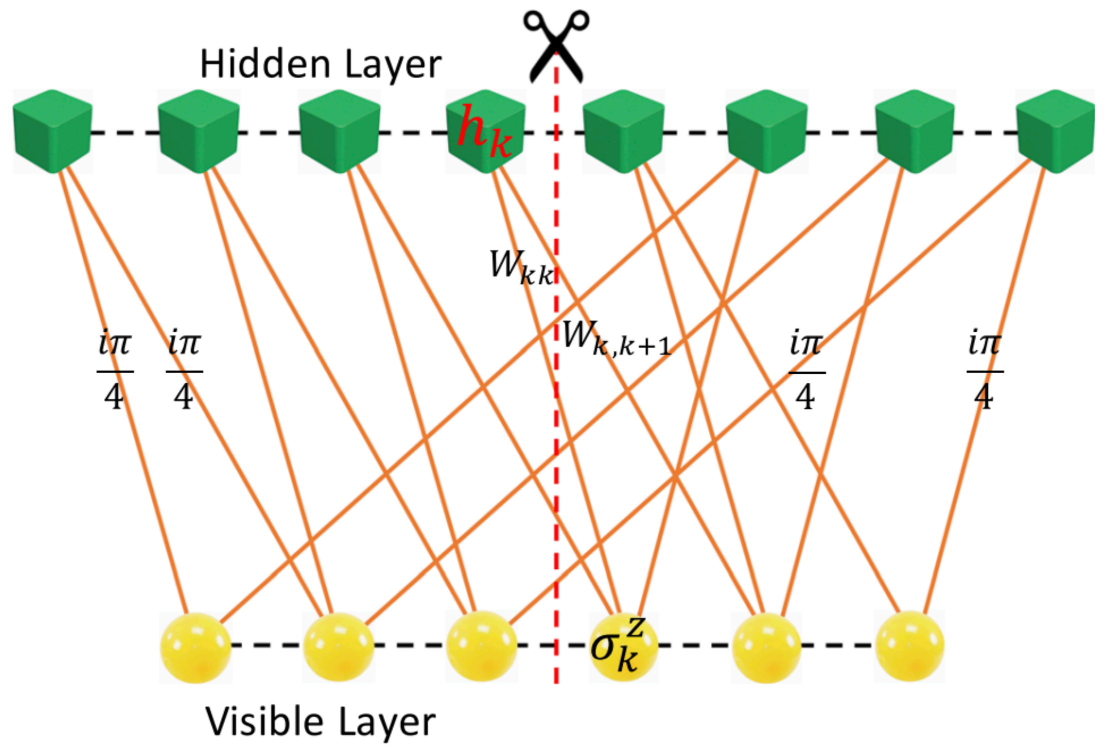
Thermal States

Part of the story for closed systems:

Quantum Entanglement in Neural Network States

[Dong-Ling Deng, Xiaopeng Li, and S. Das Sarma, 1701.04844]



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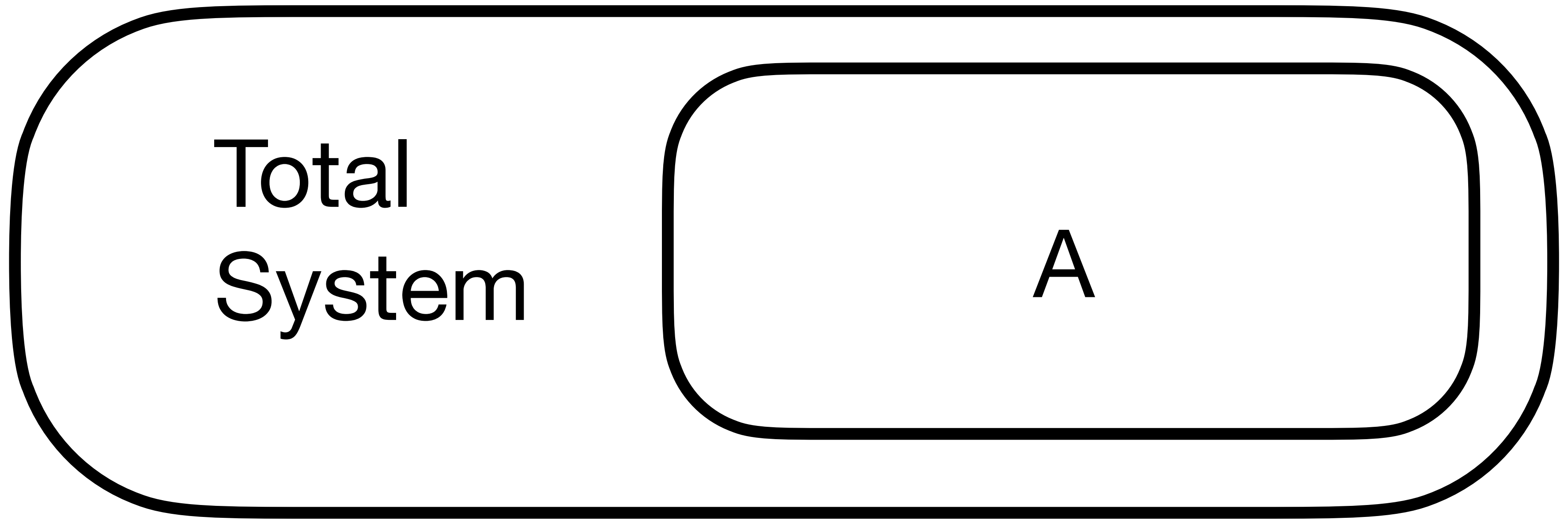

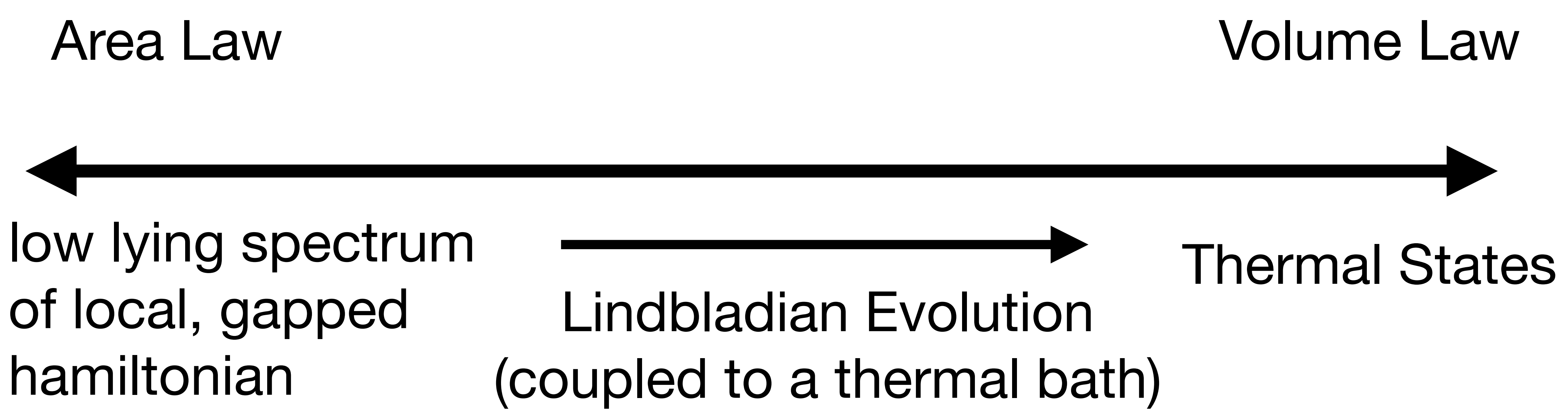

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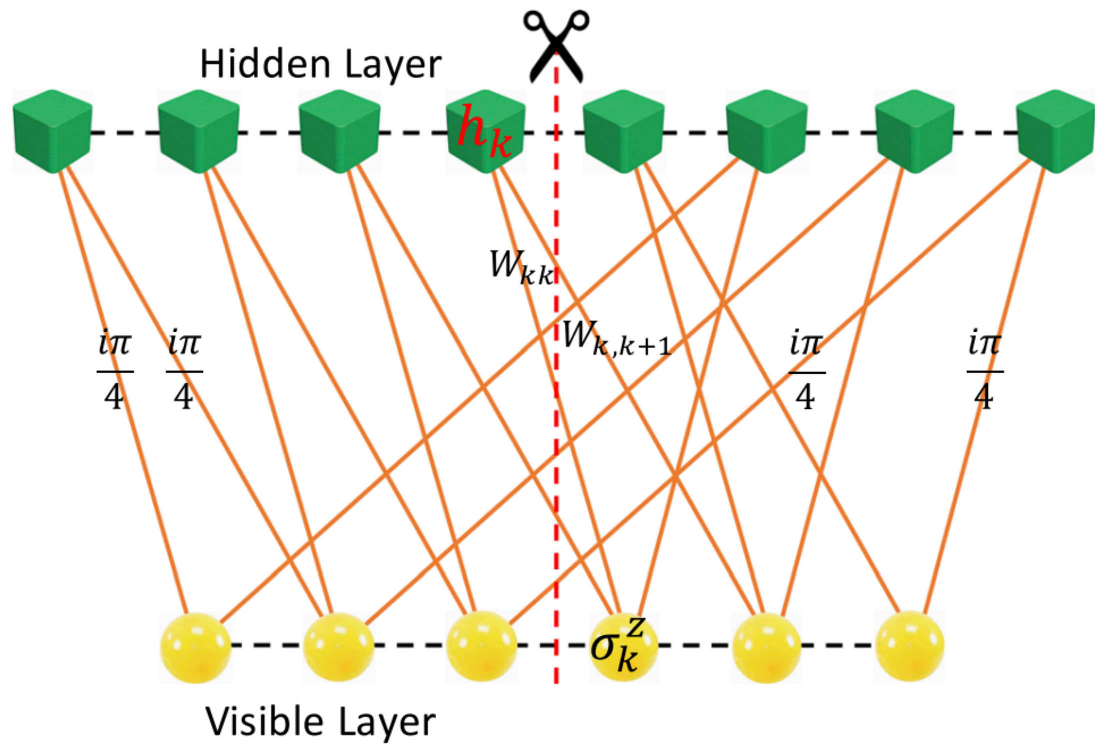
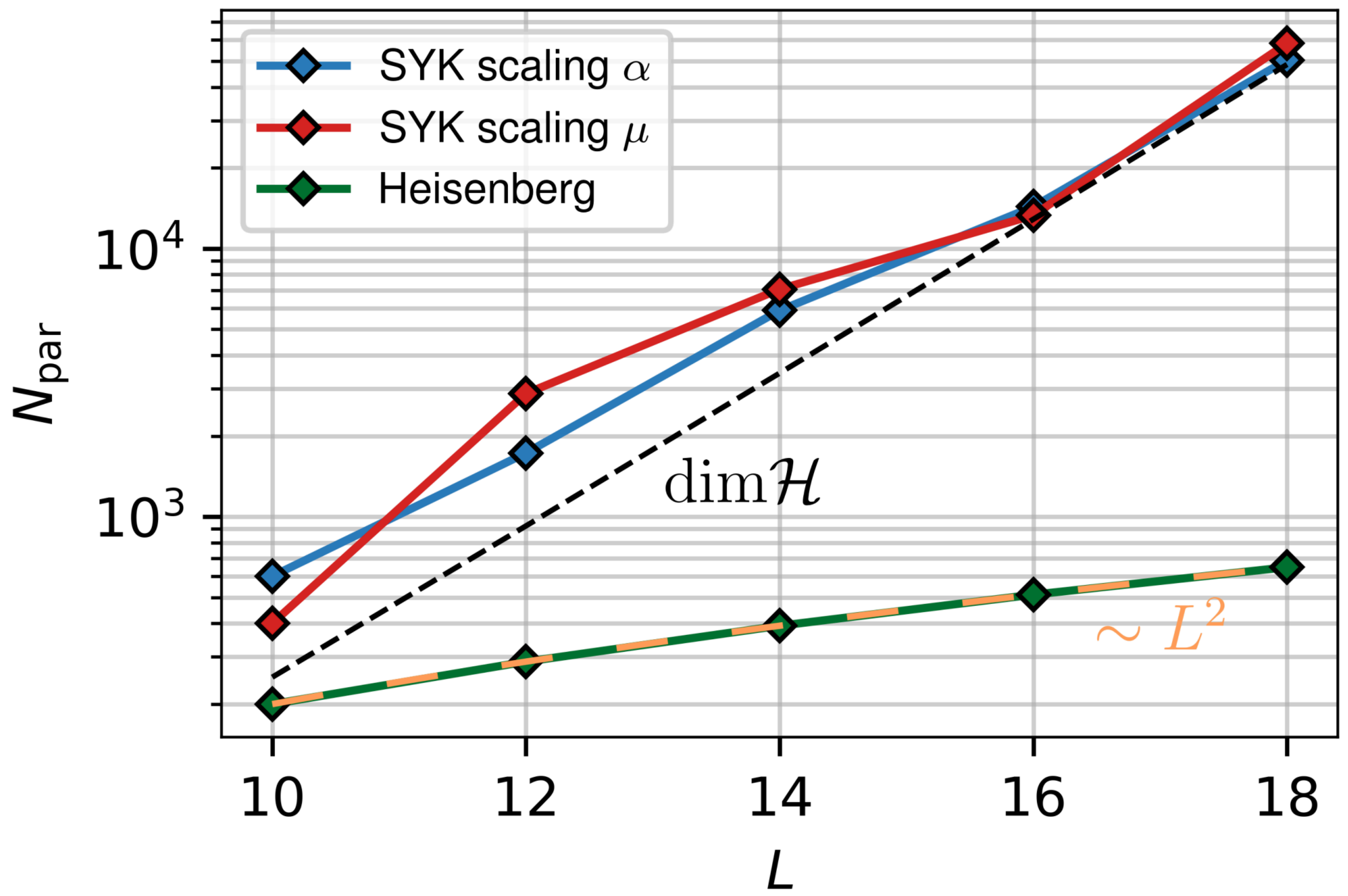


Can neural quantum states learn volume-law ground states?

[Giacomo Passetti, Damian Hofmann, Pit Neitemeier, Lukas Grunwald, Michael A. Sentef, and Dante M. Kennes 2212.02204]

$$\hat{H}_{\mathrm{SYK}}(J) = \frac{1}{(2L)^{3/2}} \sum_{ijkl} J_{ij;kl}\, \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l,$$



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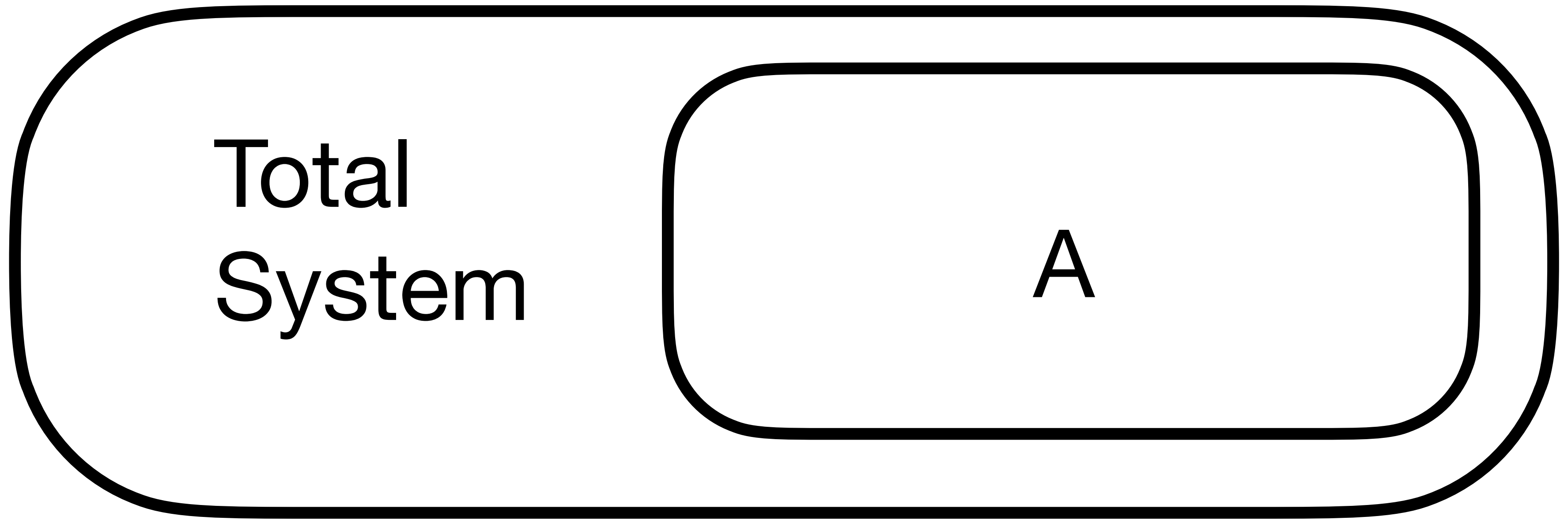

