Title: [Virtual] Exploring Quantum Science with Machine Learning

Speakers: Di Luo

Collection: Machine Learning for Quantum Many-Body Systems

Date: June 12, 2023 - 10:00 AM

URL: https://pirsa.org/23060028

Abstract: ZOOM: https://pitp.zoom.us/j/94595394881?pwd=OUZSSXpzYlhFcGlIRm81Y3VaYVpCQT09

Exploring Quantum Science with Machine Learning

Di Luo
IAIFI Fellow, MIT

1

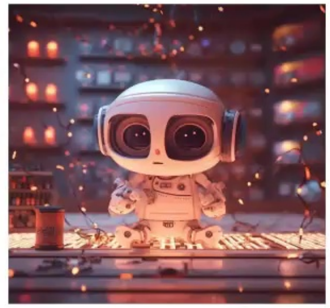
AI for Quantum Many-body Physics & Quantum Information Science

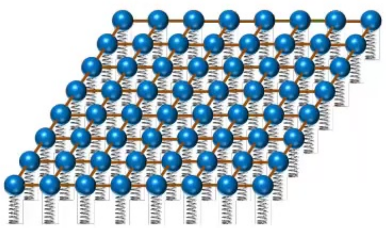
IAIFI: The NSF AI Institute for Artificial Intelligence and Fundamental Interactions

Quantum Many-body Simulation & Quantum Information Science

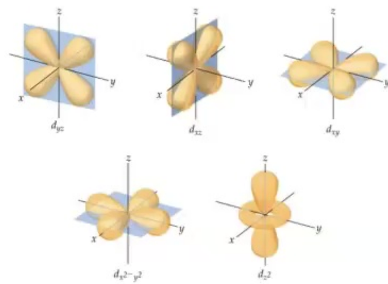
C2QA: Co-design Center for Quantum Advantage

AI for Quantum

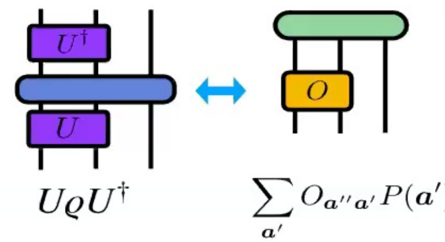




High energy physics



Condensed matter physics



Quantum information science

ChatGPT

AU

Challenges of Quantum Many-body Physics Simulation

Quantum many-body physics simulation involves simulating the behavior of a large number of interacting quantum systems. This is a challenging task due to the exponential growth of the dimensionality of the Hilbert space with the number of particles in the system. This makes it difficult to simulate systems with a large number of particles using classical computers. Additionally, the complexity of the interactions between the particles, such as those described by the Coulomb force, also makes simulation difficult. Other challenges include dealing with decoherence and the need for efficient algorithms for manipulating and measuring large quantum states.

Quantum Many-body Physics Simulation

Spectrum calculation

$$H|\psi> = E|\psi>$$

Eg. phase diagram, excited states, steady states

Real time evolution

$$H(t)\,|\,\psi(t)\rangle = i\hbar \frac{d}{dt}\,|\,\psi(t)\rangle$$

Eg. quantum chaos, quantum circuit simulation, dynamics of gauge theories

Challenges:

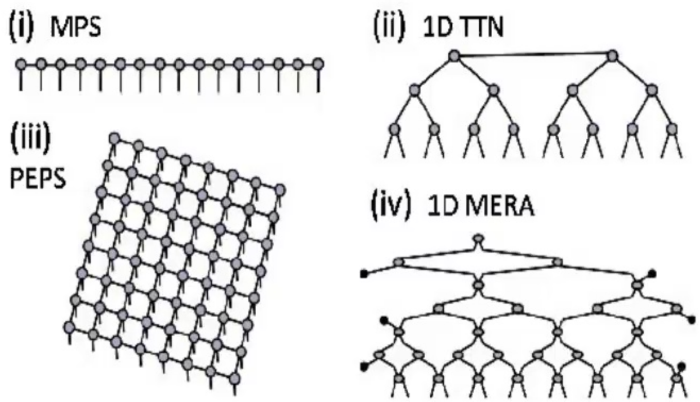
- Sign problem: non-positive real number / complex number
- high dimensionality: Hilbert space scales exponentially with particles

Ongoing Efforts: Tensor Network

Tensor network: tensor decomposition of high dimensional objects

High rank tensor

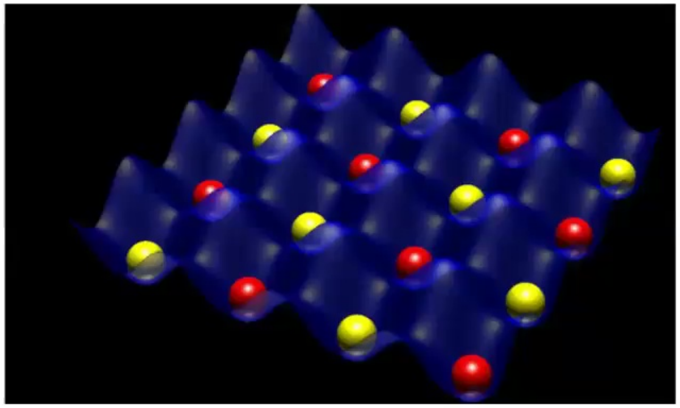
$$T_{i,j,k,l} =$$



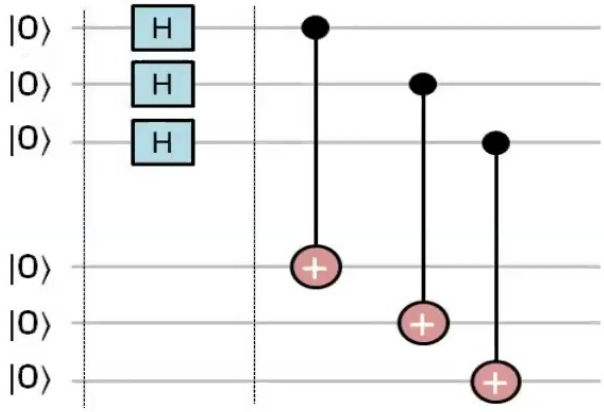
- Efficient for 1 dimensional system due to area law
- Challenges exist for two or three dimensional physics system

Ongoing Efforts: Quantum Computation

Quantum computation: naturally represents and operates on quantum objects



Analog quantum computation



Digital quantum computation

- Natural for quantum dynamics, could be used for ground state problems
- Challenges exist under current technology

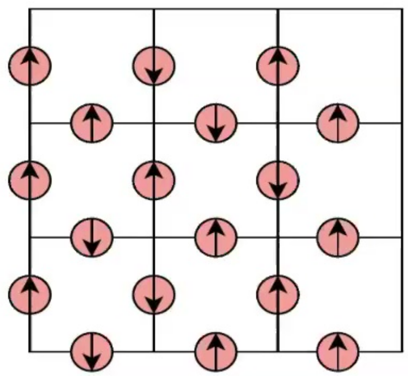
Neural Quantum States

For a n-particle (spin ½) system:

2^n x 2^n hermitian matrix ←

$$H|\psi> \; = E|\psi>$$

2^n vector

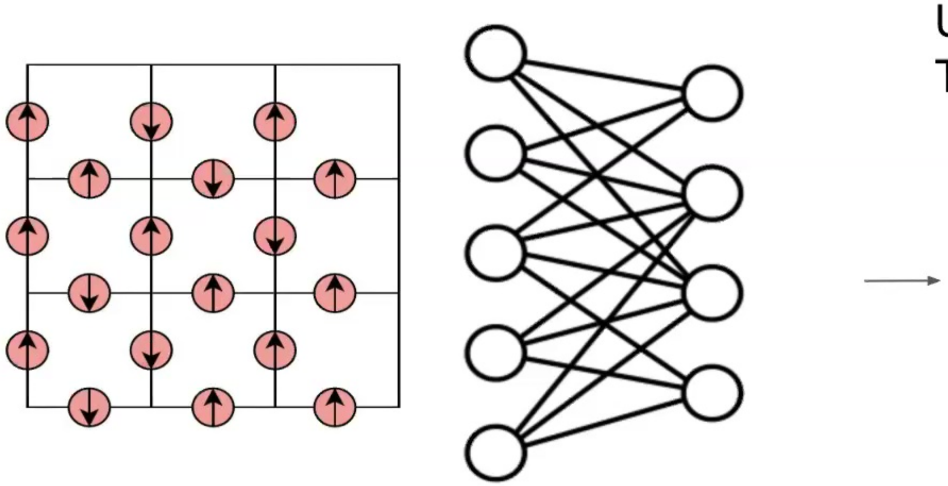


Superposition of 2^n configurations!

Q: Can machine learning help to find the best superposition of configurations?

Neural Quantum States

Neural network: low dimensional representation of high dimensional objects



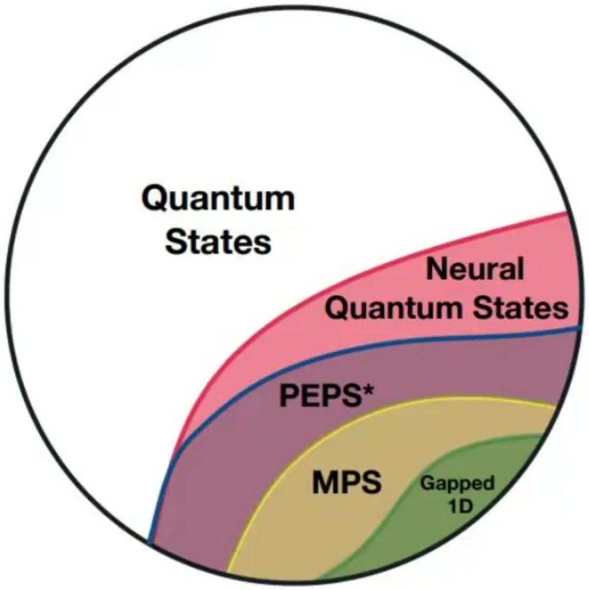
Configuration $\boldsymbol{x}$

Universal Approximation Theorem [Cybenko]

$$\Psi(x)$$

Wave function amplitude [Carleo]

Neural Quantum States



Or Sharir, Amnon Shashua, Giuseppe Carleo
https://arxiv.org/abs/2103.10293

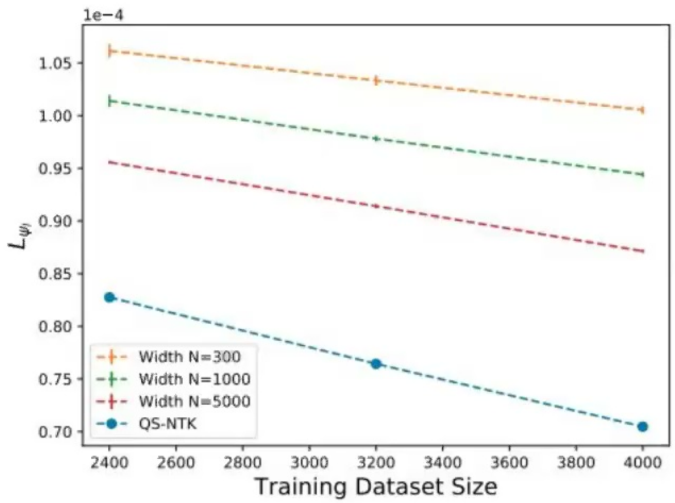
Neural Network Quantum State:

- It is able to represent volume law state
- Exact representation for Jastrow, stabilizer states
- Variational simulation for theories with sign problems