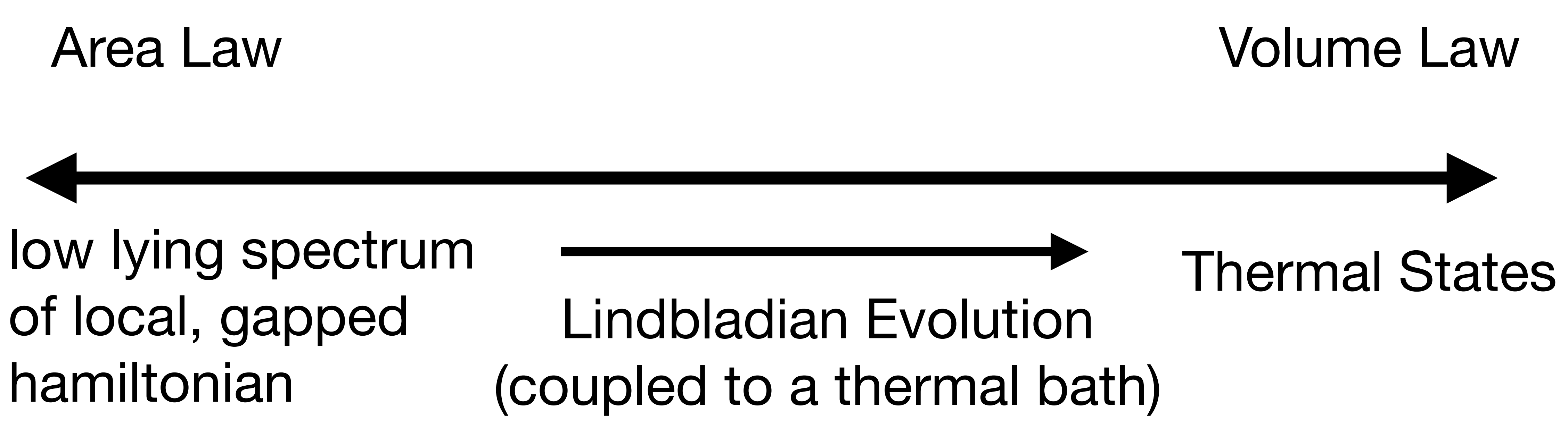

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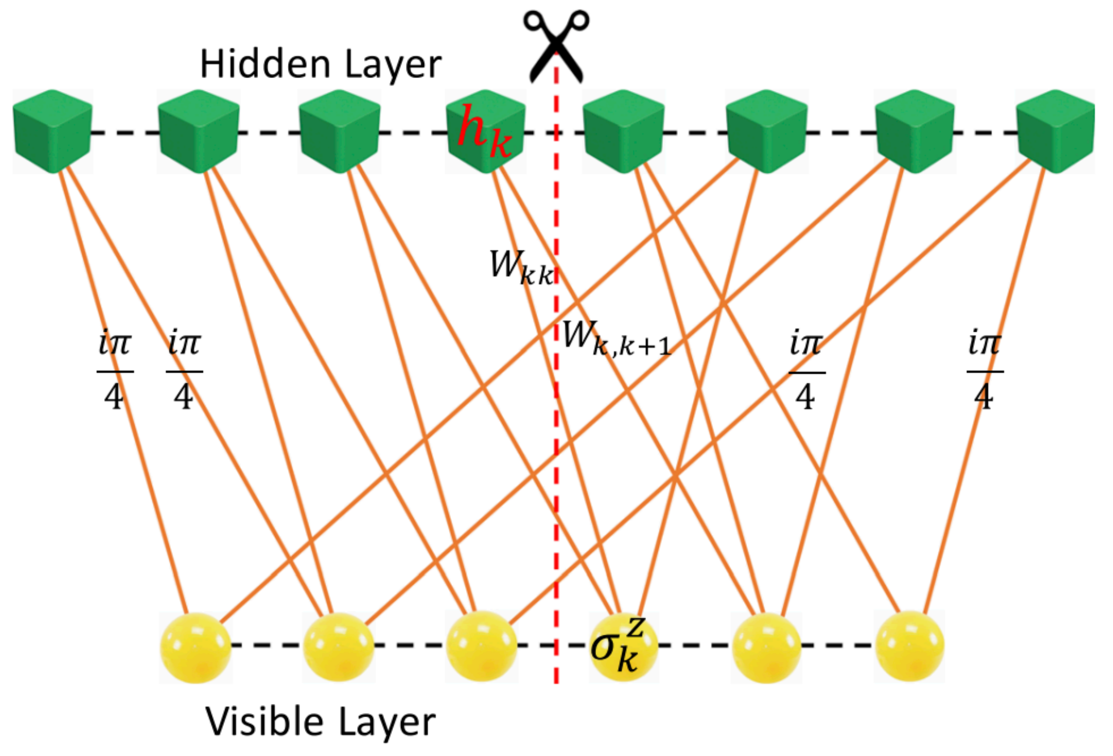

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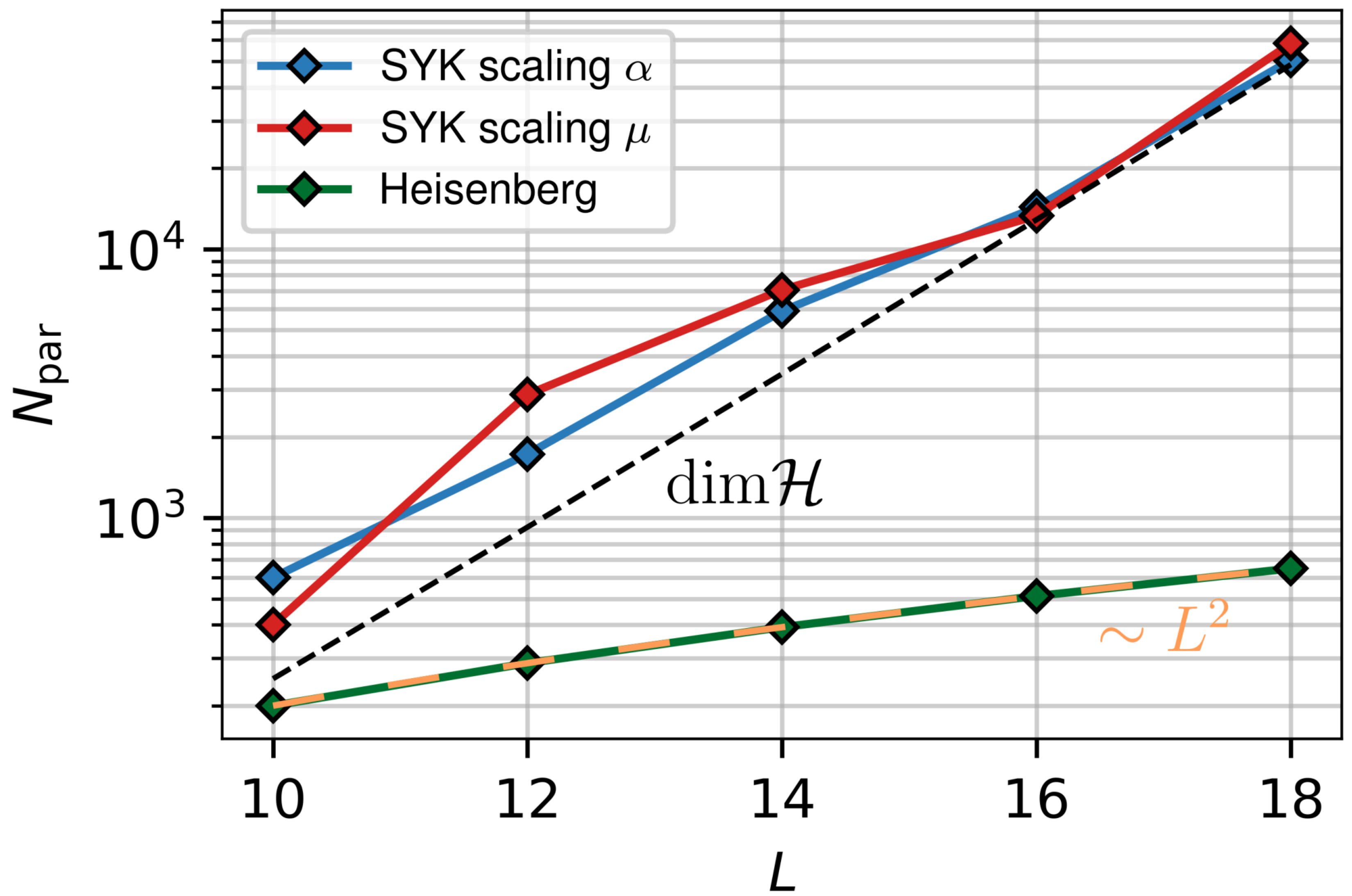
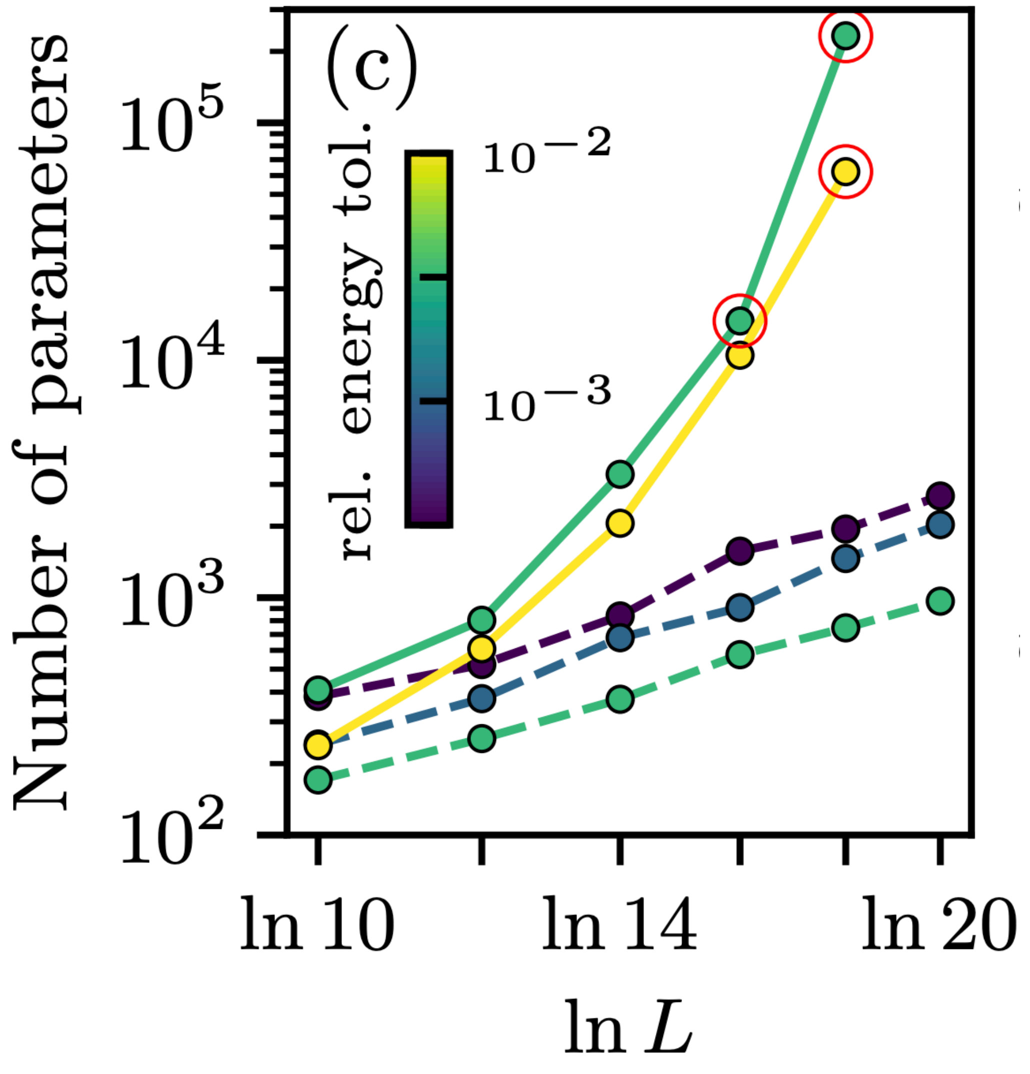


Comment on: Can neural quantum states learn volume-law ground states?

[Zakari Denis, Alessandro Sinibaldi, Giuseppe Carleo, 2309.11534]



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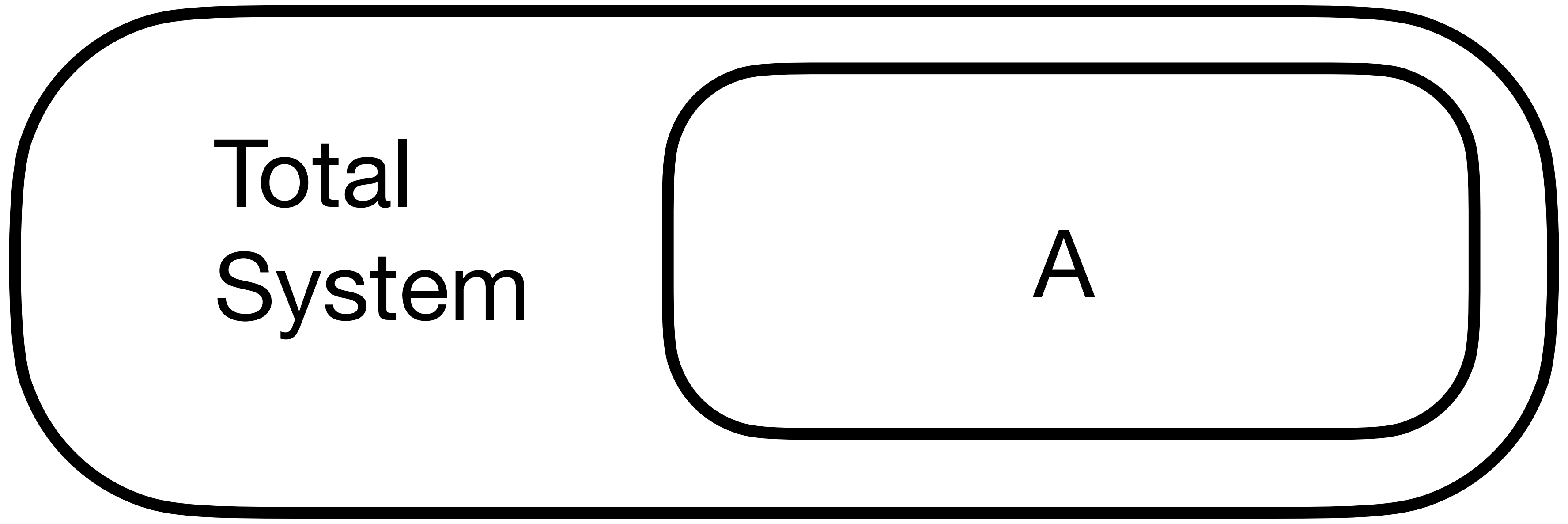

Area Law ⟵⟶ Volume Law

low lying spectrum of local, gapped hamiltonian ⟶ Lindbladian Evolution (coupled to a thermal bath) ⟶ Thermal States

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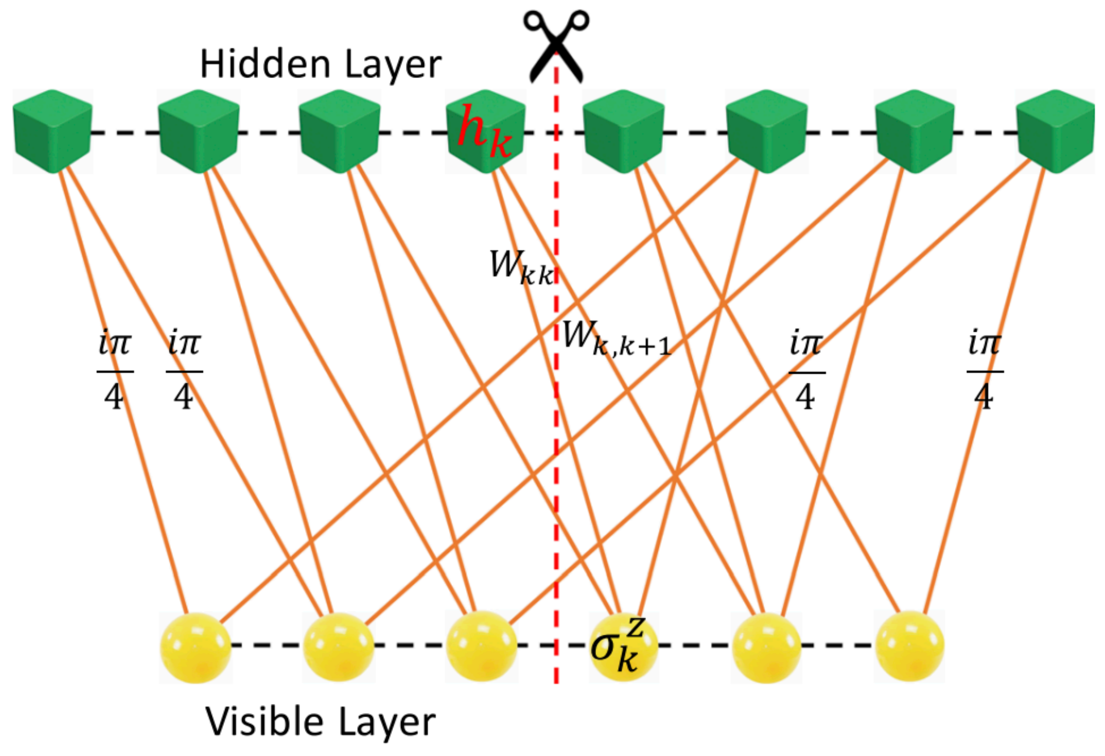

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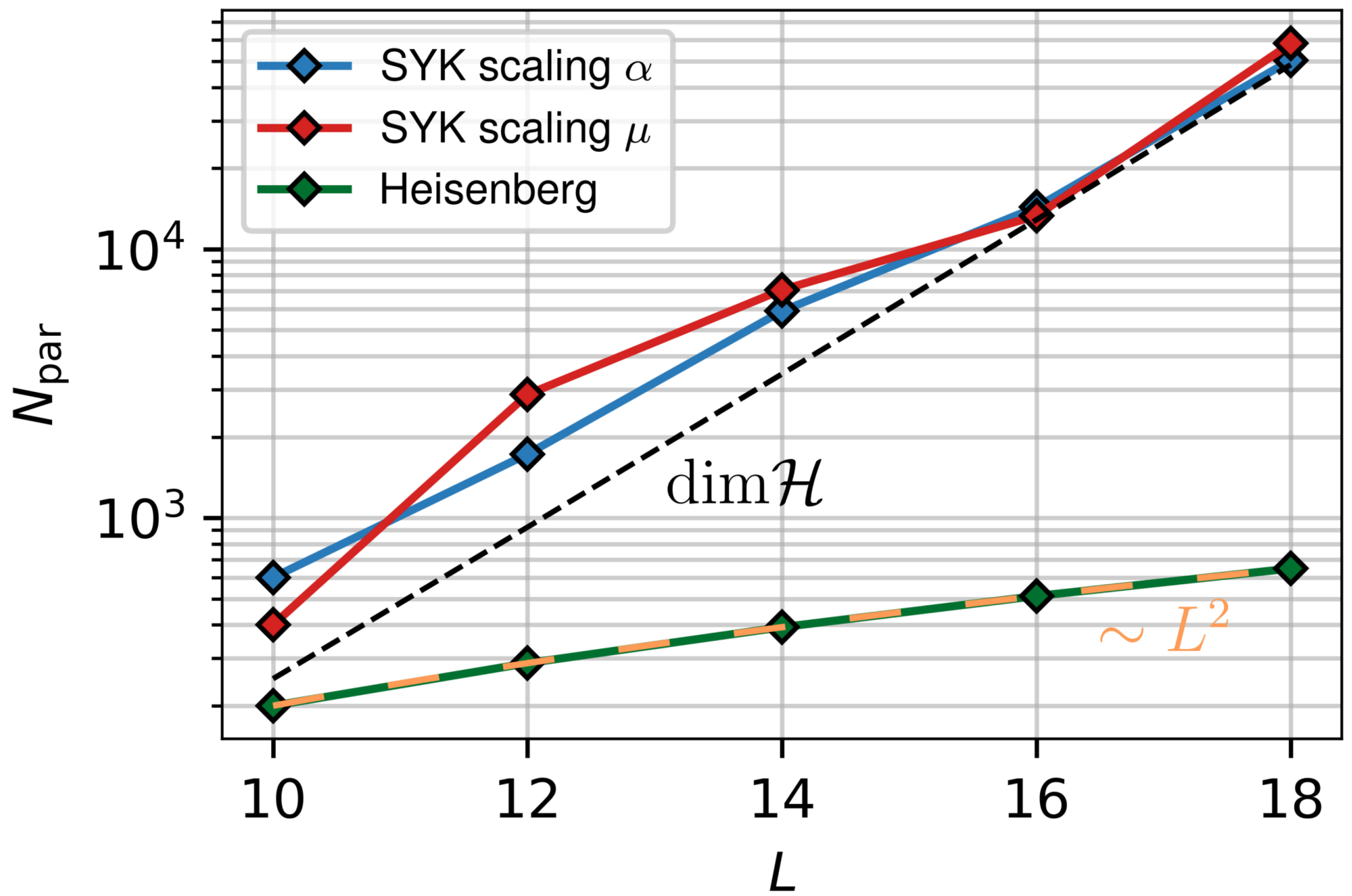

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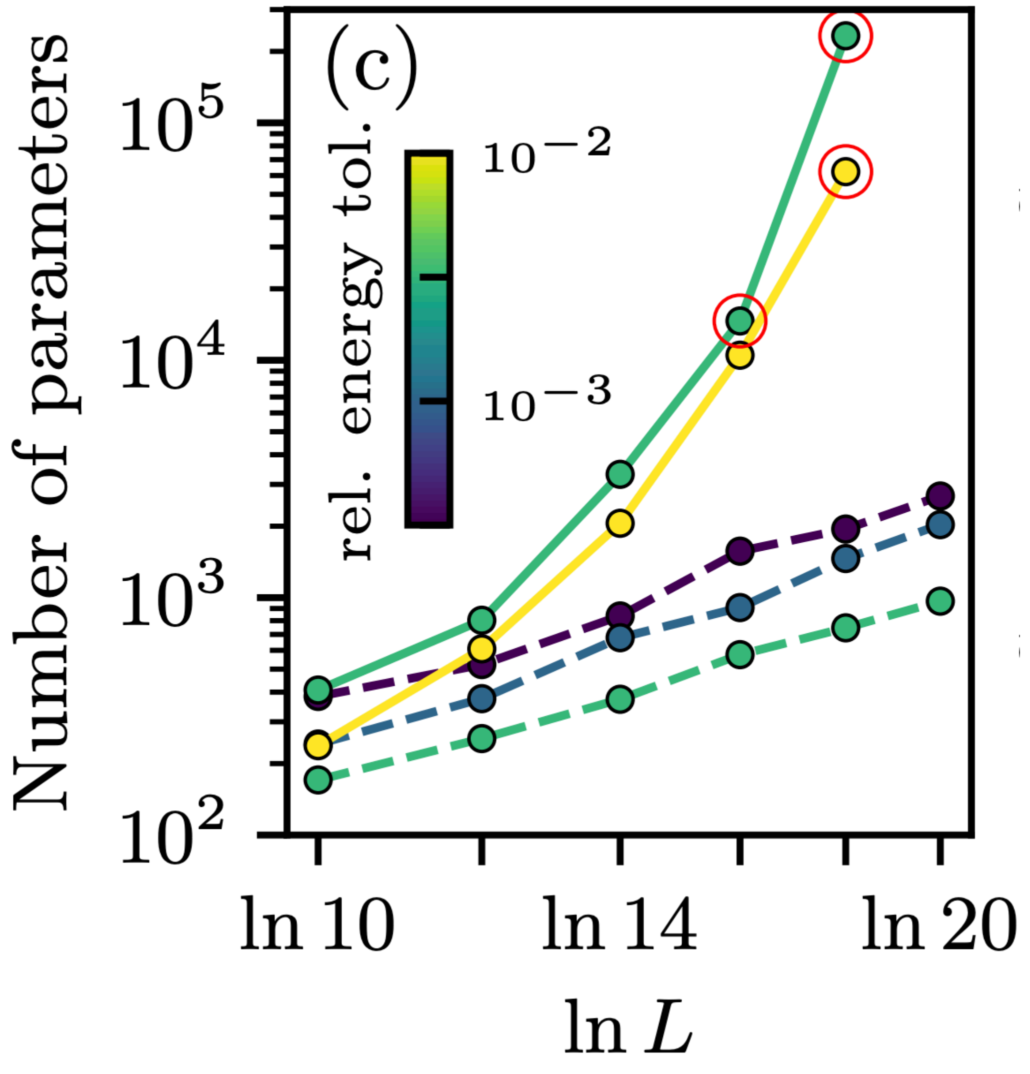


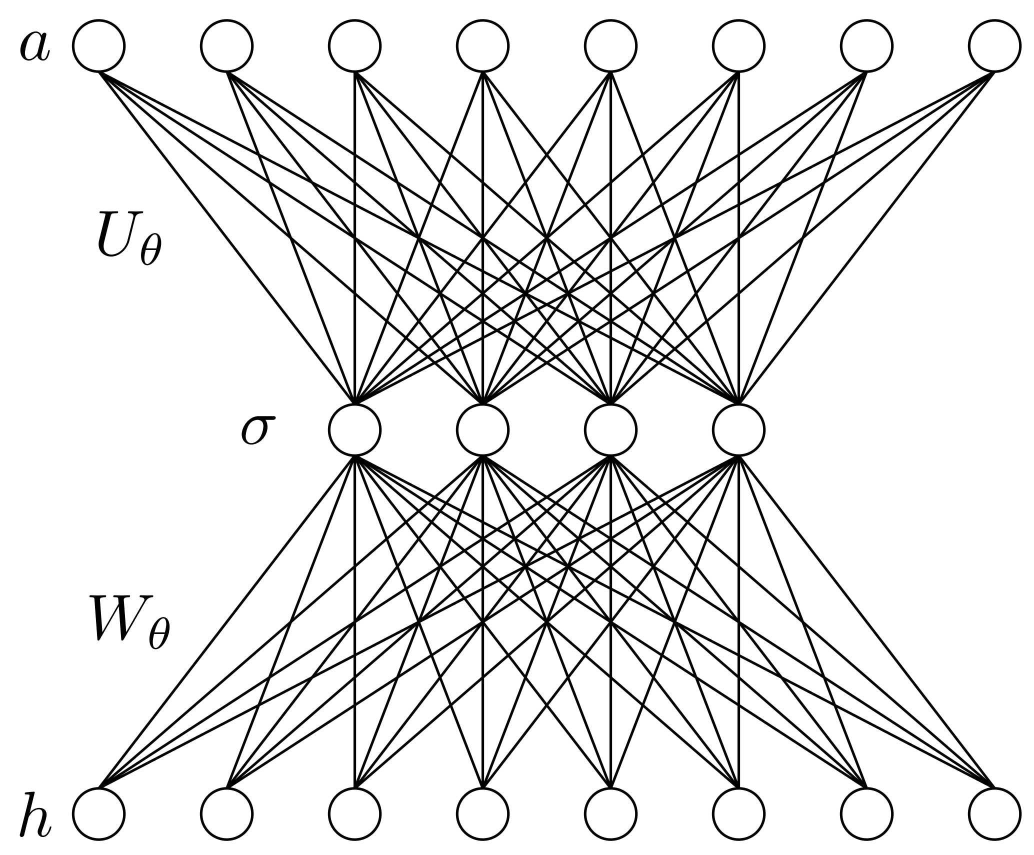
Bound on Entanglement in Neural Quantum States

[Nisarga Paul, 2510.11797]

Theorem. *(Entanglement bound)* Let $\Psi(\boldsymbol{s})$ be a feed-forward NQS on n spins with k scalar nonlinearities. We have that $\Psi(\boldsymbol{s}) = \mathcal{G}(t_1(\boldsymbol{s}), \ldots, t_\mu(\boldsymbol{s}))$ where $t_i(\boldsymbol{s})$ are affine features and $\mu \leq k+1$. Suppose $\mathcal{G}$ extends analytically and remains bounded in a complex neighborhood of each of its real arguments, in a manner independent of n. Let A be a subset of the n spins and let S_A be the von Neumann entropy of the reduced density matrix $\rho_A = \mathrm{Tr}_{\bar{A}} |\Psi\rangle\langle\Psi|$. Then the entropy grows at most linearly with μ and at most logarithmically in n:

$$S_A = O(\mu \log n). \quad (3)$$

Neural Density Operators



$$p(\sigma, a, h) = \tfrac{1}{2}\exp(a^T U\sigma + h^T W\sigma + d^T a + b^T\sigma + c^T h)$$

Sum over hidden bits

$$\langle \sigma, a|\psi\rangle = \textstyle\sum_h p(h, \sigma, a)$$

Trace over ancillary bits

$$\langle \sigma|\rho|\sigma'\rangle = \textstyle\sum_a \langle \sigma, a|\psi\rangle\langle\psi|\sigma', a\rangle$$

$$\log(\langle\sigma|\rho|\sigma'\rangle) = \sum_{j=1}^{L}(b_j\sigma_j + b_j^*\sigma_j') + \sum_{k=1}^{M_h L}\mathcal{X}_k + \sum_{p=1}^{M_a L}\mathcal{Y}_p,$$

$$\mathcal{X}_k = \log\cosh\left(c_k + \sum_{j=1}^{L} W_{kj}\sigma_j\right) + \log\cosh\left(c_k^* + \sum_{j=1}^{L} W_{kj}^*\sigma_j'\right),$$

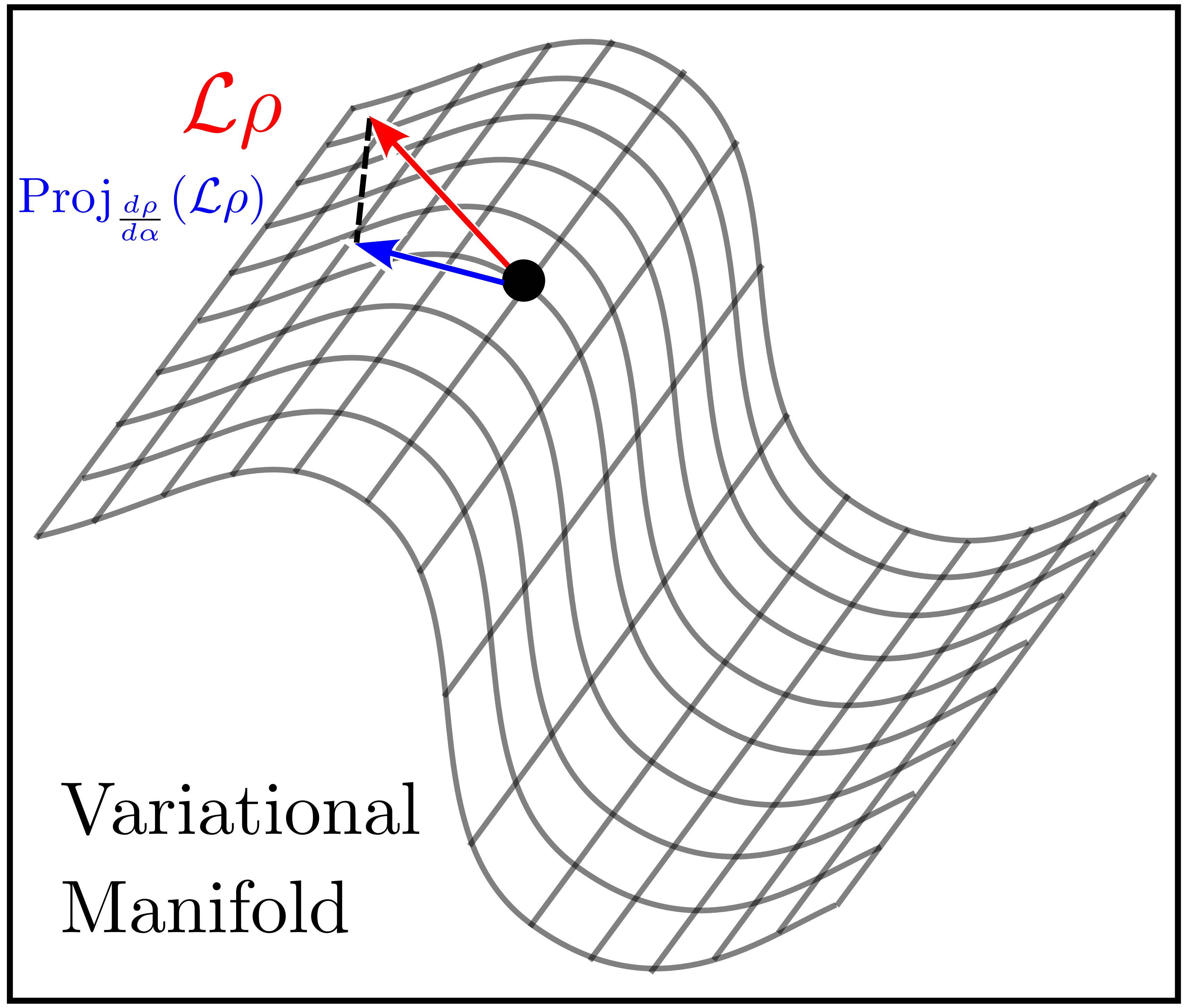
$$\mathcal{Y}_p = \log\cosh\left(d_p + d_p^* + \sum_{j=1}^{N}(U_{pj}\sigma_j + U_{pj}^*\sigma_j')\right).$$

$$\langle O\rangle = \frac{\mathrm{Tr}(\rho O)}{\mathrm{Tr}(\rho)} = \sum_\sigma \left(\frac{\langle\sigma|\rho|\sigma\rangle}{\mathrm{Tr}(\rho)}\right)\left(\frac{\langle\sigma|\rho O|\sigma\rangle}{\langle\sigma|\rho|\sigma\rangle}\right)$$

sample $\sigma \sim \langle\sigma|\rho|\sigma\rangle$,
e.g. with MCMC

evaluate local contribution to observable

Space of Density Matrices



Review: [G. Torlai, R. G. Melko: 1801.09684]