Neural Quantum States

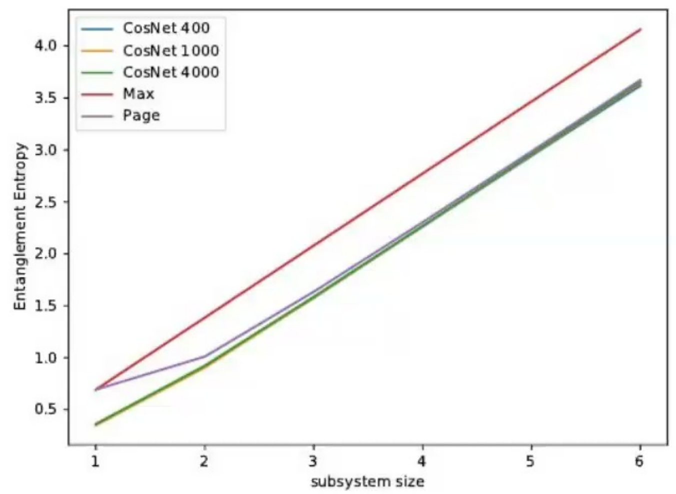
Di Luo, James Halverson, arxiv: 2112.00723

Infinite Neural Network Quantum State: Entanglement and Training Dynamics



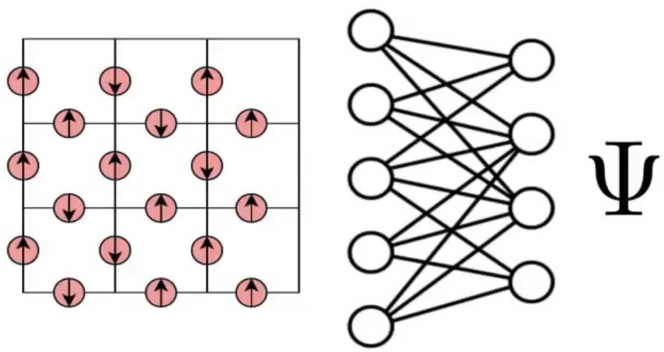
Quantum State Neural Tangent Kernel

<u>Theorem.</u> Quantum state supervised learning training is guaranteed to converge in infinite width limit.



Volume law entanglement engineering of CosNet

Neural network representation



Broken-Symmetry Ground States of the Heisenberg Model on the Pyrochlore Lattice

Nikita Astrakhantsev, Tom Westerhout, Apoorv Tiwari, Kenny Choo, Ao Chen, Mark H. Fischer, Giuseppe Carleo, and Titus Neupert
Phys. Rev. X **11**, 041021 – Published 29 October 2021

Dirac-Type Nodal Spin Liquid Revealed by Refined Quantum Many-Body Solver Using Neural-Network Wave Function, Correlation Ratio, and Level Spectroscopy

Yusuke Nomura and Masatoshi Imada
Phys. Rev. X **11**, 031034 – Published 12 August 2021

Deep-neural-network solution of the electronic Schrödinger equation

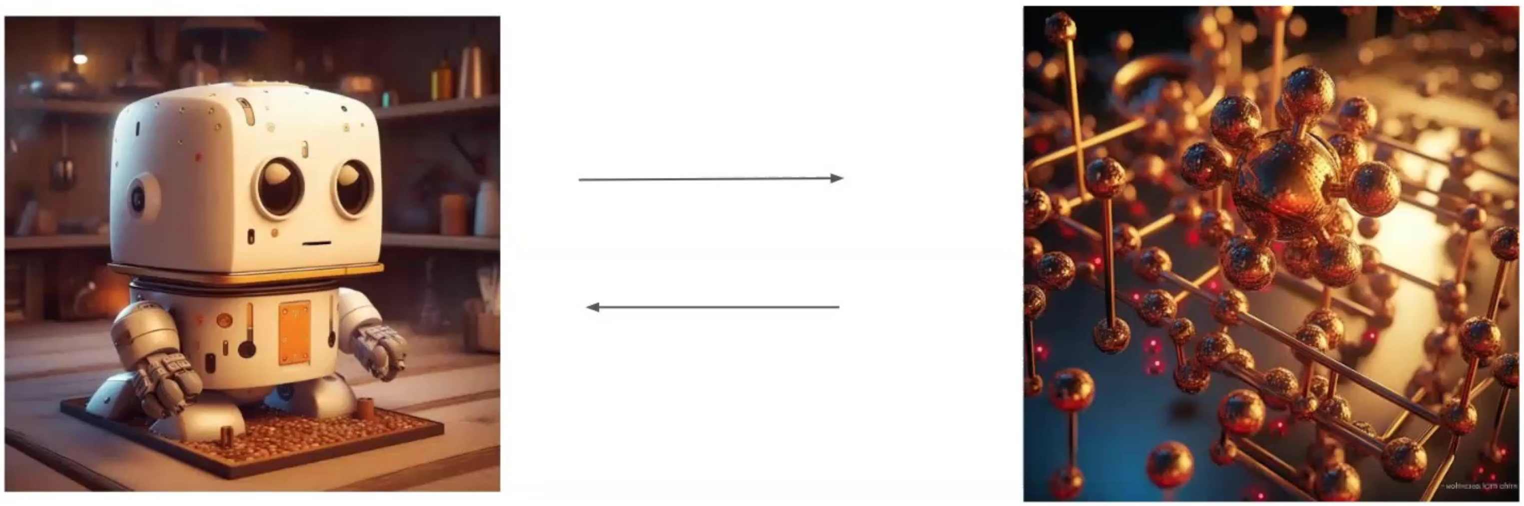
Jan Hermann, Zeno Schätzle & Frank Noé

Nature Chemistry **12**, 891–897 (2020) | Cite this article

Quantum Many-Body Dynamics in Two Dimensions with Artificial Neural Networks

Markus Schmitt and Markus Heyl
Phys. Rev. Lett. **125**, 100503 – Published 2 September 2020

AI for Quantum: Strongly Correlated Physics



Electronic Structure Study

Hamiltonian → Method → Materials Property
Phase Diagram

Method → Variational Wave Function

Variational wave function
in electronic structure study

R → Variational Wave Function → Ψ(R)

Variational Wave Function →

Goal:

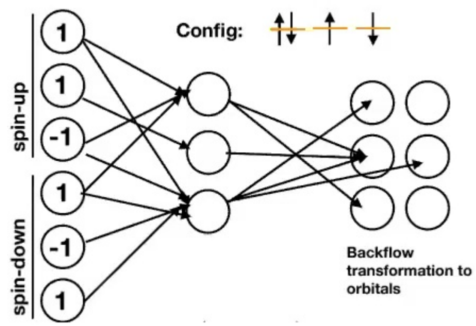
Lower energy,
Obey symmetry,
Right in mean field limit,
….

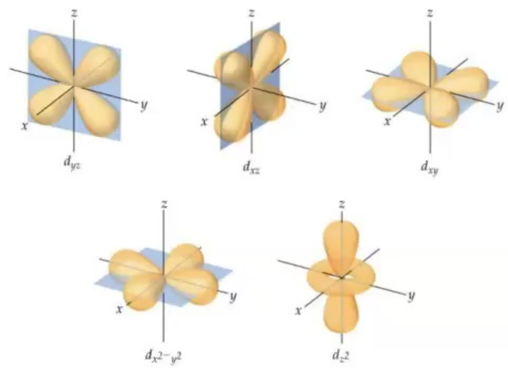
Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Backflow Transformations via Neural Networks for Quantum Many-Body Wave-Functions

--- Develop anti-symmetry neural network for fermionic simulations

$$\Psi(\cdots, x_i, \cdots, x_j, \cdots) = -\Psi(\cdots, x_j, \cdots, x_i, \cdots)$$





18

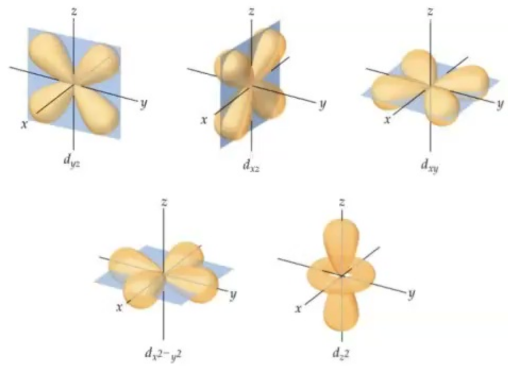
Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Neural Network Backflow

Jastrow

+

Backflow
Slater Determinant



Pro: include correlation effect

Con: hard to figure out good configuration dependent orbitals

Mean field solution

$$\Psi(\mathbf{r}) = det([\phi_{k\sigma}(r_{i,\sigma})])$$

?

Backflow transformation

[Feynman], [Sorella]

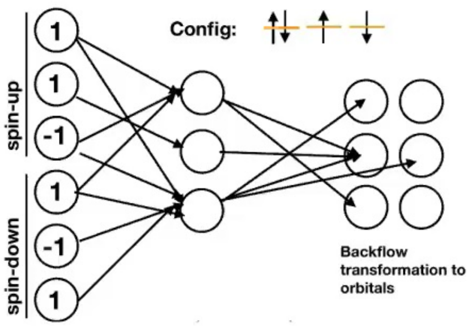
Configuration dependent orbitals

General form of backflow?

r → Determinant → $\Psi(\mathbf{r}) = det([\phi^b_{k\sigma}(r_{i,\sigma};\mathbf{r})])$

Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Neural Network Backflow



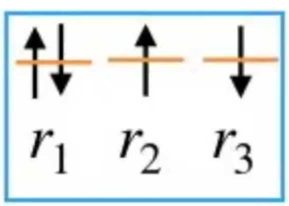
Neural network interacting orbitals

Mean field orbital

Neural network backflow output

$$\phi^b_{k\sigma}(r_{i,\sigma};\boldsymbol{r}) = \phi_{k\sigma}(r_{i,\sigma}) + a^{NN}_{ki,\sigma}(\boldsymbol{r})$$

- Configuration dependent many-particle orbital
- Allow neural network to work with fermion and change sign structure directly
- Generalization of backflow to arbitrary system



Input configuration ***r***

Determinant

$$\Psi(\mathbf{r}) = det([\phi^b_{k\sigma}(r_{i,\sigma};\mathbf{r})])$$

Neural Network Backflow

Variational Monte Carlo:

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$$

$$\partial_\theta E(\theta) = \frac{1}{N} \sum_{x\sim|\psi_\theta(x)|^2} [(E_L(x) - \langle E_L\rangle)\nabla_\theta log\psi_\theta(x)]$$

Sampling without sign problem

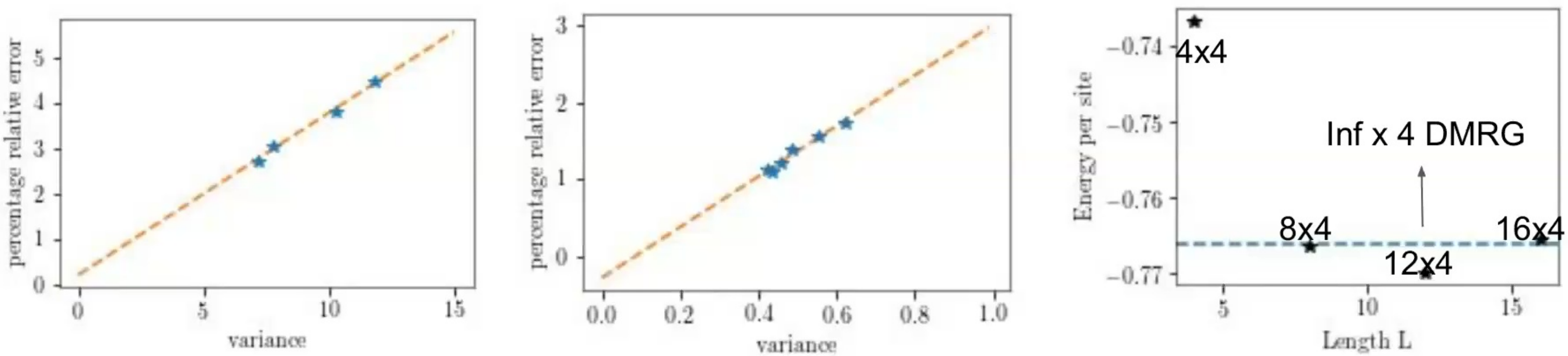
Local energy $E_L(x) = \frac{H\psi_\theta(x)}{\psi_\theta(x)}$

Parameterized wave function

Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Neural Network Backflow

Generalization of backflow to arbitrary lattice systems with complicated sign structure.



16x4 Hubbard, U/t=8, n=0.875
Variance extrapolation
error=0.209%

4x4x3 Kagome
Variance extrapolation
error=0.286%

Hubbard model,
U/t=8, n=0.875,
finite size study

Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Neural Network Backflow

- Anti-symmetric neural network
- Change sign structure directly and generalization to arbitrary lattices
- Theoretically exact and lower bound for existing backflow methods, generalization of Slater-Jastrow-Backflow hierarchy
- Further advancement in quantum chemistry: FermiNet, PauliNet

Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Neural Network Backflow

Machine learning many-electron wave functions via backflow transformations

1. **Backflow Transformations via Neural Networks for Quantum Many-Body Wave-Functions**
   Authors: D. Luo and B. K. Clark
   Phys. Rev. Lett. 122, 226401 (2019); arXiv:1807.10770
2. **Ab-Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks**
   Authors: D. Pfau, J. S. Spencer, A. G. de G. Matthews, and W. M. C. Foulkes
   arXiv:1909.02487
3. **Deep neural network solution of the electronic Schrödinger equation**
   Authors: J. Hermann, Z. Schätzle, and F. Noé
   arXiv:1909.08423

Recommended with a Commentary by Markus Holzmann, Univ. Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

https://doi.org/10.36471/JCCM_May_2020_01

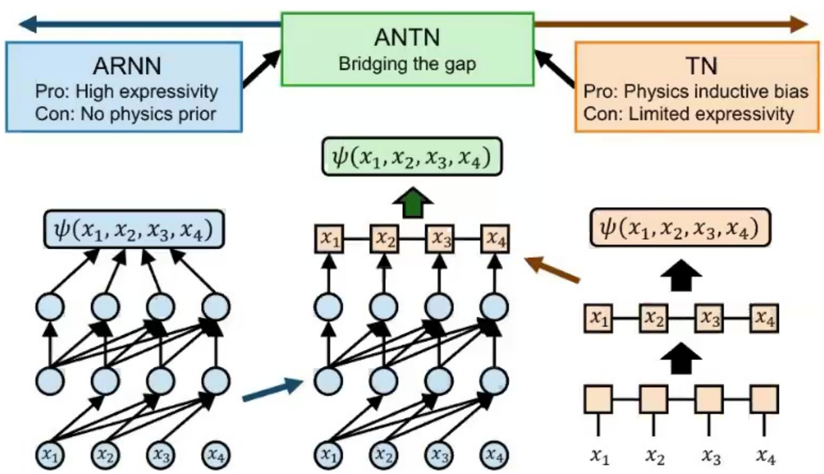
Advancement in Fermionic Simulation:

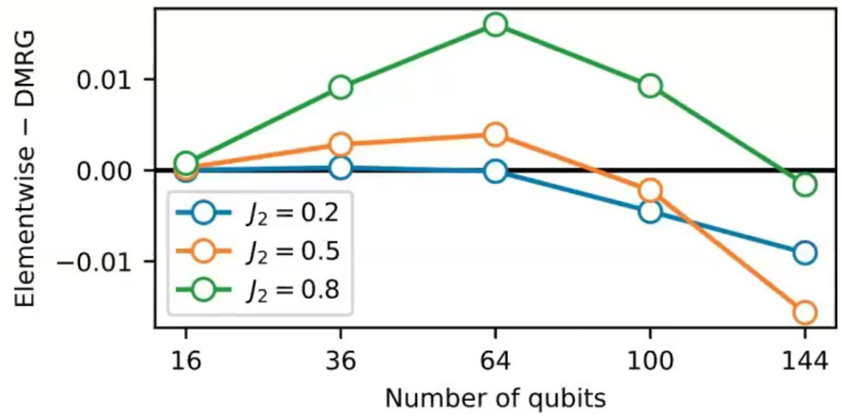
- J Stokes, JR Moreno, EA Pnevmatikakis, G Carleo, Physical Review B 102 (20), 205122
- Kenny Choo, Antonio Mezzacapo & Giuseppe Carleo, Nature Communications volume 11, 2368 (2020)
- Javier Robledo Moreno, Giuseppe Carleo, Antoine Georges, James Stokes, PNAS 119 (32)
- Hao Xie, Zi-Hang Li, Han Wang, Linfeng Zhang, Lei Wang, arxiv: 2209.06095
- Di Luo, Aidan P. Reddy, Trithep Devakul, Liang Fu, arxiv: 2303.08162
- G Pescia, J Nys, J Kim, A Lovato, G Carleo, arxiv:2305.07240
- ....

Zhuo Chen, Laker Newhouse, Eddie Chen, Di Luo, Marin Soljačić, arxiv.2304.01996

ANTN: Bridging Neural Networks and Tensor Networks for Quantum Many-Body Simulation

--- Develop Autoregressive Neural TensorNet which generalizes tensor network and autoregressive neural networks
--- Equip with exact sampling, tensor network physical inductive bias and symmetries construction





Neural POVM Simulation of Quantum Dynamics

Q: What is the connection of the quantum world and the classical world?

Wavefunction/ Density Matrix → **Probability**

Unitary Dynamics

Quantum Channel → **Quasi-stochastic Process**

Quantum world

(oscillating phase and dynamics)

'Classical' world ?

M Schmitt, M Heyl, Physical Review Letters 125 (10), 100503

Irene López Gutiérrez, Christian B. Mendl, Quantum 6, 627 (2022)

Neural POVM Simulation

Positive Operator-Valued Measurement (POVM)

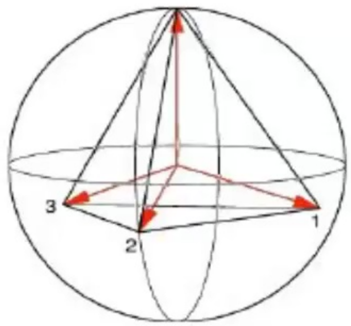
Tetrahedral POVM:

$$P_{(i)} = \mathrm{tr}(\rho M_{(i)})$$

$$M_{(i)} = \frac{1}{4}(\mathbb{1} + v_{(i)} \cdot \sigma)$$

$$v_{(1)} = (1, 1, 1) \quad v_{(2)} = (1, -1, -1)$$

$$v_{(3)} = (-1, 1, -1) \quad v_{(4)} = (-1, -1, 1)$$



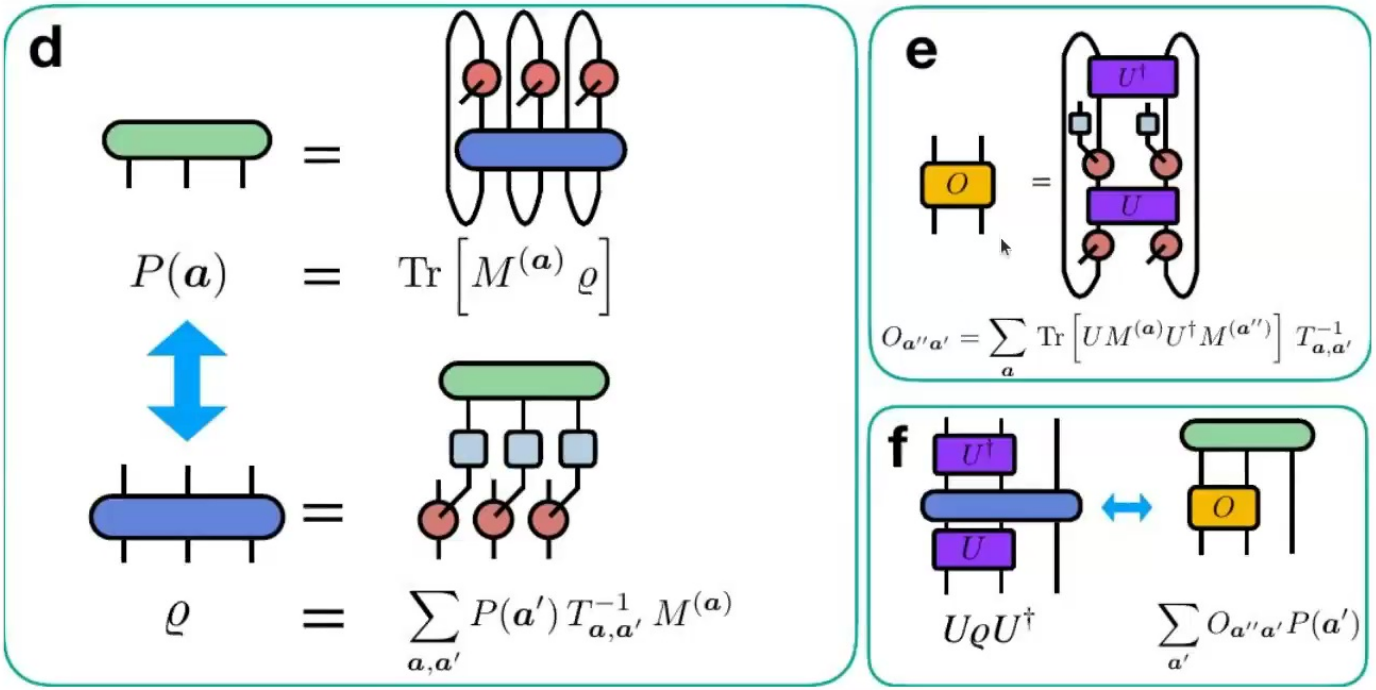
Quantum tomography

J Carrasquilla, G Torlai, RG Melko, L Aolita, Nature Machine Intelligence 1 (3), 155-161