- Want to solve $\partial_t \vec{\rho} = L\vec{\rho}$ by varying parameters α_k

$$\min_{\dot\alpha} \left\| \sum_i \dot\alpha_i \frac{\partial \rho_a}{\partial \alpha_i} - \sum_b \mathcal{L}_{ab}\rho_b \right\|_2 \implies \dot\alpha = S^{-1} f,$$

$$(O_i)_{ab} := \delta_{ab} \frac{\partial \ln(\rho_a)}{\partial \alpha_i}, \quad S_{ij} := \rho^\dagger O_i^\dagger O_j \rho + \rho^\dagger O_j^\dagger O_i \rho, \quad f_i := \rho^\dagger O_i^\dagger \mathcal{L}\rho + \rho^\dagger \mathcal{L}^\dagger O_i \rho,$$

How density matrix varies as parameters are varied

'Quantum geometric tensor'

Forces

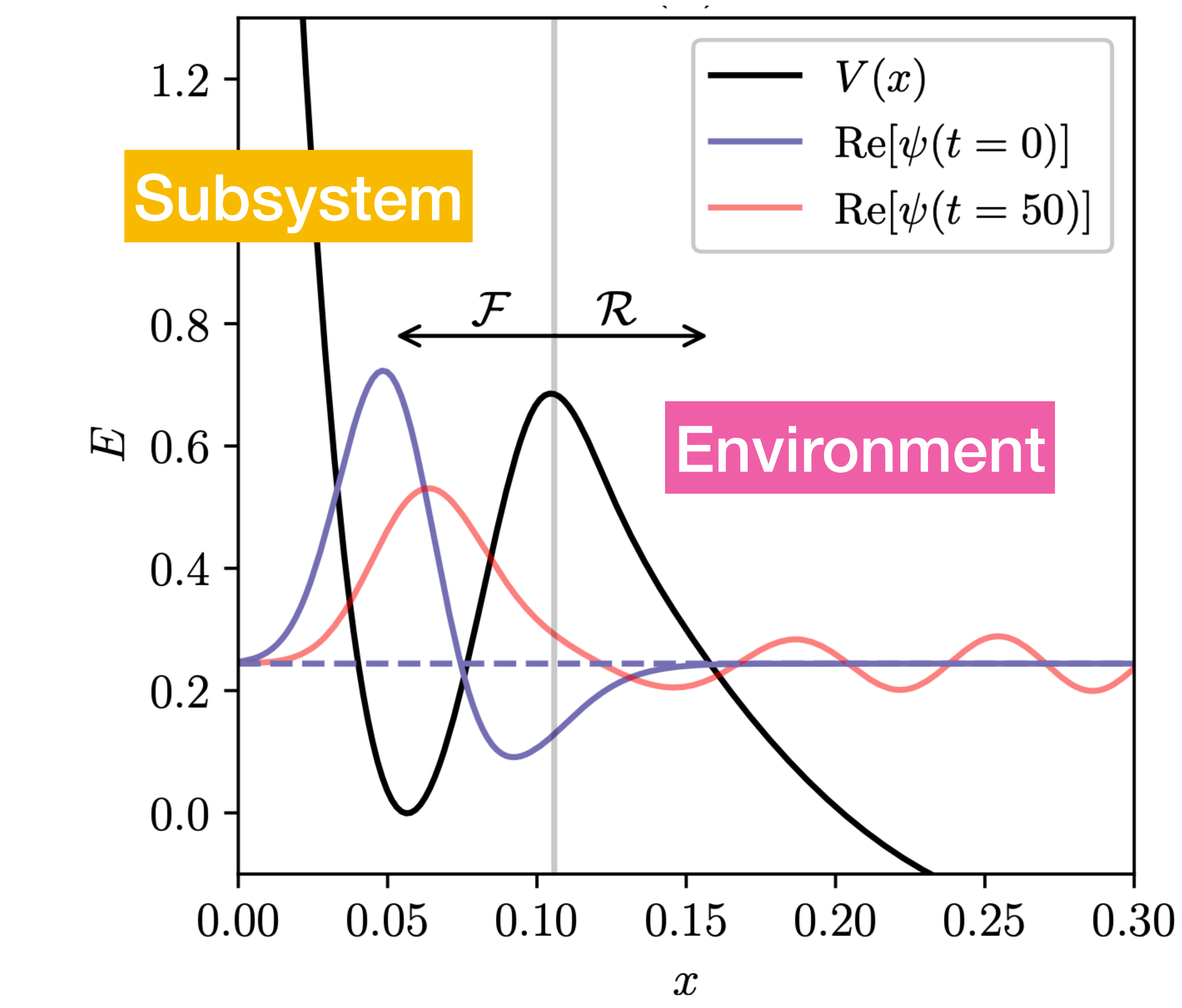
- S, f can be estimated using Monte-Carlo Markov Chains sampling from the basis elements of the doubled Hilbert Space

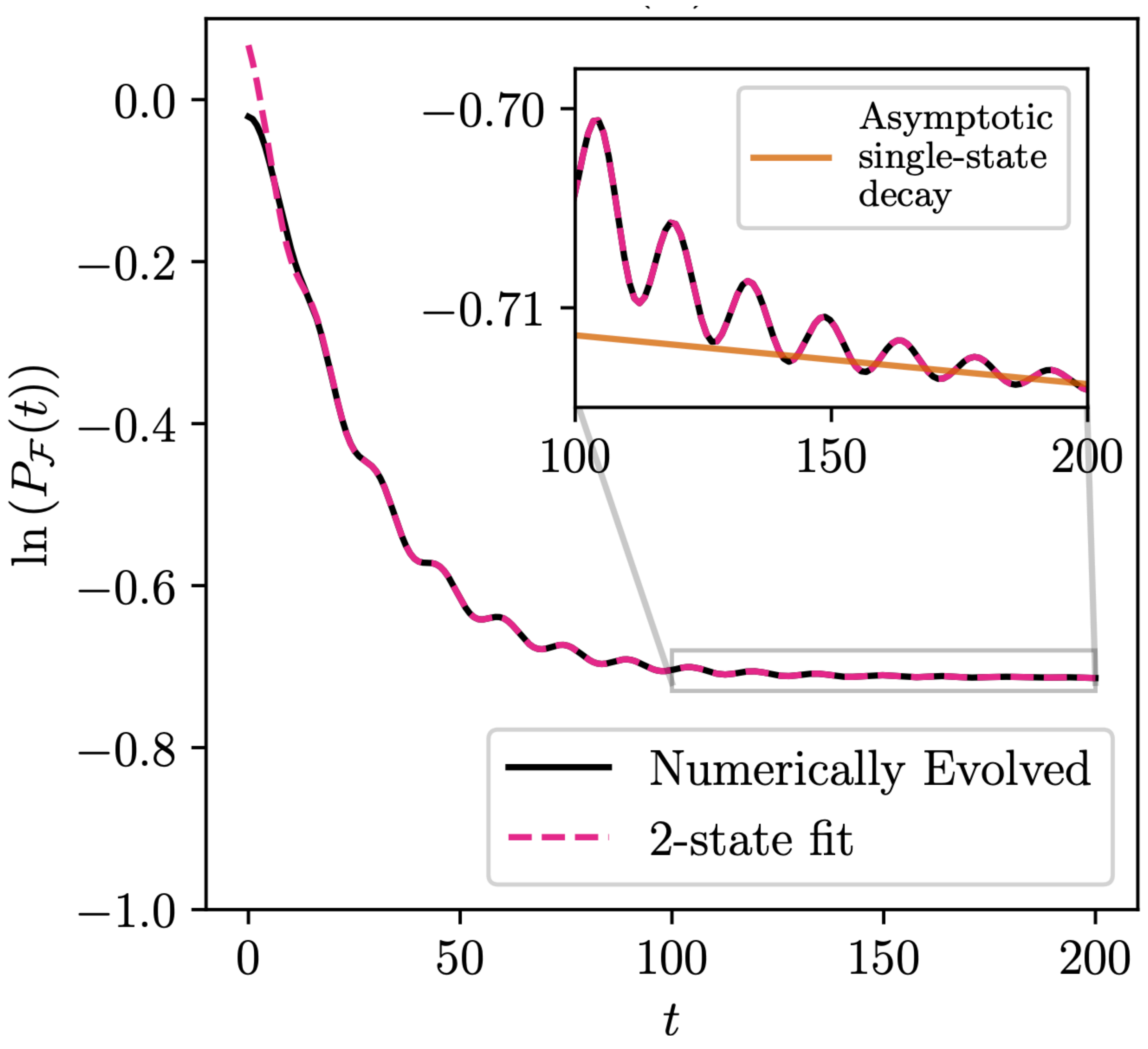
$$S_{ij} = Z \sum_a \frac{\|\rho_a\|^2}{Z} 2\mathrm{Re}\left((\mathscr{O}_i^\dagger)_{aa} (\mathscr{O}_j)_{aa} \right), \quad f_i = Z \sum_a \frac{\|\rho_a\|^2}{Z} 2\mathrm{Re}\left((\mathscr{O}_i^\dagger)_{aa} \sum_b \frac{\mathscr{L}_{ab}\rho_b}{\rho_a} \right)$$

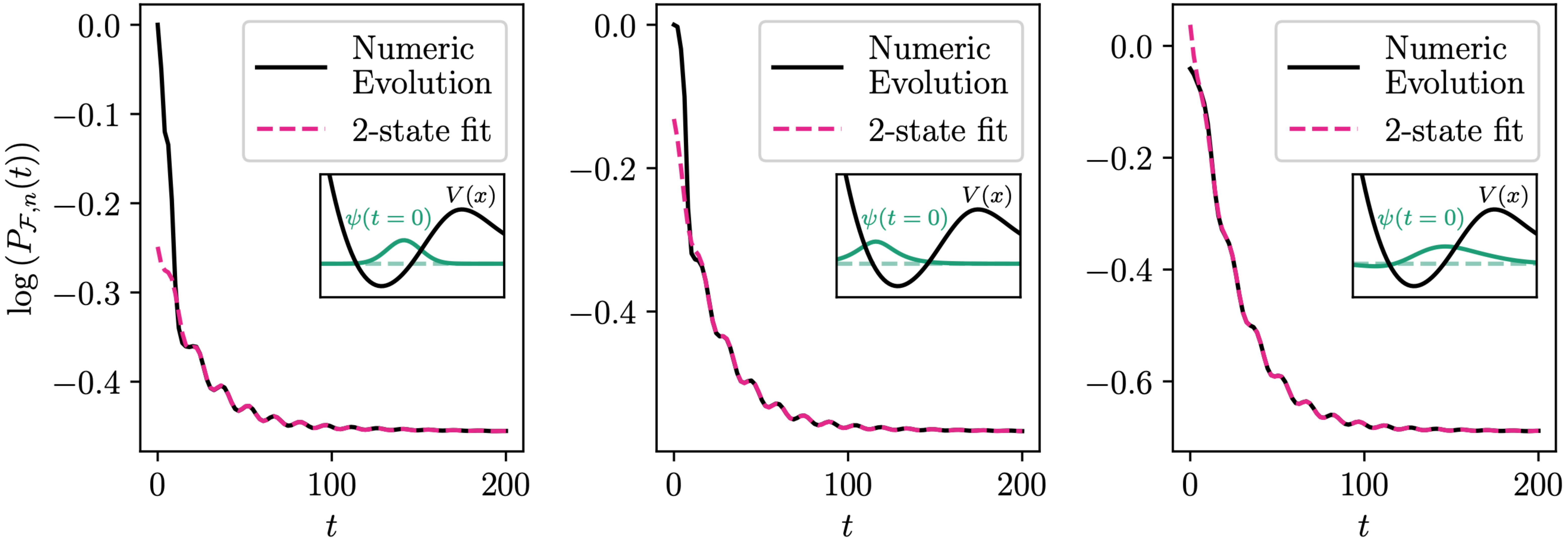
Advertisement break: Path integral predictions for pre-asymptotic false vacuum decay

with: Bruno Scheihing-Hitschfeld, Thomas Steingasser

will be here next week





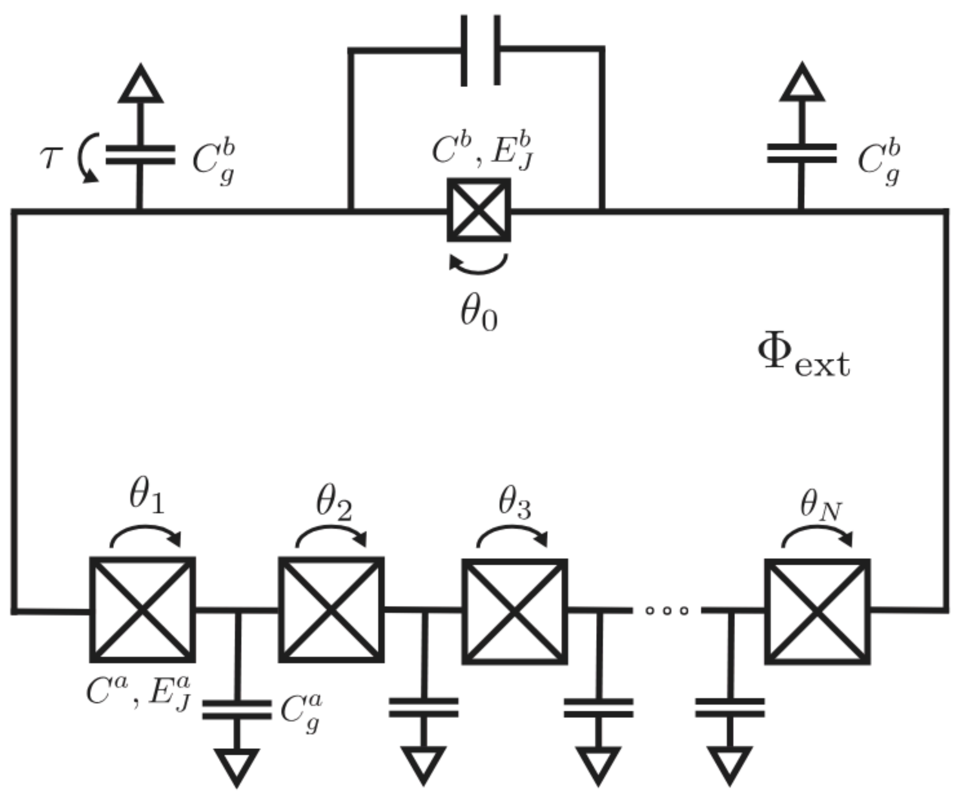


Newly developed steadyon analysis can be used to provide semiclassical predictions for lifetimes of arbitrary wavefunctions in the false vacuum!