Juan Carrasquilla, Di Luo, et al. Phys. Rev. A 104, 032610

Neural POVM Simulation: Quantum Circuits

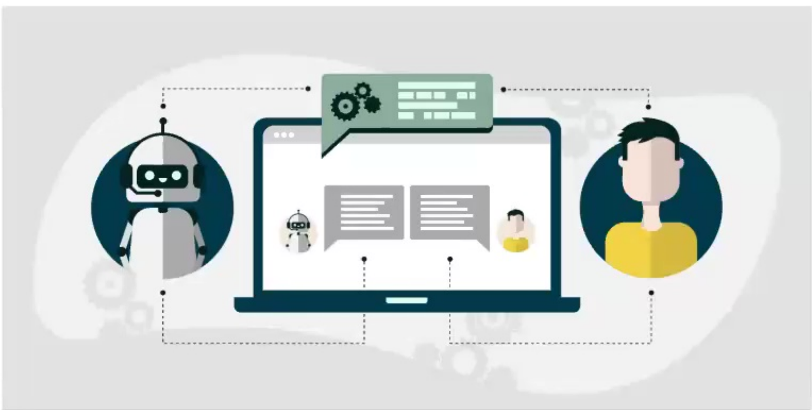
POVM simulation of quantum circuit

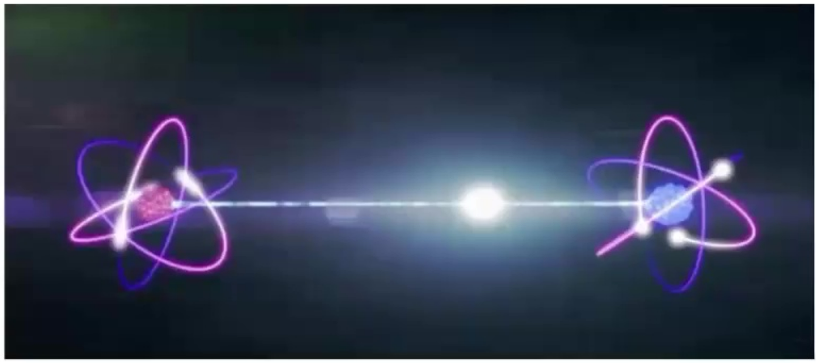


Juan Carrasquilla, Di Luo, et al. Phys. Rev. A 104, 032610

Neural POVM Simulation: Quantum Circuits

qubits as language: high dimensional distribution with long range correlation

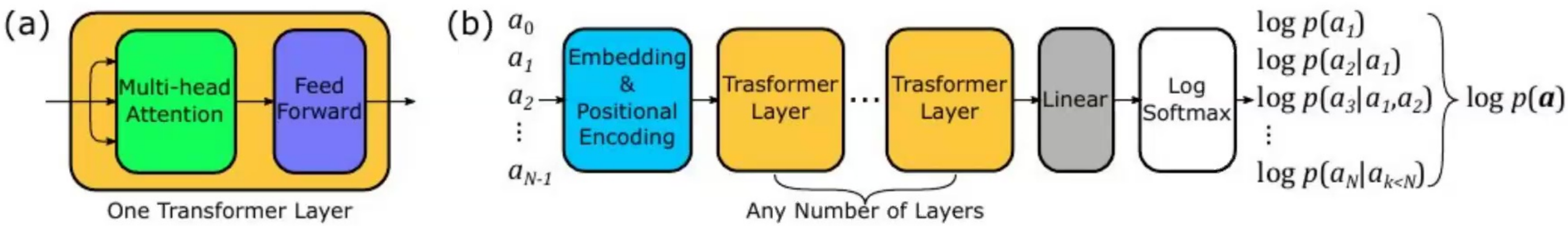




Juan Carrasquilla, Di Luo, et al. Phys. Rev. A 104, 032610

Neural POVM Simulation: Transformer Representation

$$P_\theta(a_1, \ldots, a_N) = \prod^{N} P_\theta(a_k | a_{<k}),$$



Attention is All You Need
(https://papers.nips.cc/paper/7181-attention-is-all-you-need.pdf)

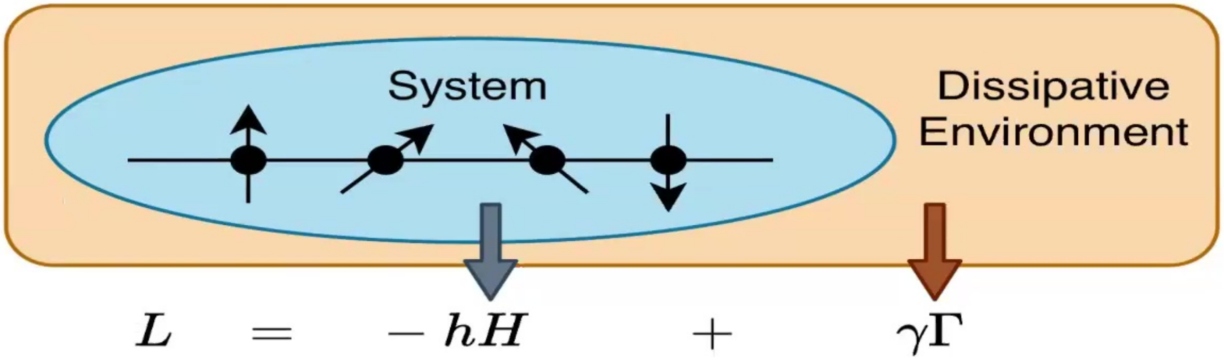
Conditional probability for exact sampling and inference

Compact representation for high dimensional distribution

Di Luo†, Zhuo Chen†, Juan Carrasquilla, Bryan K. Clark, Phys. Rev. Lett. 128, 090501

Neural POVM Simulation: Open System Dynamics

Quantum formulation: $$\dot{\rho} = \mathcal{L}\rho \equiv -i[H,\rho] + \sum_k \frac{\gamma_k}{2}\left(2\Gamma_k \rho \Gamma_k^\dagger - \{\rho, \Gamma_k^\dagger \Gamma_k\}\right)$$



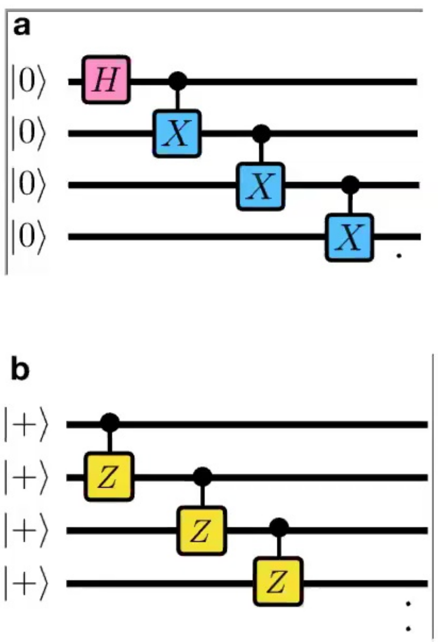
POVM formulation: $$\dot{p}(\boldsymbol{a}) = \sum_{\boldsymbol{b}} p(\boldsymbol{b}) L_{\boldsymbol{a}}^{\boldsymbol{b}} = \sum_{\boldsymbol{b}} p(\boldsymbol{b}) \left(A_{\boldsymbol{a}}^{\boldsymbol{b}} + B_{\boldsymbol{a}}^{\boldsymbol{b}}\right)$$

$$A_{\boldsymbol{a}}^{\boldsymbol{b}} = -i\,\mathrm{Tr}\left(H[N^{(\boldsymbol{b})}, M_{(\boldsymbol{a})}]\right); \qquad B_{\boldsymbol{a}}^{\boldsymbol{b}} = \sum_k \frac{\gamma_k}{2}\,\mathrm{Tr}\left(2\Gamma_k N^{(\boldsymbol{b})}\Gamma_k^\dagger M_{(\boldsymbol{a})} - \Gamma_k^\dagger \Gamma_k \{N^{(\boldsymbol{b})}, M_{(\boldsymbol{a})}\}\right).$$

Juan Carrasquilla, Di Luo, et al. Phys. Rev. A 104, 032610

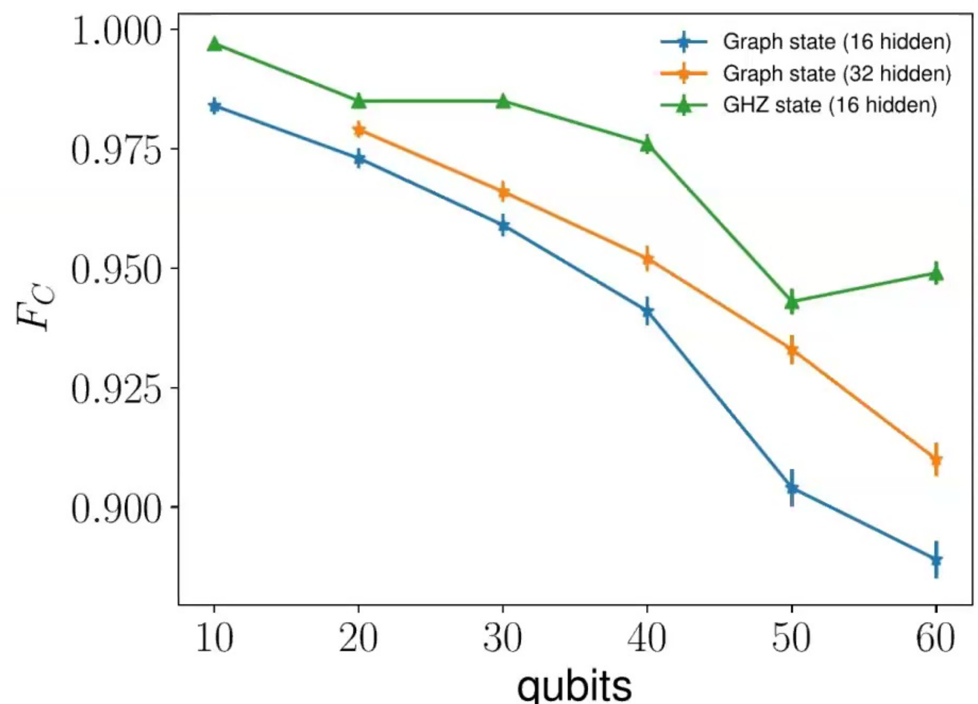
Neural POVM Simulation: Quantum Circuits

simulation of quantum state preparation



GHZ state

Graph state

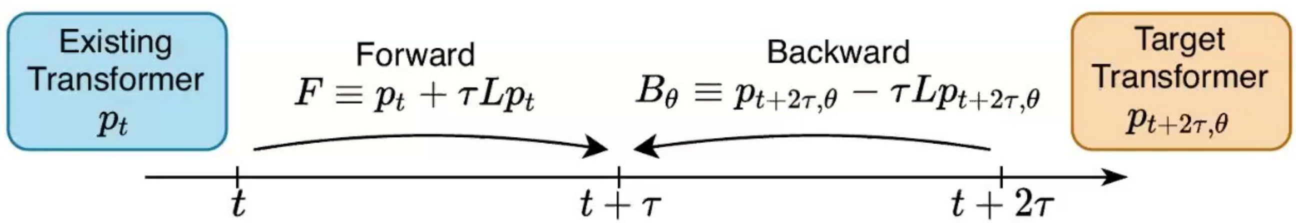


Neural POVM Simulation: Optimization

$$\dot{p}(\boldsymbol{a}) = \sum_{\boldsymbol{b}} p(\boldsymbol{b}) L_{\boldsymbol{a}}^{\boldsymbol{b}} = \sum_{\boldsymbol{b}} p(\boldsymbol{b}) \left(A_{\boldsymbol{a}}^{\boldsymbol{b}} + B_{\boldsymbol{a}}^{\boldsymbol{b}} \right)$$

Dynamics:

$$\theta = \arg\min E_{a \sim p_{t+2\tau}} \left[\frac{1}{p_{t+2\tau}(a)} \left| B_\theta(a) - F(a) \right| \right]$$



Steady state: minimize the derivative to be zero

$$\|\dot{p_\theta}\|_1 = \sum_{\boldsymbol{a}} \left| \sum_{\boldsymbol{b}} p_\theta(\boldsymbol{b}) L_{\boldsymbol{a}}^{\boldsymbol{b}} \right| = \frac{1}{N_s} \sum_{\boldsymbol{a} \sim p_\theta}^{N_s} \frac{\left| \sum_{\boldsymbol{b}} p_\theta(\boldsymbol{b}) L_{\boldsymbol{a}}^{\boldsymbol{b}} \right|}{p_\theta(\boldsymbol{a})}$$

TDVP approach: Moritz Reh, Markus Schmitt, Martin Gärttner, Physical Review Letters 127 (23), 230501

Di Luo†, Zhuo Chen†, Juan Carrasquilla, Bryan K. Clark, Phys. Rev. Lett. 128, 090501

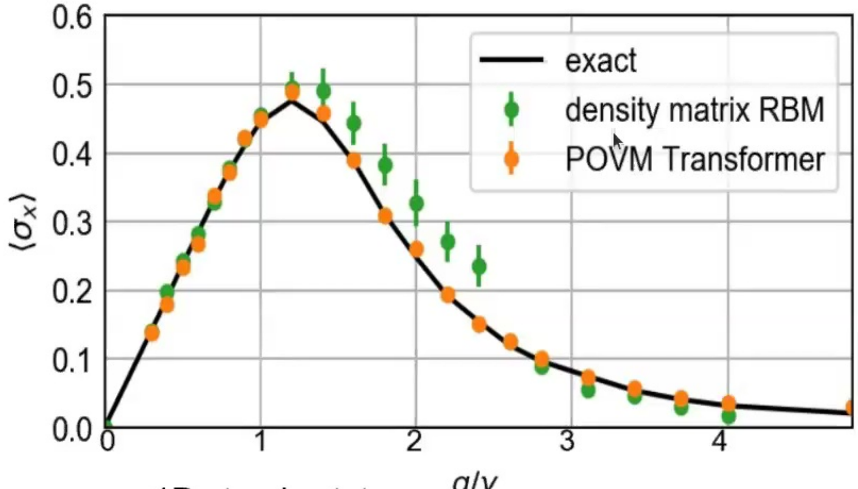
Neural POVM Simulation: Open System Dynamics

1D Dissipative Transverse Ising Chain $H = \frac{V}{4}\sum_{\langle i,j\rangle}\sigma_i^{(z)}\sigma_j^{(z)} + \frac{g}{2}\sum_k \sigma_k^{(x)}$

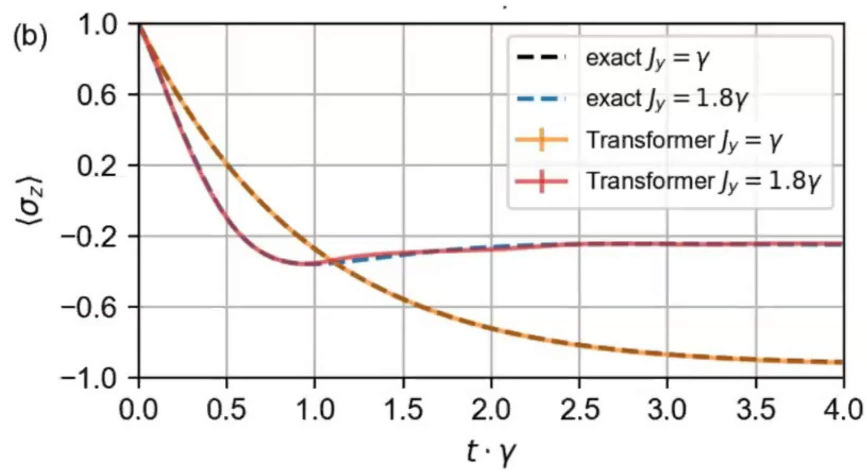
Dissipative Heisenberg Chain $H = \sum_{\langle i,j\rangle}\sum_{w=x,y,z} J_w \sigma_i^{(w)}\sigma_j^{(w)} + B\sum_k \sigma_k^{(z)}$

$$\Gamma_k = \sigma_k^{(-)} = \frac{1}{2}(\sigma_k^{(x)} - i\sigma_k^{(y)})$$

RBM data: Phys. Rev. Lett. 122, 250503



1D steady state

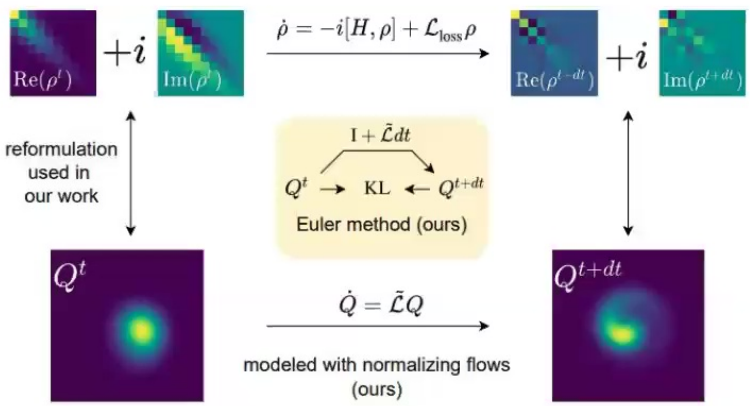


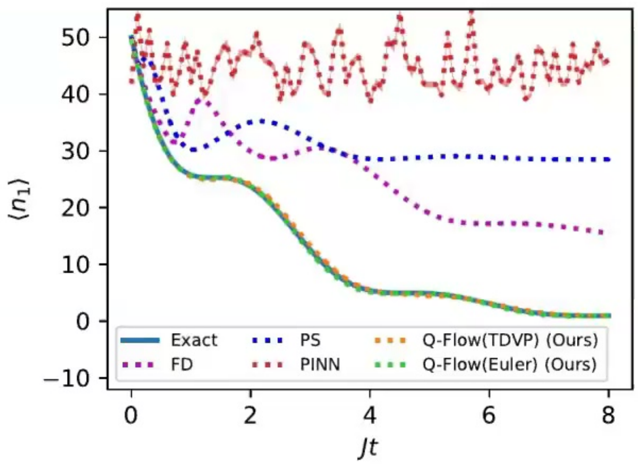
2D dynamics

35

QFlow: Generative Modeling for Differential Equations of Open Quantum Dynamics with Normalizing Flows

--- Develop flow-based models with Q function for continuous variable open quantum dynamics simulations using stochastic Euler methods and time dependent variational principle

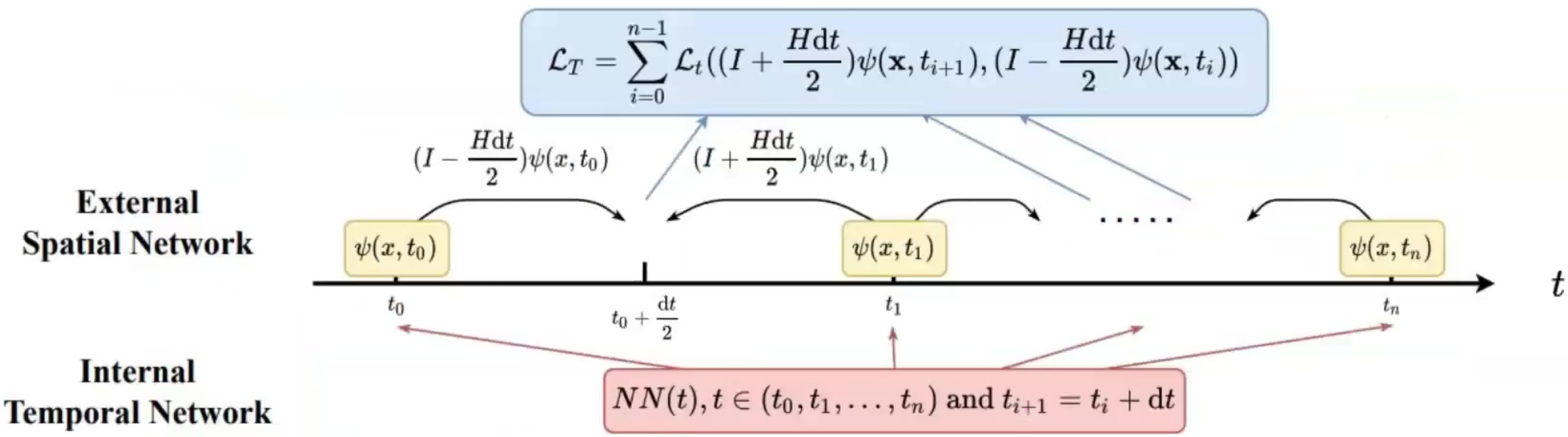




Jiangran Wang, Zhuo Chen, Di Luo, Zhizhen Zhao, Vera Mikyoung Hur, Bryan K. Clark, arxiv.2108.02200

Spacetime Neural Network for High Dimensional Quantum Dynamics

--- Develop a spacetime neural network that is able to all all the time steps dynamics simultaneously

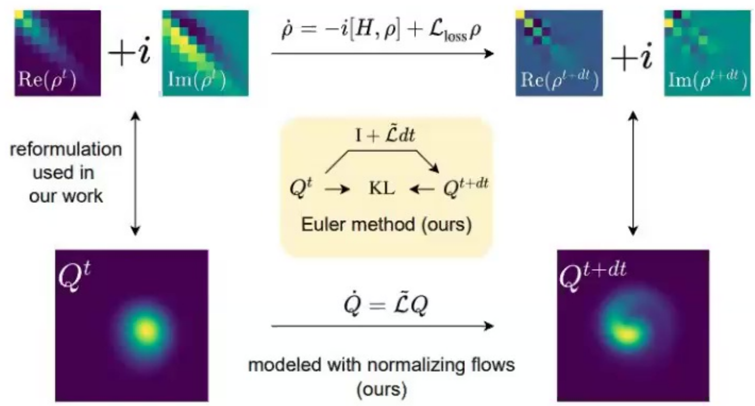


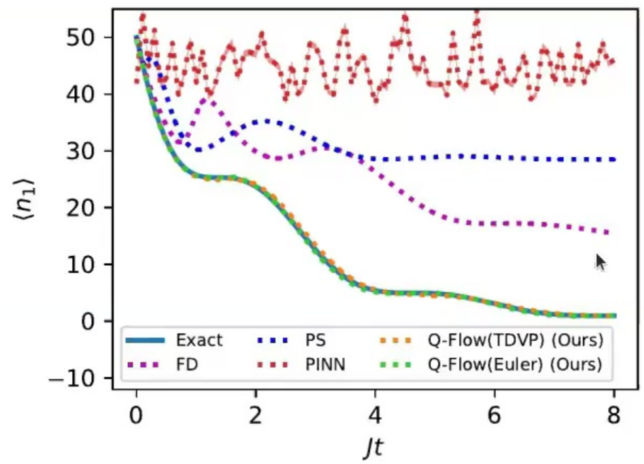
38

Owen Dugan, Peter Y. Lu, Rumen Dangovski, Di Luo, Marin Soljačić, ICML 2023

QFlow: Generative Modeling for Differential Equations of Open Quantum Dynamics with Normalizing Flows

--- Develop flow-based models with Q function for continuous variable open quantum dynamics simulations using stochastic Euler methods and time dependent variational principle





Di Luo†, Zhuo Chen†, Juan Carrasquilla, Bryan K. Clark, Phys. Rev. Lett. 128, 090501