hep-th/2511.08669,
hep-th/2511.08670

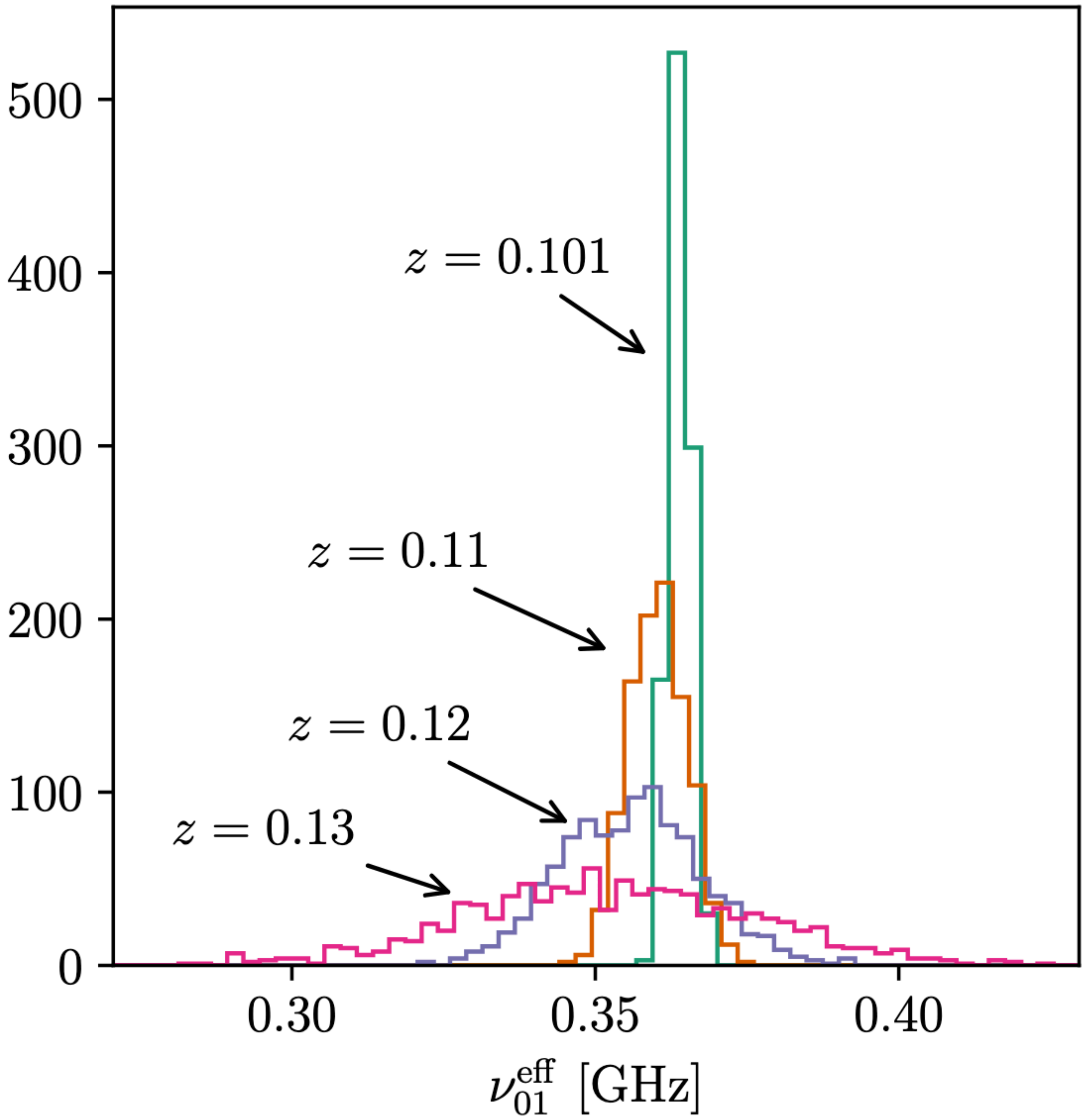
Advertisement break: Lattice field theory for superconducting circuits

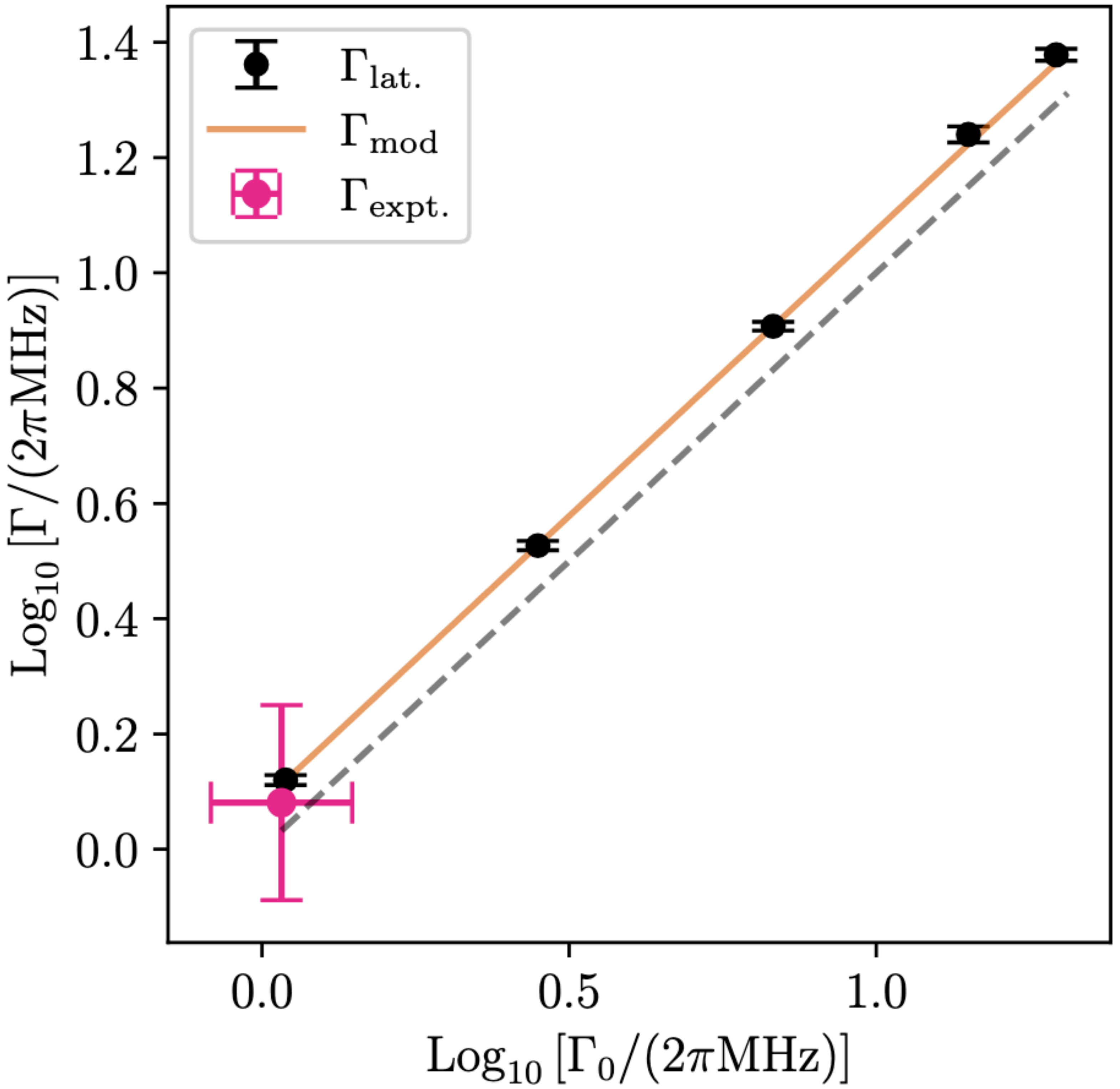
[Joshua Lin, Max Hays, Stephen Sorokanich III, Julian Bender, Phiala E. Shanahan, and Neill C. Warrington]



$$H = 2e^2 \sum_{xx'} (n_x - n_{gx}) C^{-1}_{xx'} (n_{x'} - n_{gx'}) - E_J^a \sum_x \cos\theta_x - E_J^b \cos\left(\sum_x \theta_x - \varphi_{\text{ext}}\right) , \quad (20)$$

[on arxiv Monday!]





Path-integral monte carlo can be used for any many-body quantum mechanical system, including fluxonium!

We probe ‘charge noise dephasing’ with methods inspired by Lattice-QCD.
First principles, ab-initio, systematically controlled.

(for the experts: charge-noise dephasing arises from an equivalent of a θ-term in this model! We reweight instanton sectors to numerically calculate the dephasing!)

Advertisement: Fast Quantum Monte Carlo Simulation by Random Compilation

with: John M. Martyn, Neill C. Warrington, Isaac L. Chuang, Andrew J. Daley

[out soon!]

(Did all the Lindbladian work!)

Randomly-corrected Trotterization promotes order-n Suzuki-Trotter formula to an order-(2n + 1) by inserting correction operations

[Chien Hung Cho, Dominic W. Berry, and Min-Hsiu Hsieh 2210.11281]

Key Idea: Randomized Trotterization can be better than standard trotterization, by ‘averaging out trotter errors’

1

Lindbladian

↓

Master Equation Unravelling

↓

Random Trotterization

2

Path Integral Monte Carlo

↓

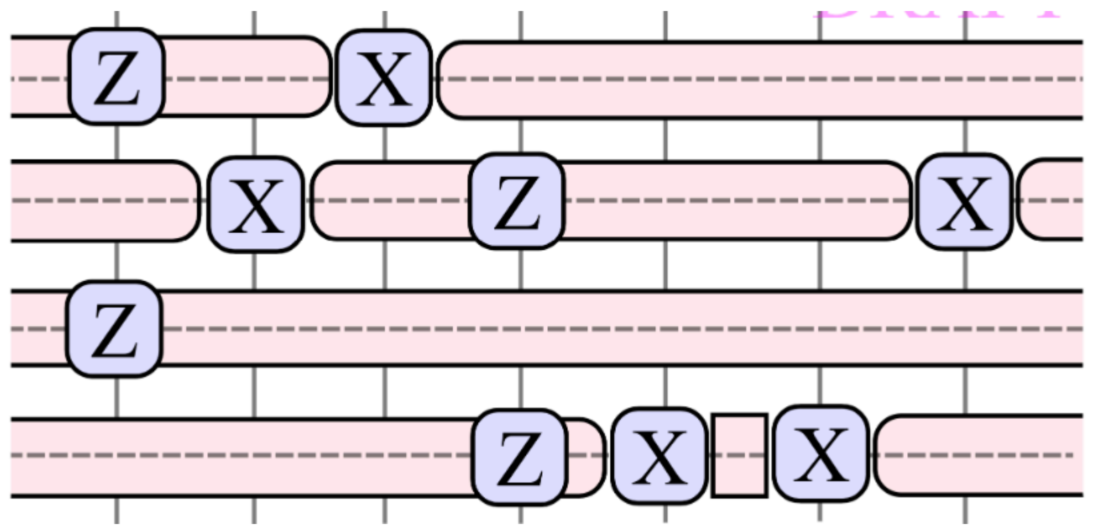
Random Action (QDRIFT)

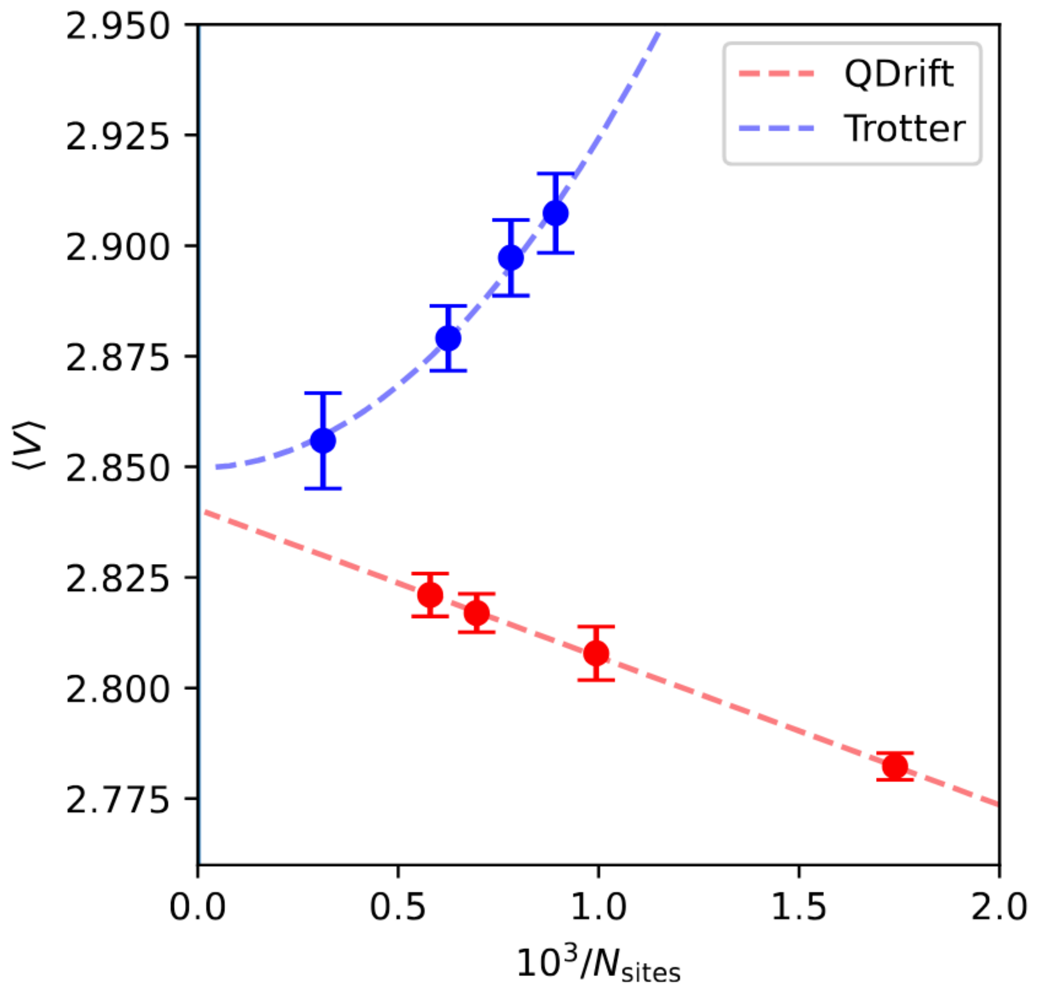
(requires long-range interactions for a benefit)

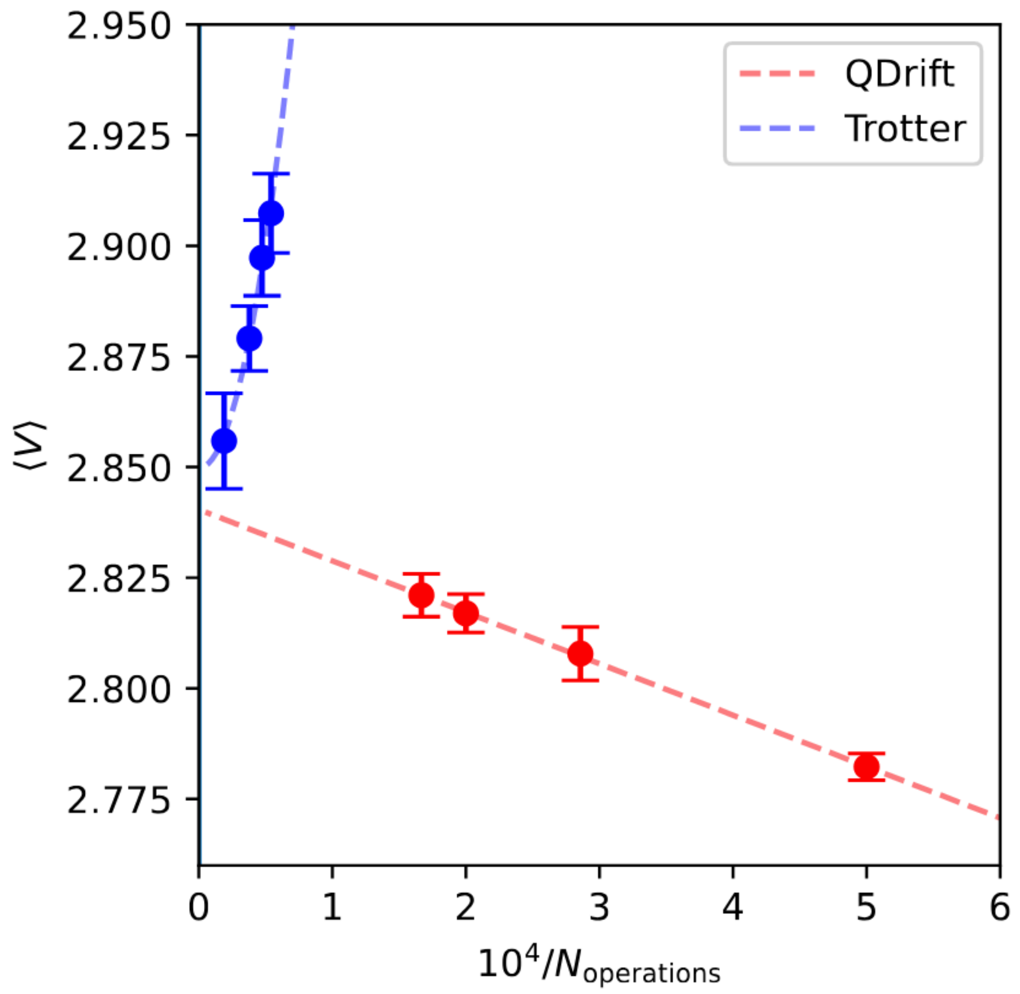
QDrift replaces the standard Euclidean-time action with a randomized one, resulting in a faster continuum limit