Neural POVM Simulation: Open System Dynamics

1D Dissipative Transverse Ising Chain

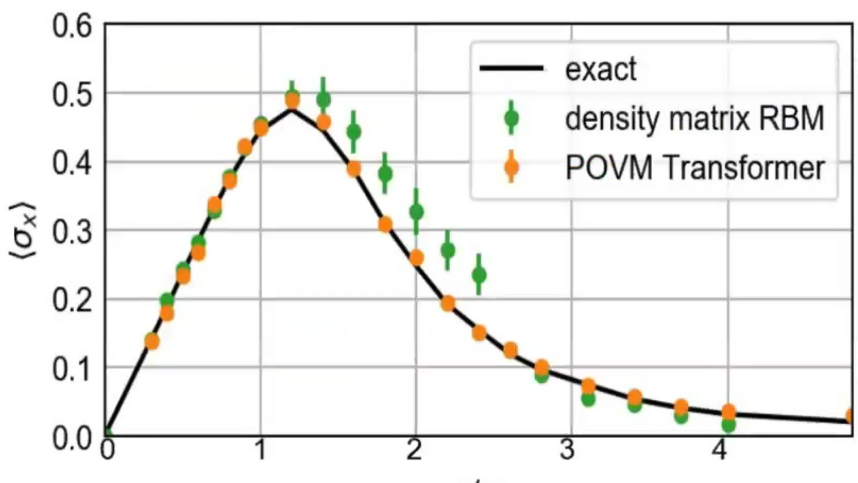
$$H = \frac{V}{4}\sum_{\langle i,j\rangle}\sigma_i^{(z)}\sigma_j^{(z)} + \frac{g}{2}\sum_k \sigma_k^{(x)}$$

Dissipative Heisenberg Chain

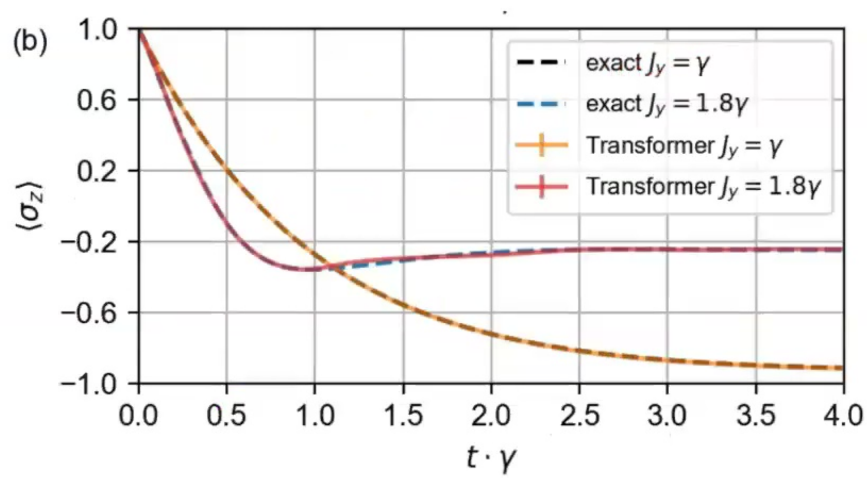
$$H = \sum_{\langle i,j\rangle}\sum_{w=x,y,z} J_w \sigma_i^{(w)}\sigma_j^{(w)} + B\sum_k \sigma_k^{(z)}$$

$$\Gamma_k = \sigma_k^{(-)} = \frac{1}{2}(\sigma_k^{(x)} - i\sigma_k^{(y)})$$

RBM data: Phys. Rev. Lett. 122, 250503



1D steady state

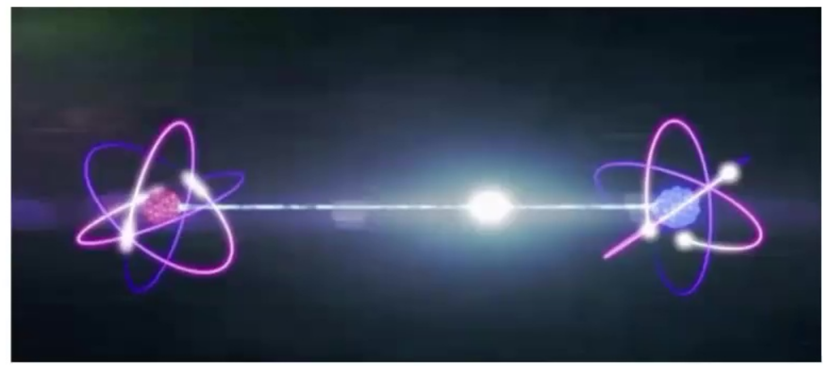


2D dynamics

Juan Carrasquilla, Di Luo, et al. Phys. Rev. A 104, 032610

Neural POVM Simulation: Quantum Circuits

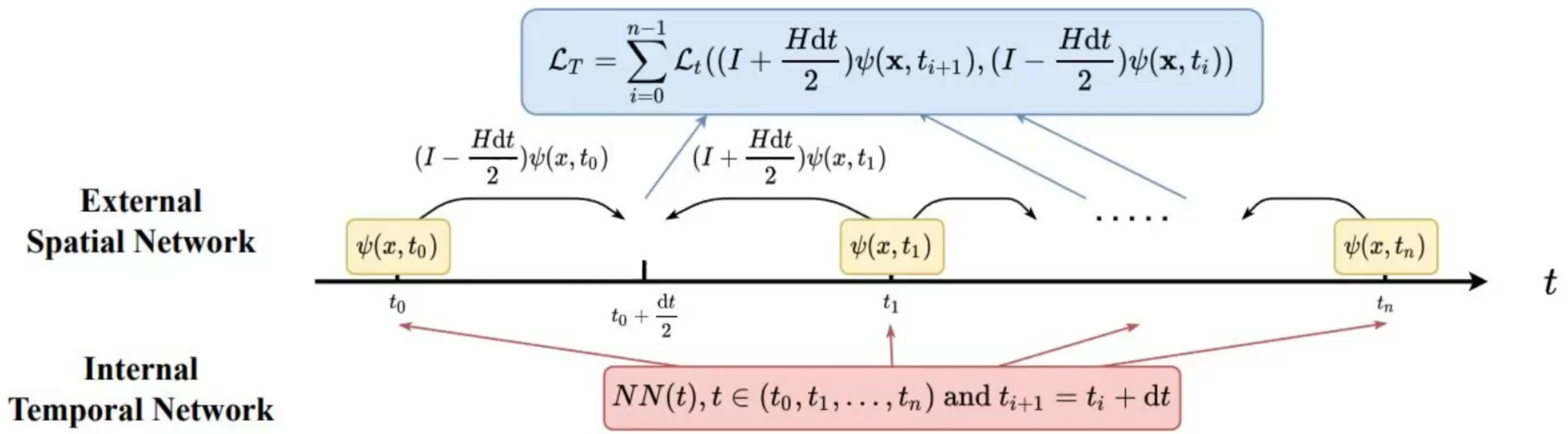
qubits as language: high dimensional distribution with long range correlation



Jiangran Wang, Zhuo Chen, Di Luo, Zhizhen Zhao, Vera Mikyoung Hur, Bryan K. Clark, arxiv.2108.02200

Spacetime Neural Network for High Dimensional Quantum Dynamics

--- Develop a spacetime neural network that is able to all all the time steps dynamics simultaneously



Neural POVM Simulation of Quantum Dynamics

Q: What is the connection of the quantum world and the classical world?

Quantum world		'Classical' world ?
Wavefunction/ Density Matrix	→	**Probability**
Unitary Dynamics		
Quantum Channel	→	**Quasi-stochastic Process**

Quantum world

(oscillating phase and dynamics)

'Classical' world ?

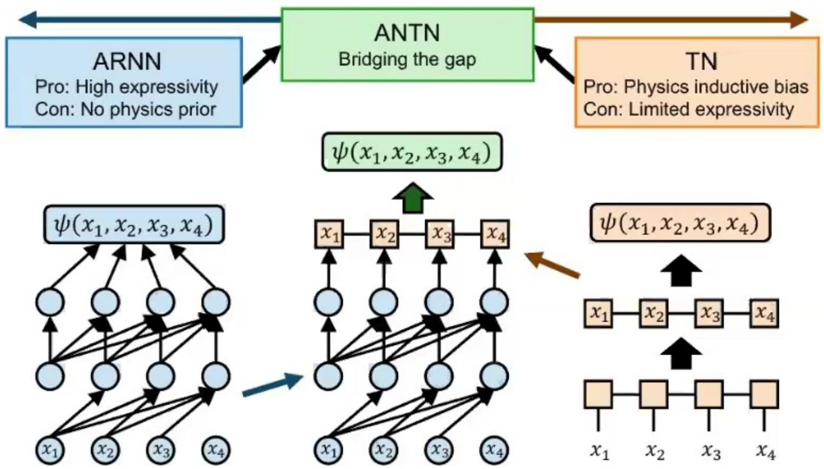
M Schmitt, M Heyl, Physical Review Letters 125 (10), 100503

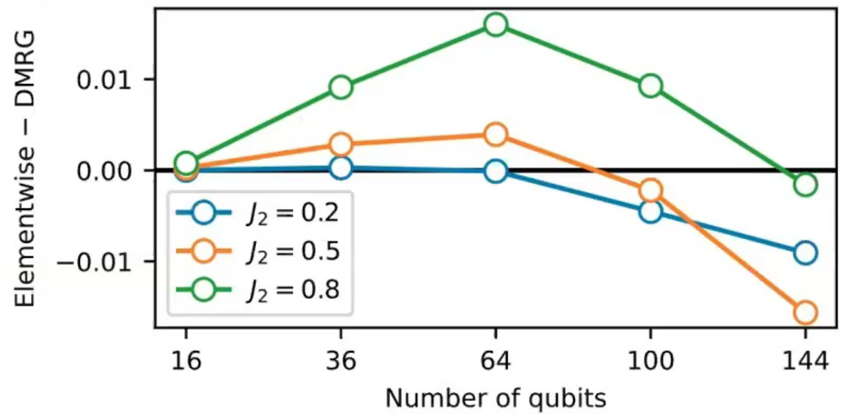
Irene López Gutiérrez, Christian B. Mendl, Quantum 6, 627 (2022)

Zhuo Chen, Laker Newhouse, Eddie Chen, Di Luo, Marin Soljačić, arxiv.2304.01996

ANTN: Bridging Neural Networks and Tensor Networks for Quantum Many-Body Simulation

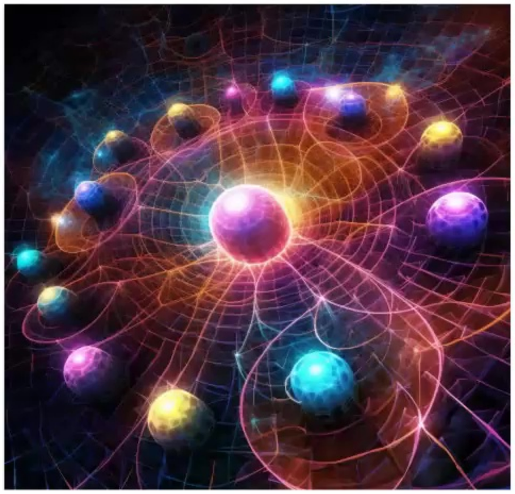
--- Develop Autoregressive Neural TensorNet which generalizes tensor network and autoregressive neural networks
--- Equip with exact sampling, tensor network physical inductive bias and symmetries construction