[Earl Campbell, 1811.08017]

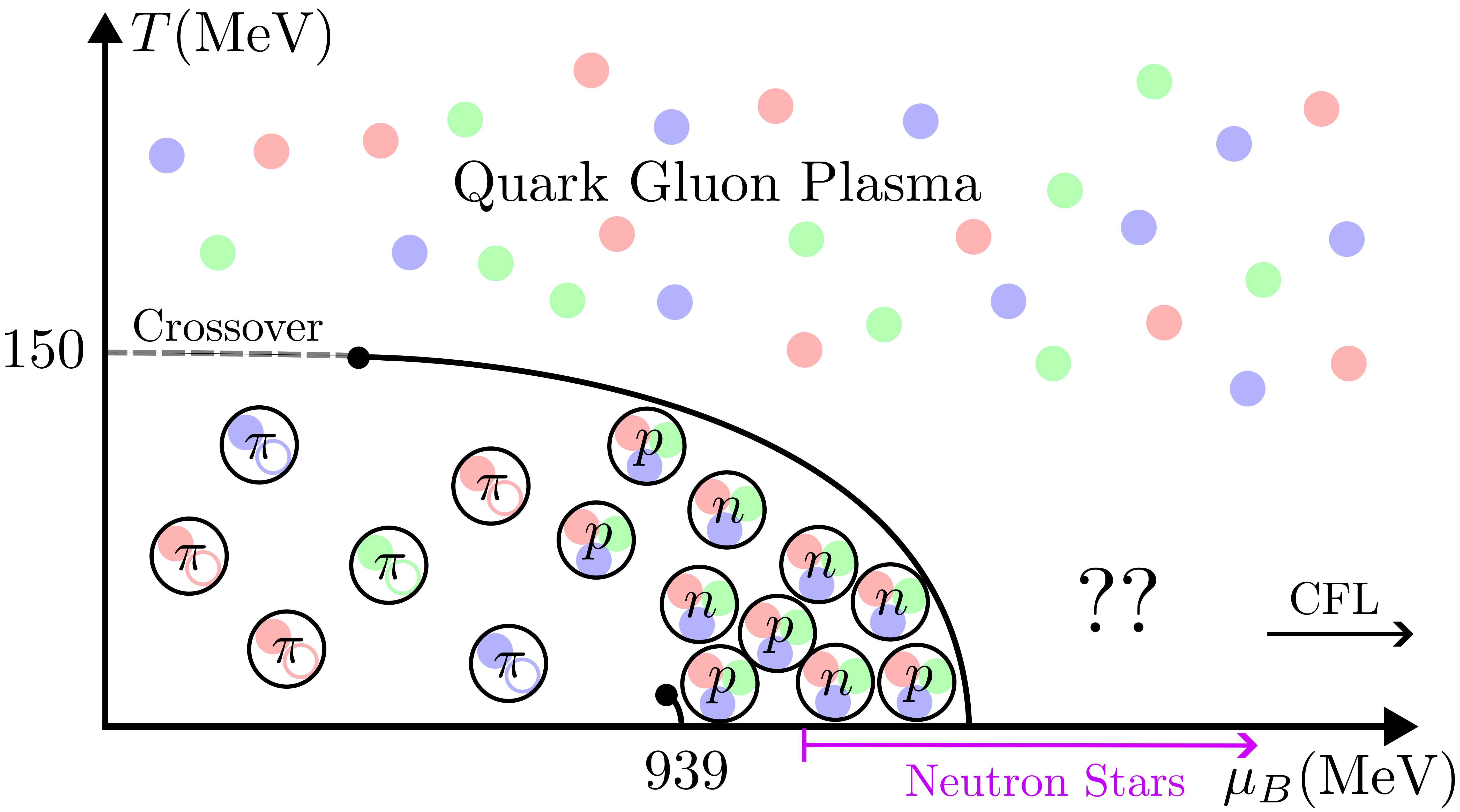
$$H = -J \sum_{i,j=1,\ i\neq j}^{n} \frac{Z_i Z_j}{|i-j|^2} - h \sum_{i=1}^{n} X_i.$$



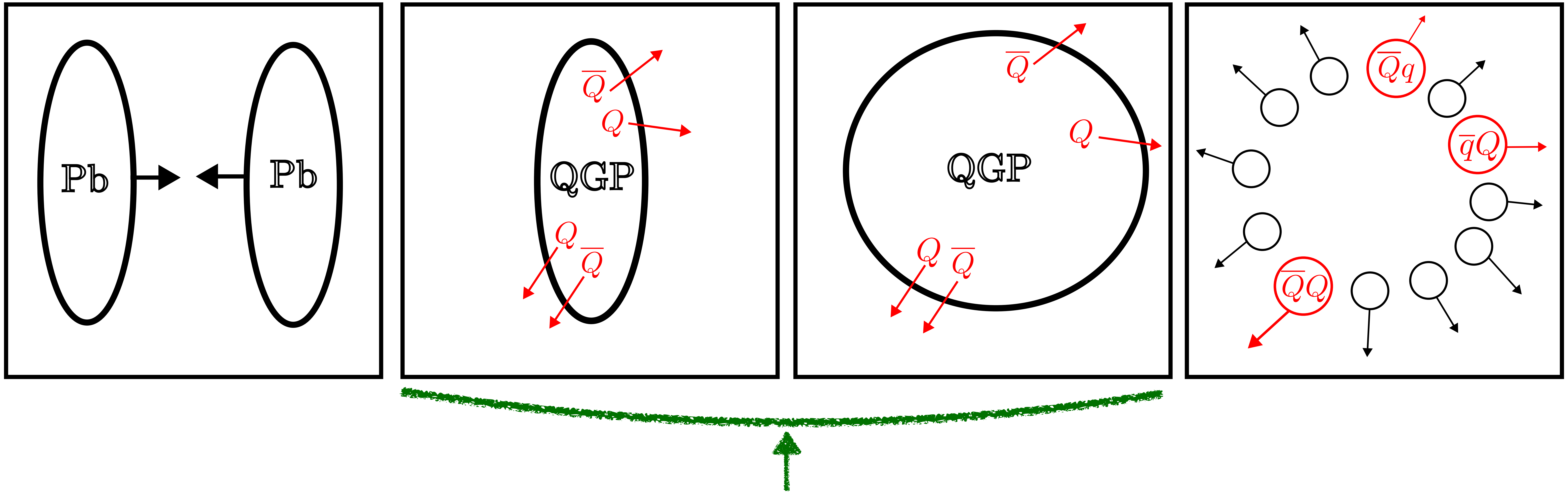




Conjectured Phase Diagram of QCD



Heavy Quarkonia in the QGP



- GOAL: Numerically study the heavy quark dynamics in the thermal QGP medium from first principles (as much as possible)

- PROBLEM: How to simulate quantum systems when dimension of Hilbert Space is very large?

Bottom Quarks within the QGP in full QCD

Schwinger Model Open Quantum System

NRQCD Open Quantum System

"The functional master equation can generate master equations for systems with an arbitrary finite number of heavy quarks in the QGP."

[Yukinao Akamatsu, 1209.5068, 1403.5783]

$$\mathcal{L}\rho(t) = \frac{d\rho}{dt} = -i[H,\rho] + \int \mathrm{d}^3x\mathrm{d}^3y\; D(x,y)\left(\tilde{O}^A(x)\rho(t)\tilde{O}^{A\dagger}(y) - \frac{1}{2}\{\tilde{O}^{A\dagger}(y)\tilde{O}^A(x),\rho\}\right)$$

$$\tilde{O}^A(x) = O^A(x) - \frac{1}{4T}[H, O^A(x)], \quad O^A(x) = \left[\psi_+^\dagger T^A\psi_+ - \psi_-^\dagger T^{*A}\psi_-\right](x)$$

$$\begin{aligned} H + \Delta H = &\int \mathrm{d}^3\vec{x}\; \psi_+^\dagger\frac{\nabla^2}{2M}\psi_+(x) + \psi_-^\dagger\frac{\nabla^2}{2M}\psi_-(x) \\ &+ \int \mathrm{d}^3\vec{x}\mathrm{d}^3\vec{y}\; \Sigma(|\vec{x}-\vec{y}|)\Big[-(\psi_+^\dagger T^A\psi_+)(\vec{x})(\psi_-^\dagger T^{*A}\psi_-)(\vec{y}) - (\psi_-^\dagger T^{*A}\psi_-)(\vec{x})(\psi_+^\dagger T^A\psi_+)(\vec{y}) \\ &\qquad + (\psi_+^\dagger T^A\psi_+)(\vec{x})(\psi_+^\dagger T^A\psi_+)(\vec{y}) + (\psi_-^\dagger T^{*A}\psi_-)(\vec{x})(\psi_-^\dagger T^{*A}\psi_-)(\vec{y})\Big] \end{aligned}$$

pNRQCD Open Quantum System

[Nora Brambilla, Miguel A. Escobedo, Joan Soto, Antonio Vairo 1612.07248, 1711.04515]

$$\frac{d\rho(t)}{dt} = -i[H,\rho(t)] + \sum_n\left[C_i^n\rho(t)C_i^{n\dagger} - \frac{1}{2}\left\{C_i^{n\dagger}C_i^n, \rho(t)\right\}\right]$$

$$H = \begin{pmatrix} h_s + \frac{r^2}{2}\gamma & 0 \\ 0 & h_o + \frac{N_c^2-2}{2(N_c^2-1)}\frac{r^2}{2}\gamma \end{pmatrix} \quad C_i^0 = \sqrt{\frac{\kappa}{N_c^2-1}}r_i\begin{pmatrix} 0 & 1 \\ \sqrt{N_c^2-1} & 0\end{pmatrix} \quad C_i^1 = \sqrt{\frac{\kappa(N_c^2-4)}{2(N_c^2-1)}}r_i\begin{pmatrix} 0 & 0 \\ 0 & 1\end{pmatrix}.$$

Caldeira Leggett

$$H = \frac{p^2}{M} - \frac{\alpha}{r} + \gamma\frac{r^2}{2} + \frac{\kappa}{4MT}\{r,p\}$$

$$C = \sqrt{\kappa}\left(r + \frac{ip}{2MT}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}\rho(t) = -i[H,\rho] + C\rho C^\dagger - \frac{1}{2}\left\{C^\dagger C, \rho\right\}$$

[A. O. Caldeira and A. J. Leggett Phys. Rev. Lett. **48**, 1571 (1982)]

- Schwinger Model is a QCD-like theory in 1+1d dimensions that is used as a testbed for numerical methods

$$\mathscr{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(i\partial_\mu - eA_\mu - m)\psi + g\phi\bar{\psi}\psi + \mathscr{L}_\phi$$

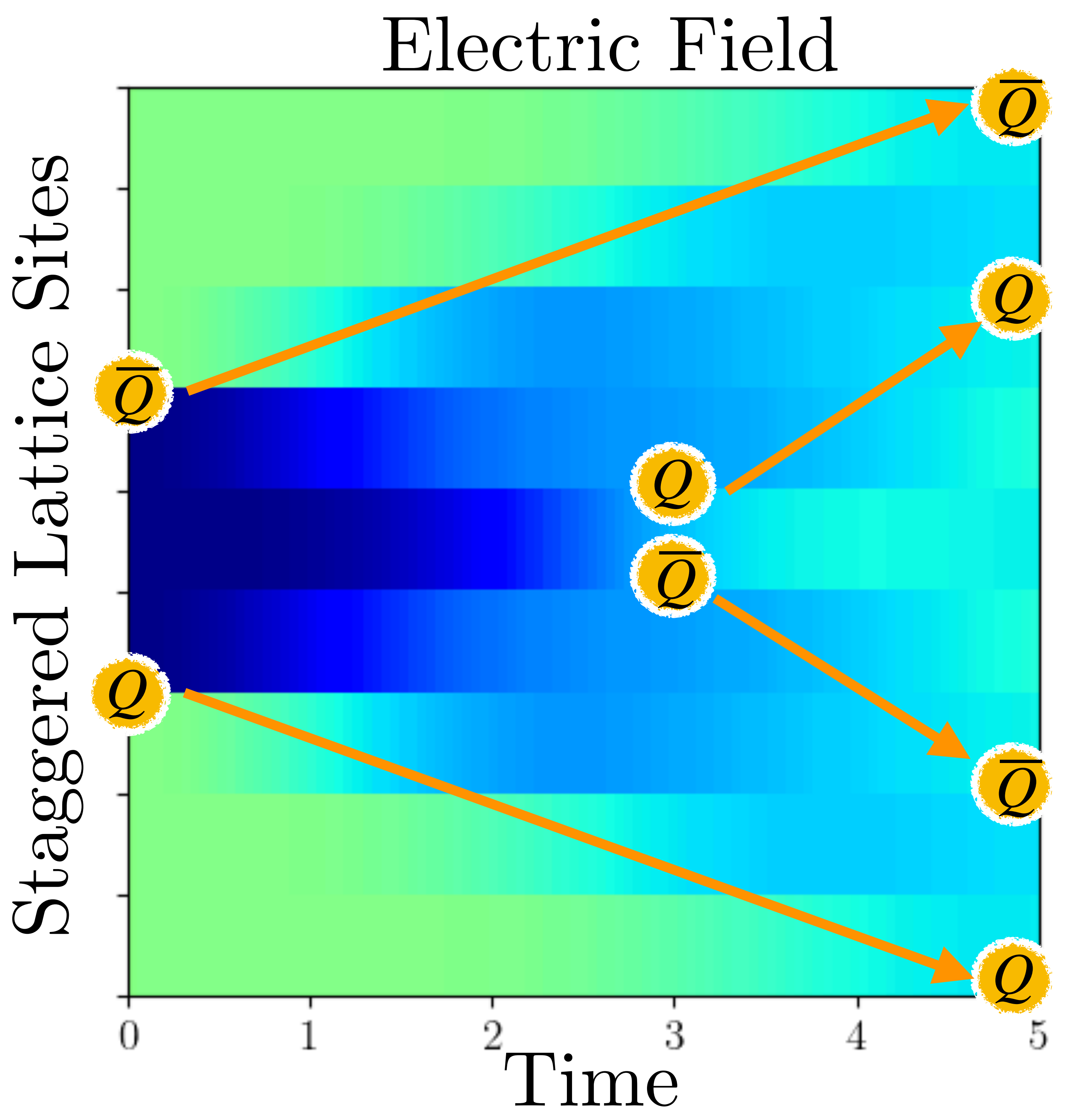
$U(1)$-charged fermion ("quark")

Environmental d.o.f. that are integrated out ("QGP")

- Performing this procedure, a lattice-Lindblad equation is derived:

$$L\rho(t) := \frac{d\rho(t)}{dt} = -i\left[H,\rho(t)\right] + a^2\sum_{i,j} D_{ij}\left(\widetilde{O}_i\rho(t)\widetilde{O}_j^\dagger - \frac{1}{2}\left\{\widetilde{O}_j^\dagger\widetilde{O}_i,\rho(t)\right\}\right)$$

$$\widetilde{O}_i \equiv O_i - \frac{1}{4T}[H,O_i],\quad \widetilde{O}_i^\dagger \equiv O_i + \frac{1}{4T}[H,O_i]$$



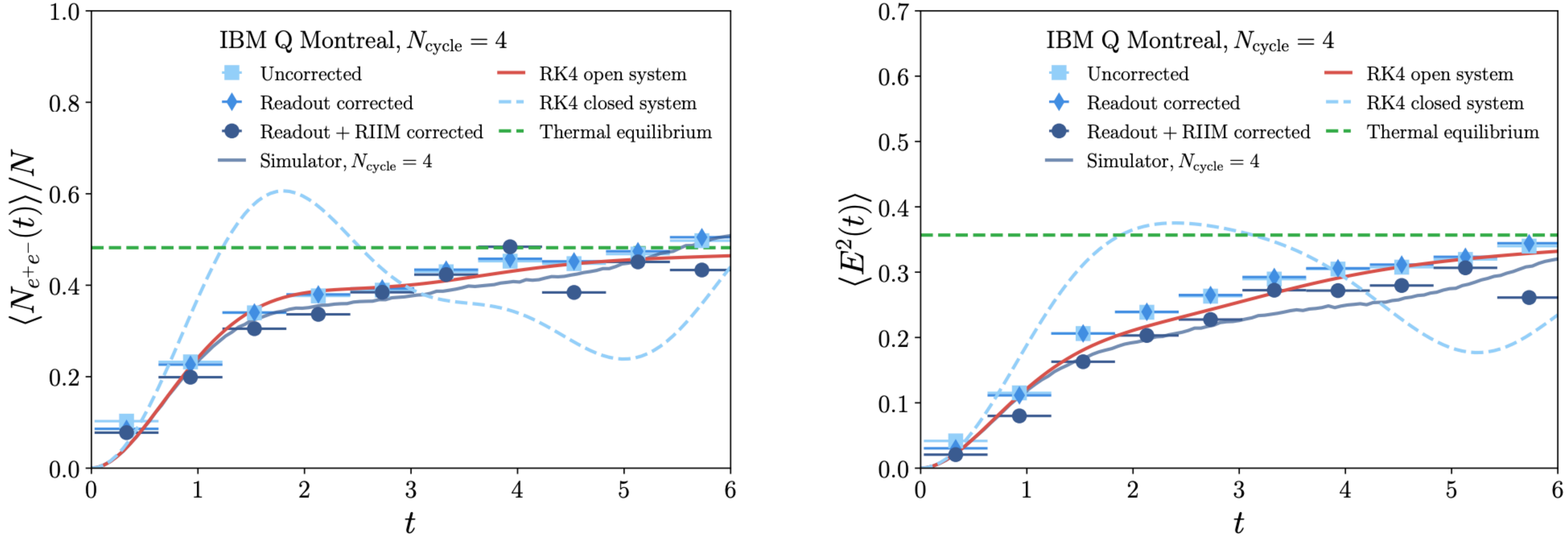
[K. Lee, J. Mulligan, F. Ringer, X. Yao: 2308.03878]

$$L = 10 \implies \text{dim} = (2^{10})^2 \sim 10^6$$

$$L = 20 \implies \text{dim} = (2^{20})^2 \sim 10^{12}$$

Quantum Computing Investigations

[Wibe A. de Jong, Kyle Lee, James Mulligan, Mateusz Ploskon, Felix Ringer, and Xiaojun Yao, 2106.08394]



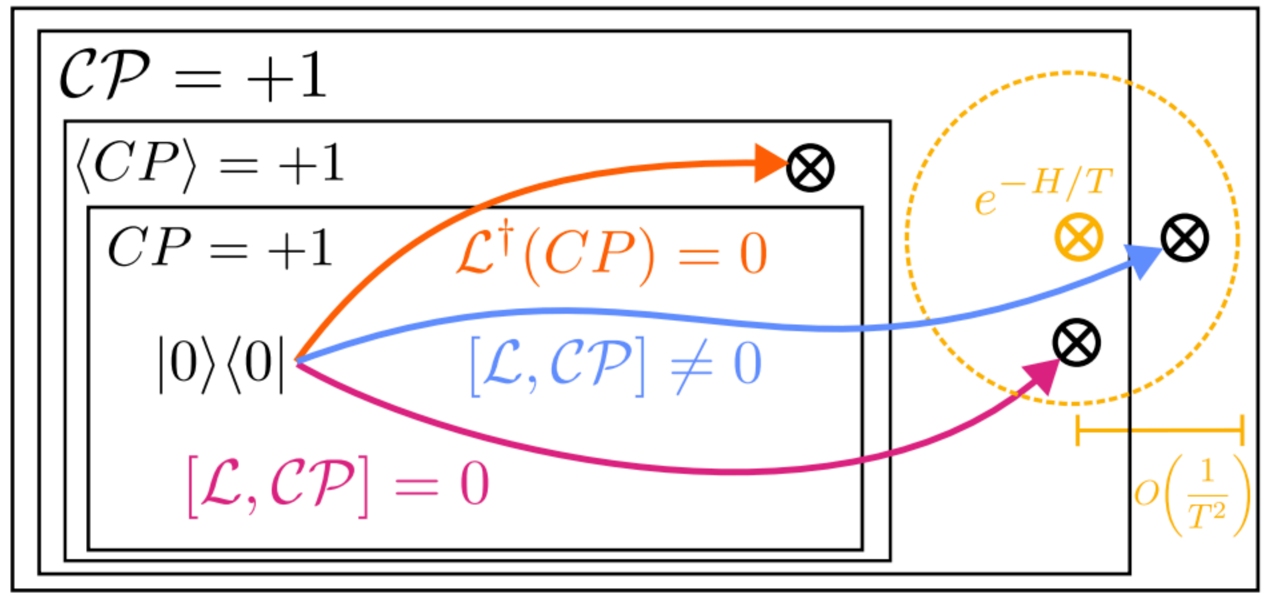
(N_{sites} = 2, Schwinger Model Open Quantum System)

[Symmetries and conserved quantities in lindblad master equations, V. V. Albert and L. Jiang]

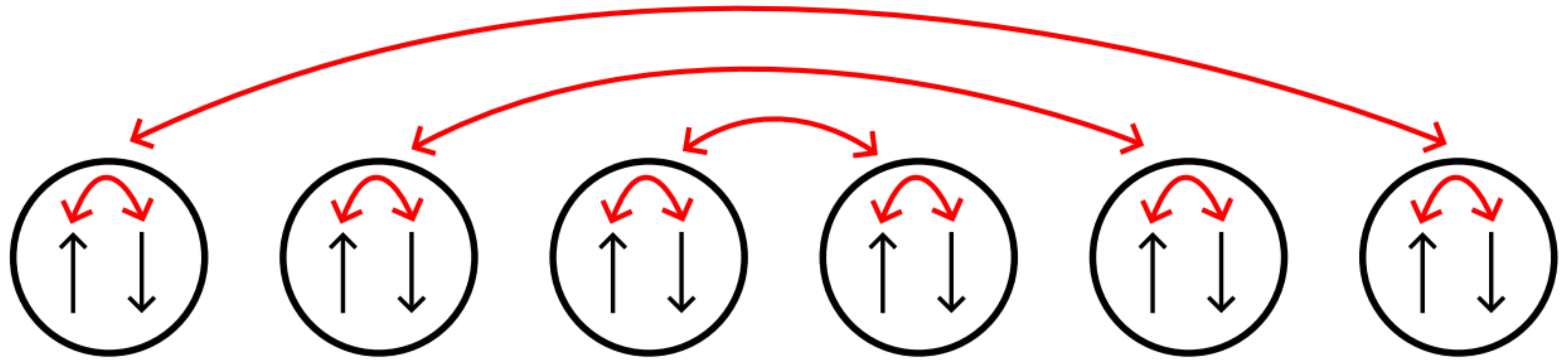
(2402.06607)

$$\begin{array}{ccc} & [Q,H]=[Q,F_l]=0 \quad \forall l & \\ \Leftrightarrow & & \Downarrow \\ \frac{d}{dt}Q=\mathcal{L}^\dagger(Q)=0 & \Rightarrow & [\mathcal{Q},\mathcal{L}]=0 \end{array}$$

(a) Relationship between discrete conserved charges Q and dynamical symmetries [75]. F_l are the diagonalized jump operators corresponding to the Lindbladian $\mathcal{L}$, see Equation (A.4). $\mathcal{Q} = Q \otimes Q$ is the charge super-operator, and $\mathcal{L}^\dagger(Q)$ notates the Heisenberg evolution of Q.



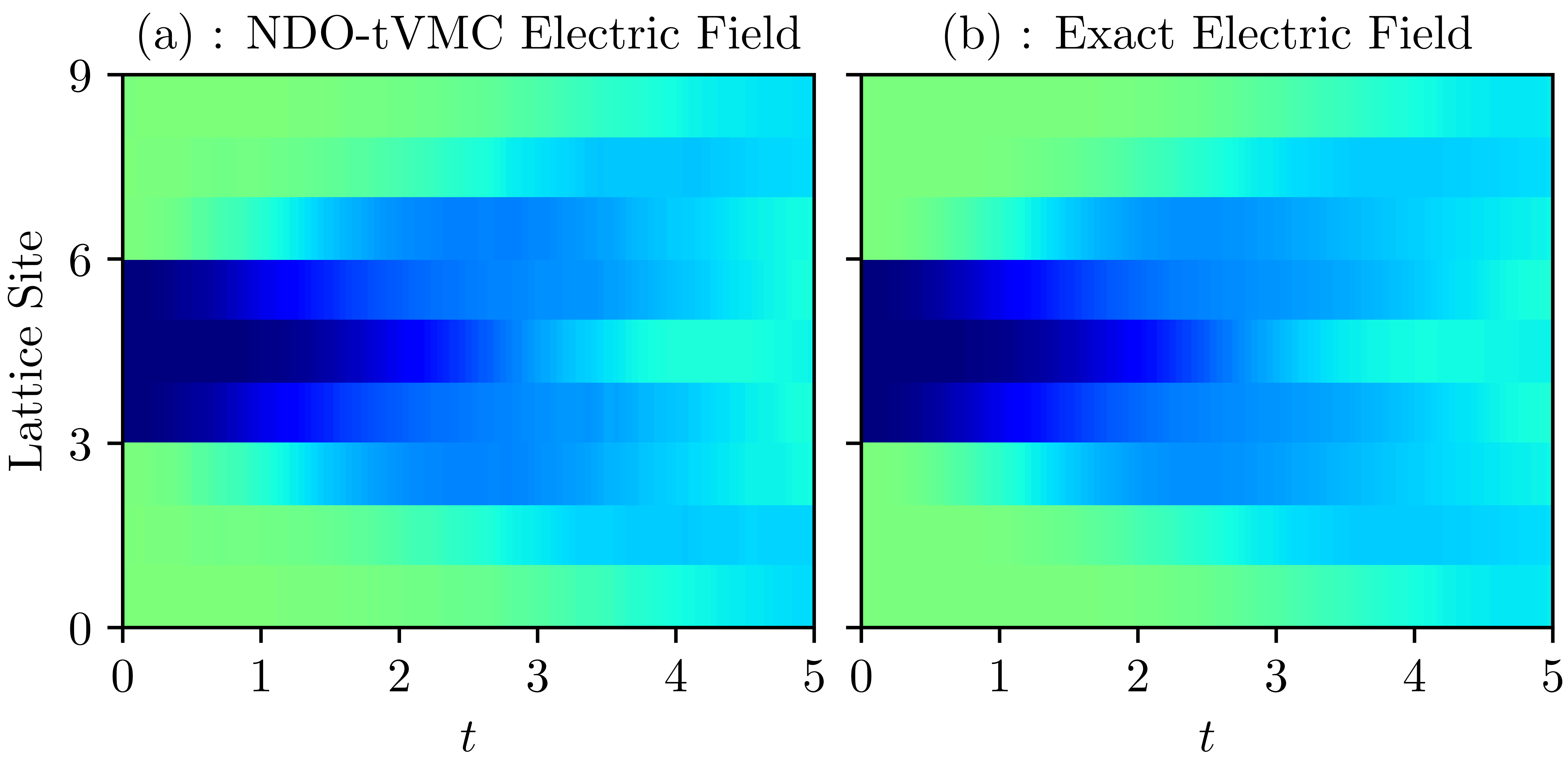
(b) Different evolutions and steady states depending on the CP-nature of the coupling matrix. The pictured initial state is the free ground state. Orange depicts strong CP conservation, maroon depicts weak CP conservation and blue depicts no CP conservation.



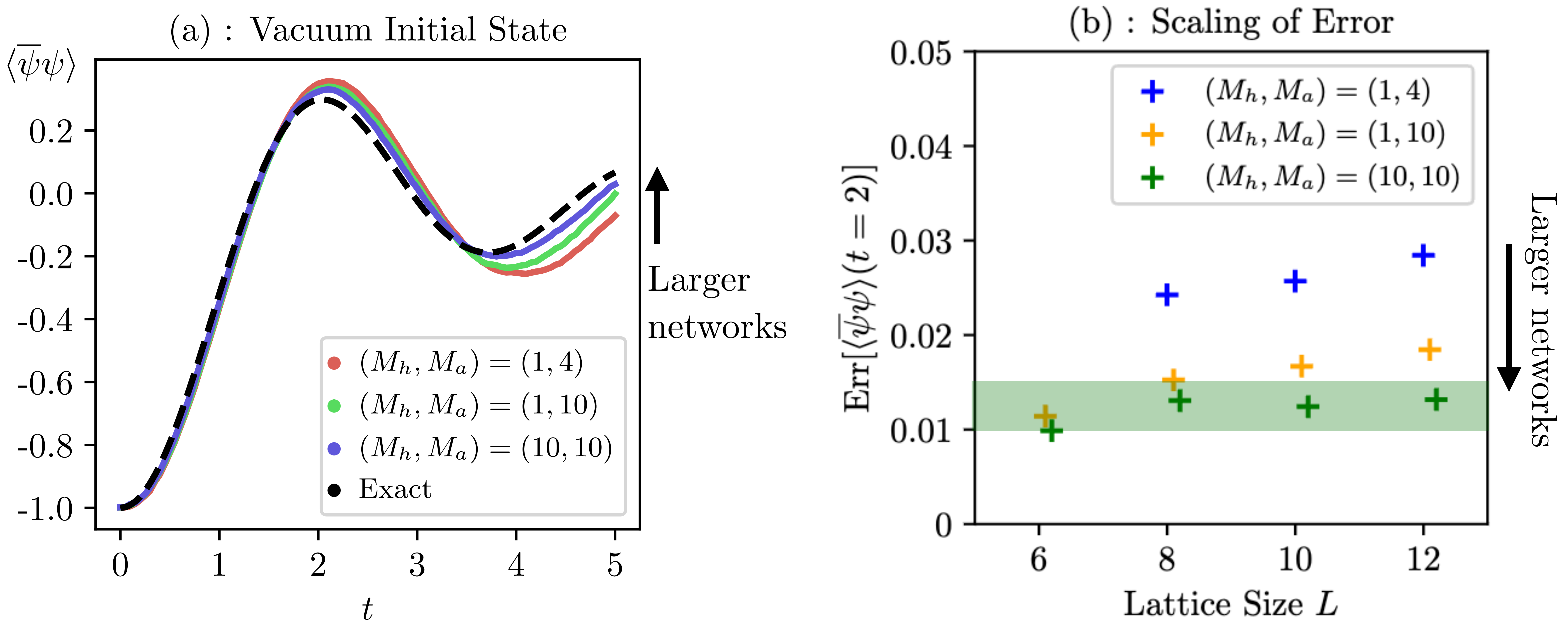
(c) Schematic of the CP operator, which is a combination of a bond-reflection S and swapping $\uparrow,\downarrow$ on each staggered site, where $\uparrow,\downarrow$ represent the spin-$\frac{1}{2}$ basis of σ^z. Note that there are no individual C, P symmetries - in particular $[H,S] \neq 0$, and $[H, \prod \sigma_x] \neq 0$.

Electric Field Comparisons on L = 10

◆ Neural Networks reproduce exact simulations on small system sizes!