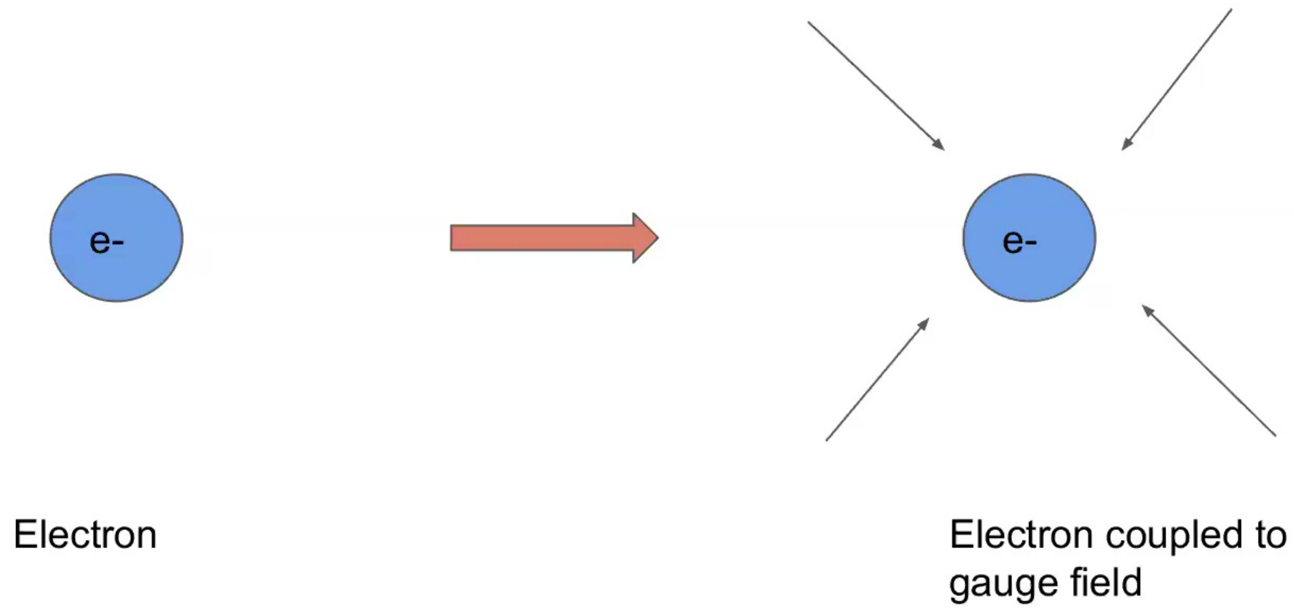


AI for Quantum: Real-time Quantum Dynamics

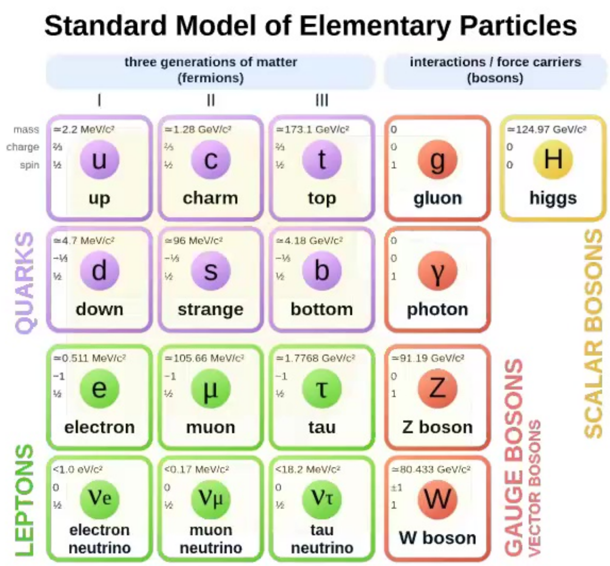
AI for Quantum: Quantum Field Theories



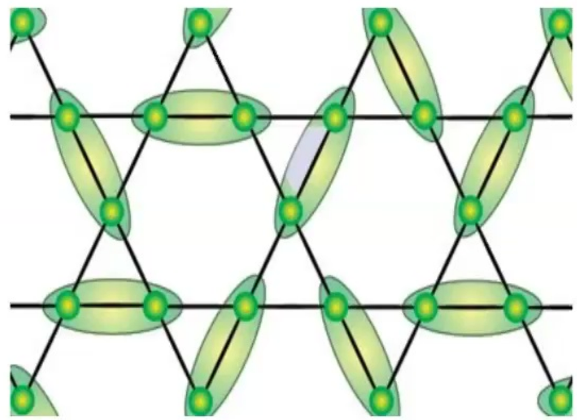
Motivations: Simulation of Gauge Theory



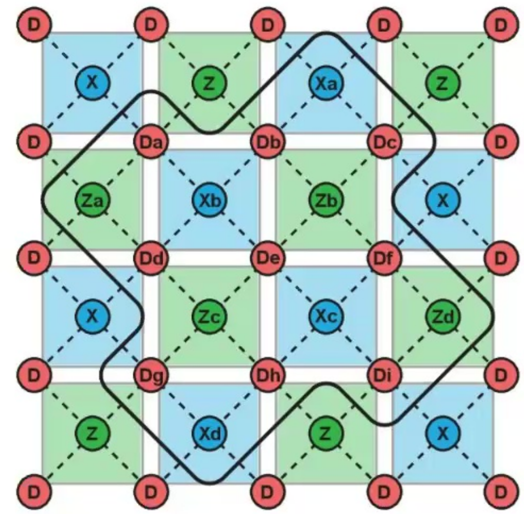
Motivations: Simulation of Gauge Theory



High energy



Condensed matter



Quantum error correction

Challenges: Simulation of Gauge Theory

- *High dimension Hilbert space*
- *Sign problems*
- *Gauge symmetries*
- *Continuous field variables*
- *Continuous limit*

New Exploration

- Gauge Equivariant Neural Network

  (Phys. Rev. Lett. 127, 276402, arxiv. 2211.03198)

- Gauge-Fermion FlowNet for 2+1D QED at Finite Density

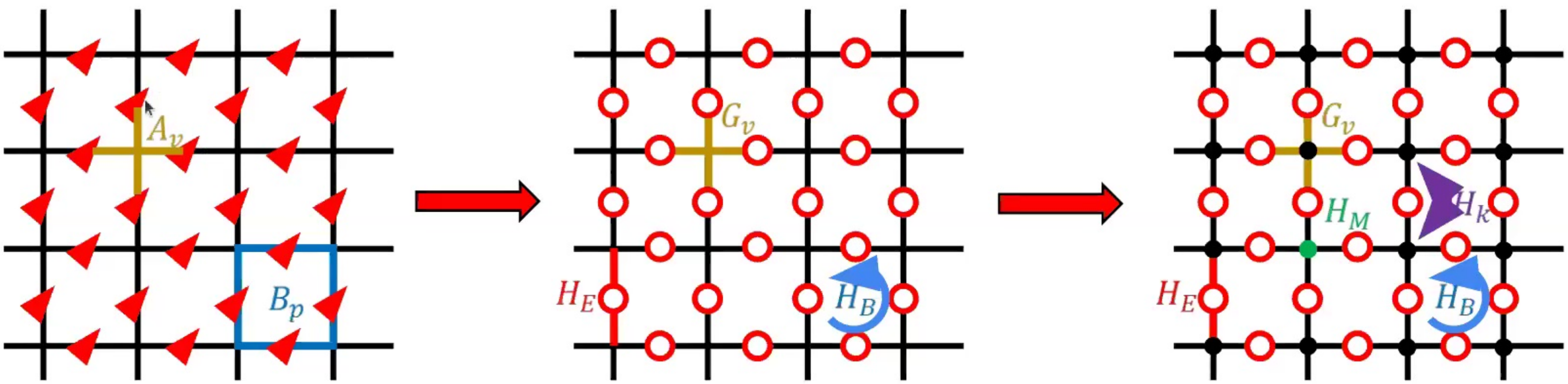
  (Phys. Rev. Lett. 122, 226401, arxiv.2101.07243, arxiv. 2212.06835)

- Neural Quantum Field State for continuum Quantum Field Theories

  (arxiv. 2212.00782)

Motivations: Simulation of Quantum Field Theories

$\mathbb{Z}_2$ toric code model | U(1) pure gauge theory | U(1) gauge theory with fermions



$\mathbb{Z}_2$ gauge theory
A_v: Gauss's law

Continuous gauge theory
Infinite degree of freedom

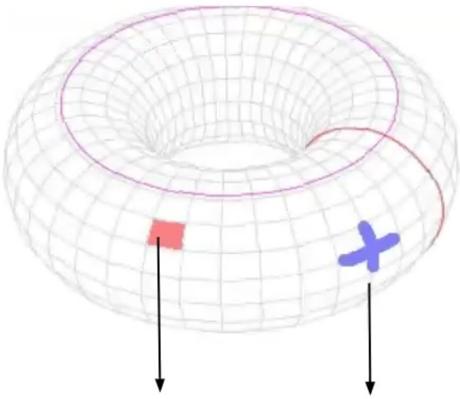
Gauge field fermion interaction
Fermionic sign problem

Di Luo, Giuseppe Carleo, Bryan Clark, James Stokes. Phys. Rev. Lett. 127, 276402

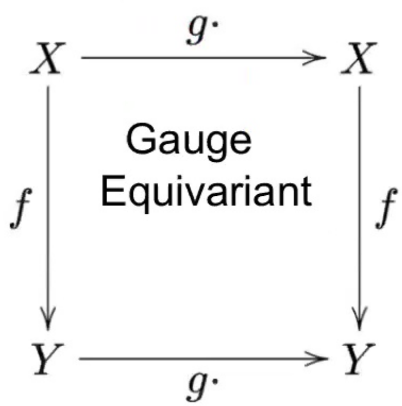
Gauge Equivariant Neural Network for Quantum Lattice Gauge Theories

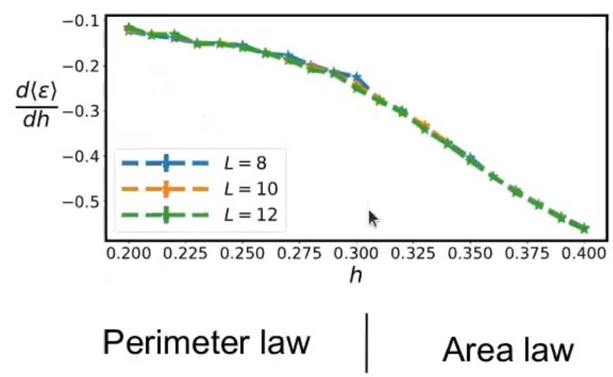
--- Develop gauge equivariant neural network for simulating quantum lattice gauge models
--- Exact representation for Toric code, Kitaev D(G) model, Fracton ground states and applications to transverse field Toric code phase transition

$$\mathcal{H}_{\text{gauge}} = \{|\psi\rangle \in \mathcal{H} : G_v|\psi\rangle = |\psi\rangle \ \forall v \in V\} \qquad \psi(G_v x) = \psi(x)$$



$W_f := \prod_{e \in f} Z_e \quad G_v := \prod_{e \ni v} X_e$





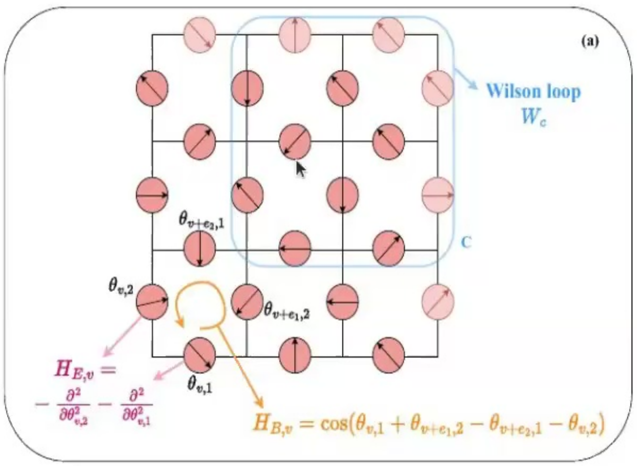
Di Luo†, Shunyue Yuan†, James Stokes, Bryan Clark. arxiv. 2211.03198