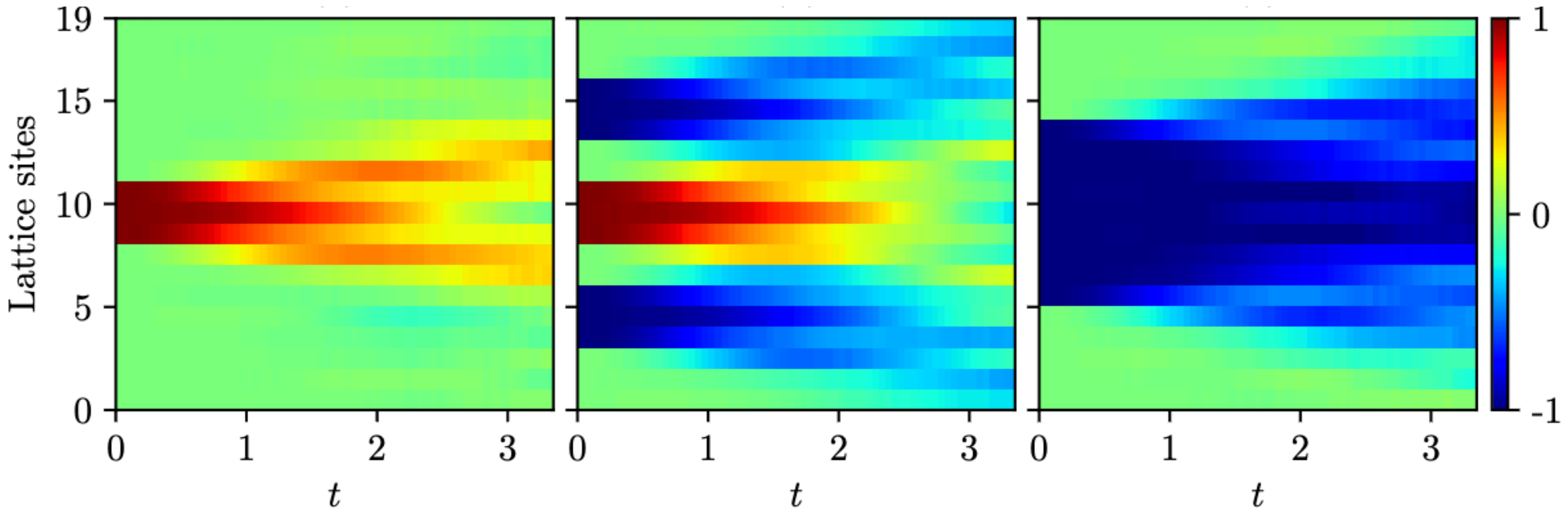


(2210 parameters, parametrising a 63504 dimensional space)



◆ Systematic Errors introduced by Neural Network Ansatz are under control

Real-time simulations on L = 20

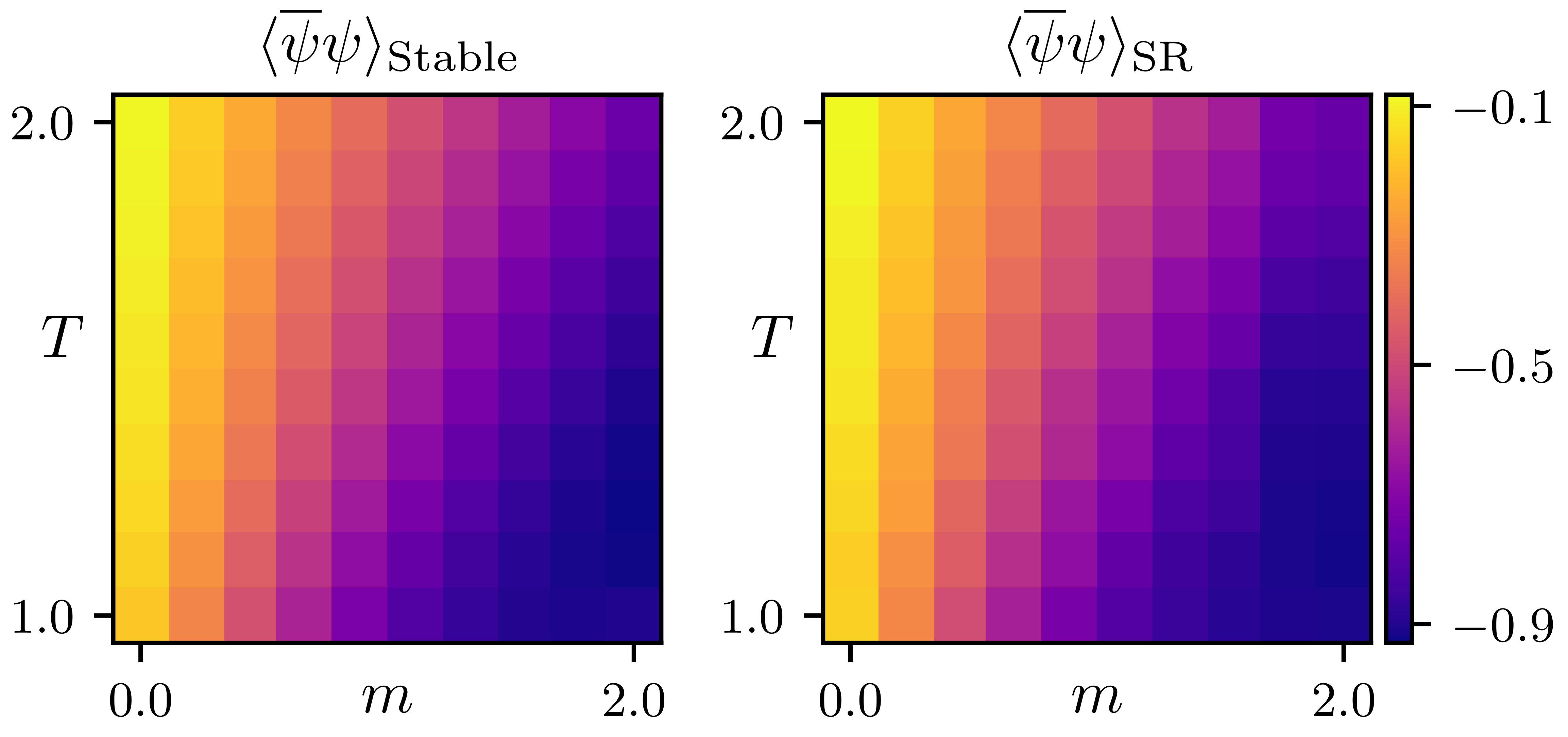


- String breaking due to formation of e+e- pair
- String-String interactions
- Long string dynamics

(9280 real parameters, parametrising a $3 \cdot 10^{10}$ dimensional space)

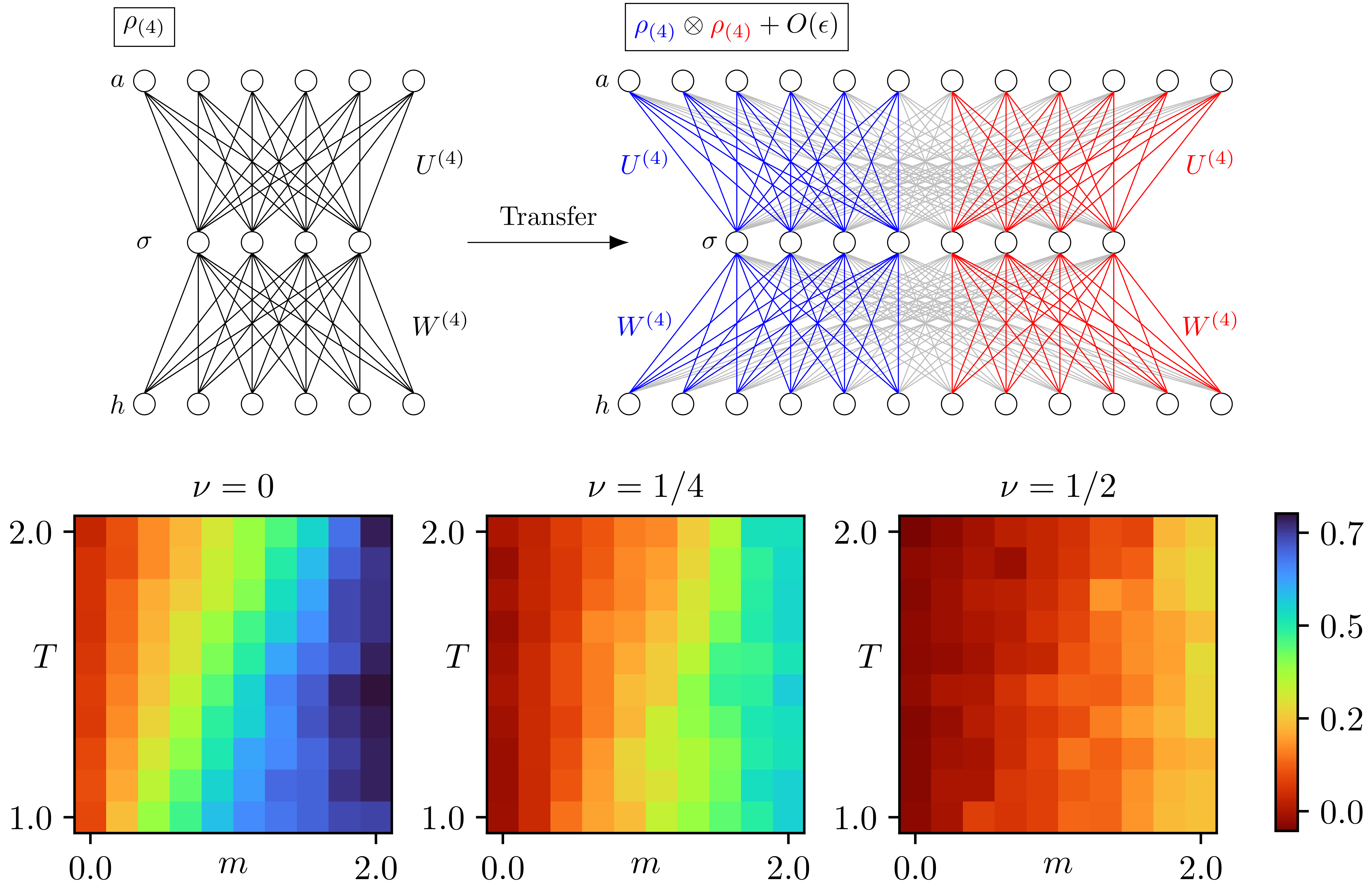
- In the long-time limit, Lindbladian dynamics drives the state towards the thermal state.

Exact Chiral condensate ML chiral condensate



Good agreement on L=4 (small system sizes!)

Transfer learning to larger lattice sizes



Lessons

Upshot

- First demonstration that systematic errors are under control for Open Quantum System evolution using Neural Networks in a lattice gauge theory

Toward the future

with Tom Magorsch, Nora Brambilla, Phiala Shanahan

Schwinger Model OQS → (p)NRQCD OQS

"strictly more physical"

Latent Space Purification (NDO) → AGHDO

[Giacomo Torlai and Roger G. Melko 1801.09684]

[Michael J. Hartmann, Giuseppe Carleo 1902.05131]

[Filippo Vicentini, Riccardo Rossi, and Giuseppe Carleo 2206.13488]

(+ universal approximation, strictly more general ansatz)

(Autoregressive nature means no need for MCMC sampling)

(Mapping spin system structure onto
nonrelativistic problem is strange though!)

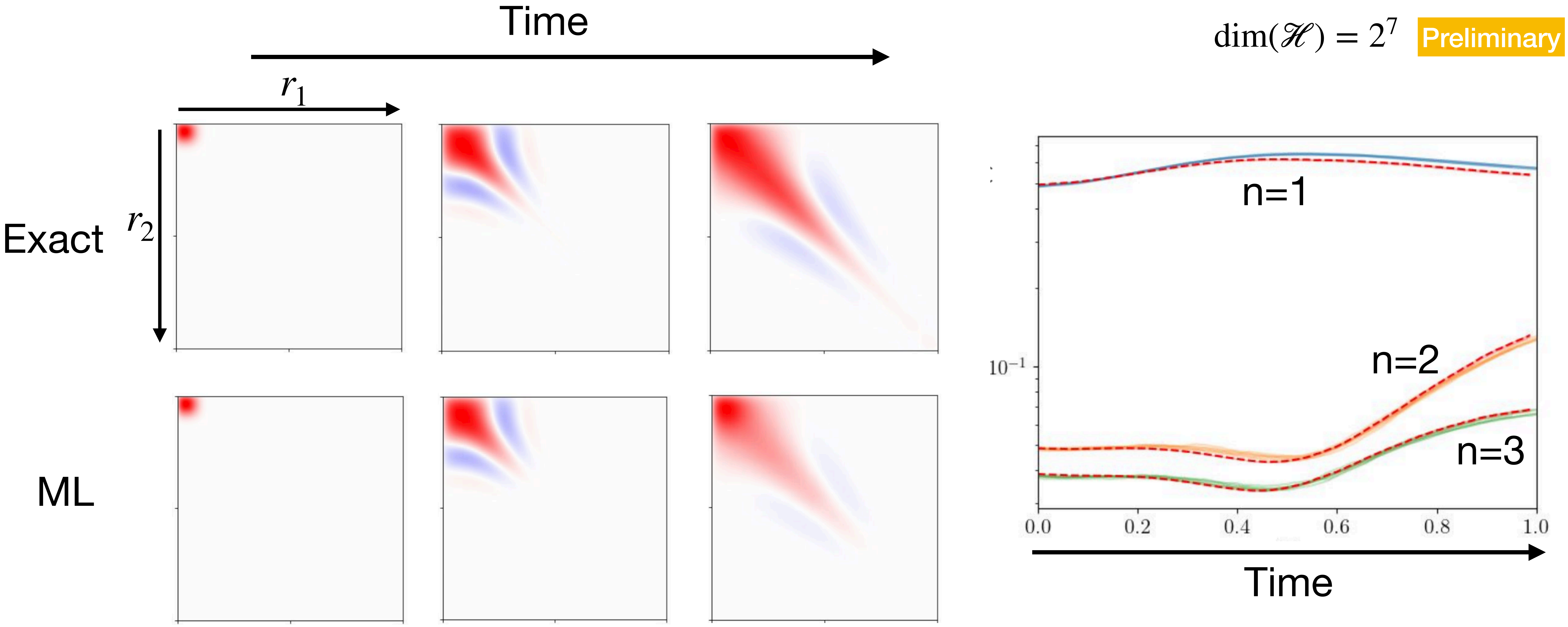
tVMC → projected-tVMC

[Giuseppe Carleo, Federico Becca, Marco Schiró, Michele Fabrizio, 1109.2516]

[Alessandro Sinibaldi, Clemens Giuliani, Giuseppe Carleo, Filippo Vicentini, 2305.14294]

(fixes exponentially large sample size requirement)

$\dim(\mathscr{H}) = 2^7$ Preliminary



Joshua Lin (joshua.lin@anl.gov)

Considering going Neural?

What are the competing numerical methods?

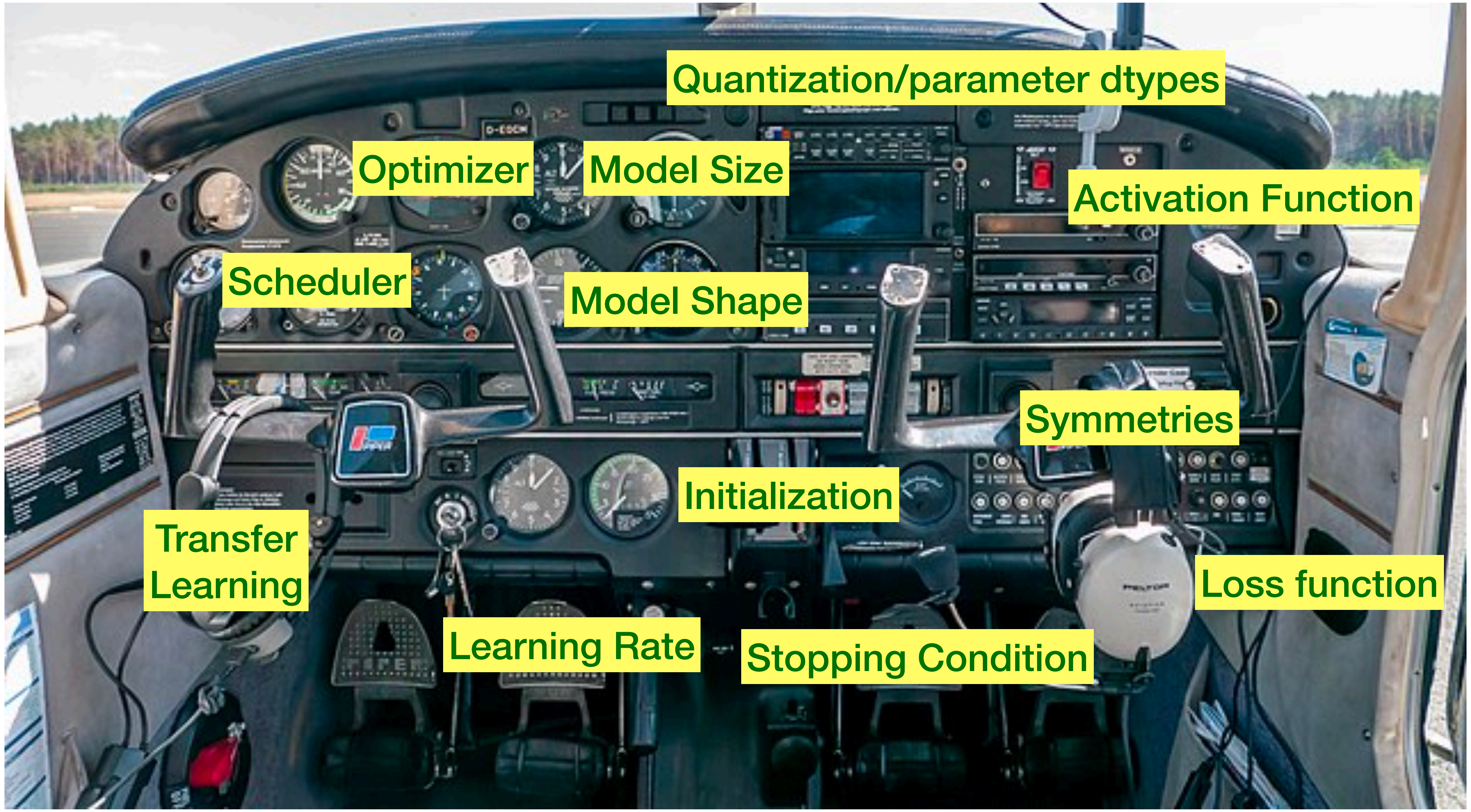
Does your system have interesting physics that *only* shows up for very large Hilbert space sizes?

Does your Hilbert space have many symmetries that can be exploited?

Is there an appropriate architecture?

Can you find people to train your networks?

What training a model feels like



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Thank you!