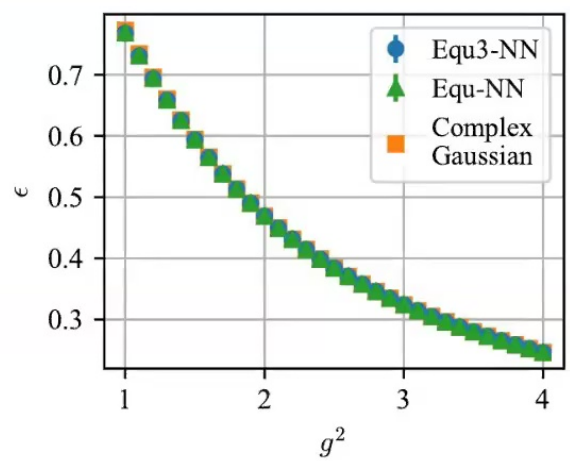
Gauge Equivariant Neural Network for 2+1D U(1) Gauge Theory Simulations in Hamiltonian Formulation

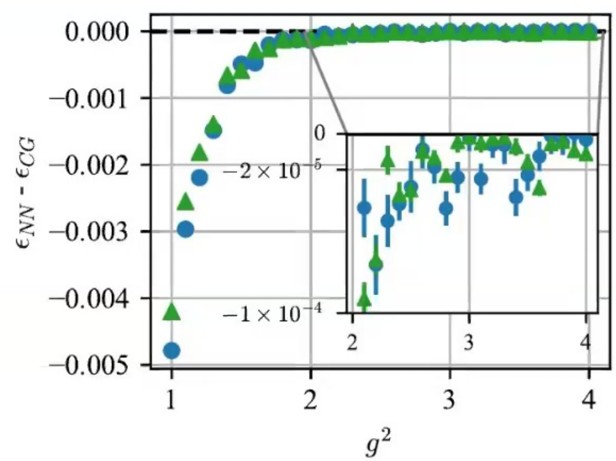
--- *Develop gauge equivariant neural network for simulating continuous-variable quantum lattice gauge models*

--- Comparable results in weak coupling regimes and improved performance in strong coupling regimes

$$\Psi(\cdots, \theta_{v,\delta}, \cdots) = \Psi(\cdots, \theta_{v,\delta} + \alpha_{v+e_\delta} - \alpha_v, \cdots)$$





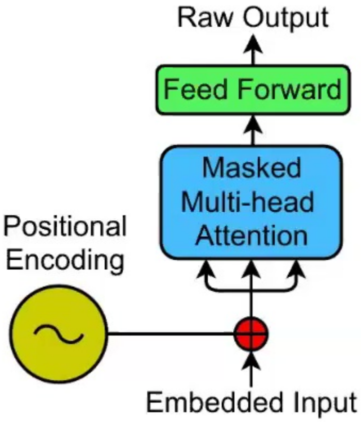


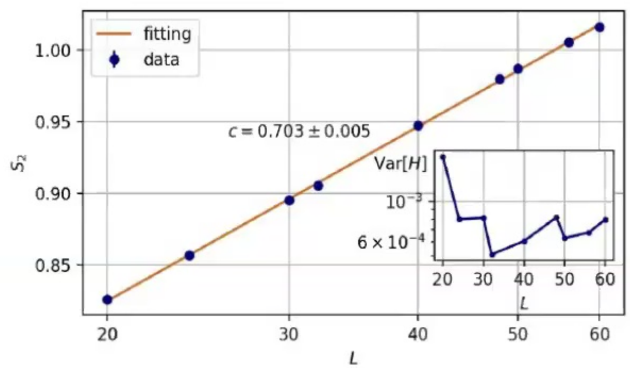
Di Luo†, Zhuo Chen†, Kaiwen Hu, Zhizhen Zhao, Vera Hu, Bryan Clark. arxiv: 2012.05232

Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network for Quantum Lattice Models

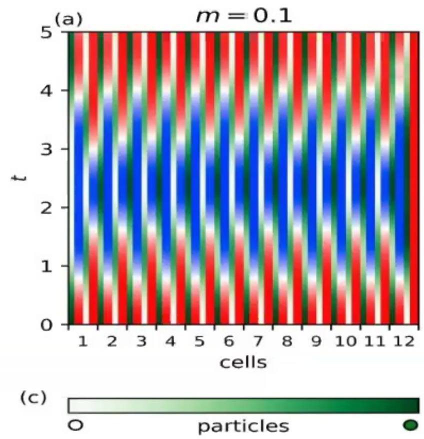
--- Develop autoregressive neural network that satisfies gauge constraints and algebraic constraints with applications to quantum link models, toric codes, Fracton, anyonic models

$$f(x_1, x_2, ..., x_n) = \prod_i^n f(x_i | x_{i<})$$





Anyon central charge



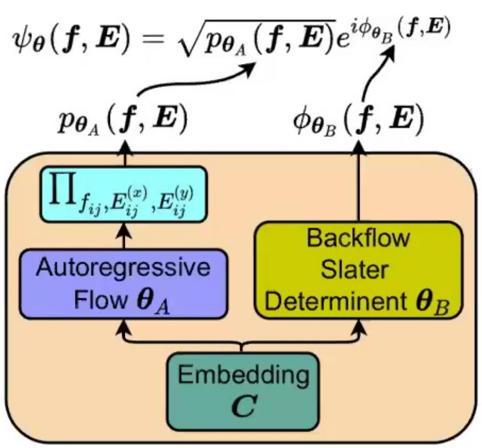
1+1-D QED real-time dynamics

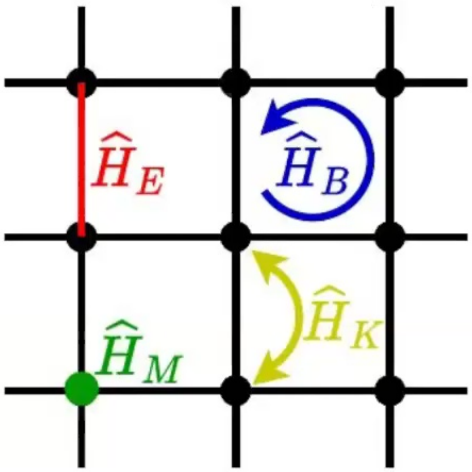
Zhuo Chen†, Di Luo†, Kaiwen Hu, Bryan Clark. arxiv. 2212.06835

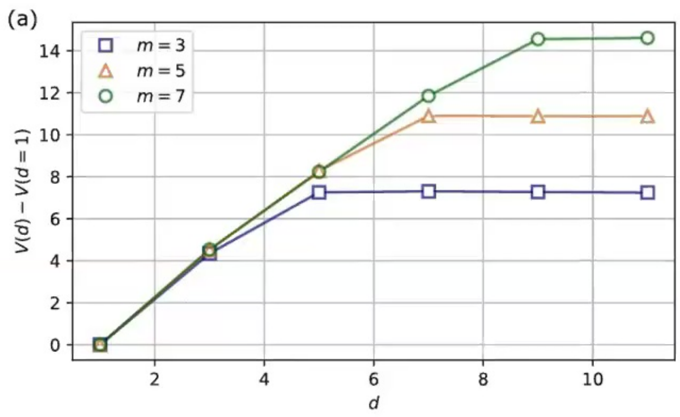
Simulating 2+1D Lattice Quantum Electrodynamics at Finite Density with Neural Flow Wavefunctions

--- Develop Gauge-Fermion FlowNet, which represents U(1) gauge field without cutoff, obey Gauss's law, samples without auto-correlation time and variationally simulates model with sign problems.

--- Simulate 2+1D QED at finite density to study string breaking, charge crystal phase transition and magnetic phase transition.



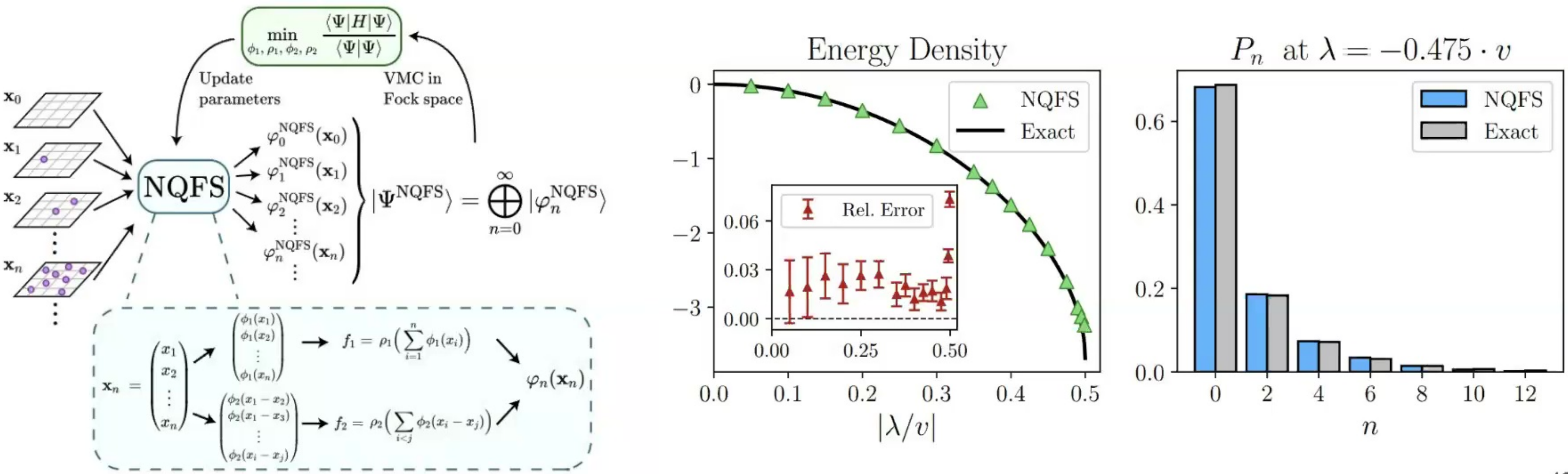




John M. Martyn, Khadijeh Najafi, Di Luo. arxiv. 2212.00782

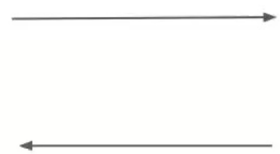
Variational Neural-Network Ansatz for Continuum Quantum Field Theory

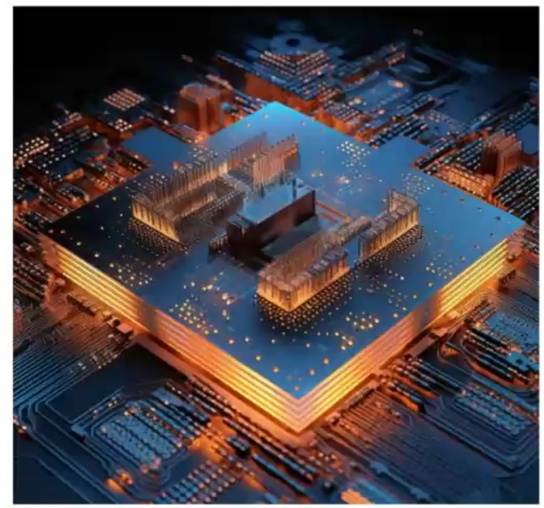
--- Develop neural quantum field state for continuum quantum field theory with applications to Lieb-Liniger Model, Calogero-Sutherland Model, Regularized Klein-Gordon Model.



49

AI for Quantum: Quantum Information Science

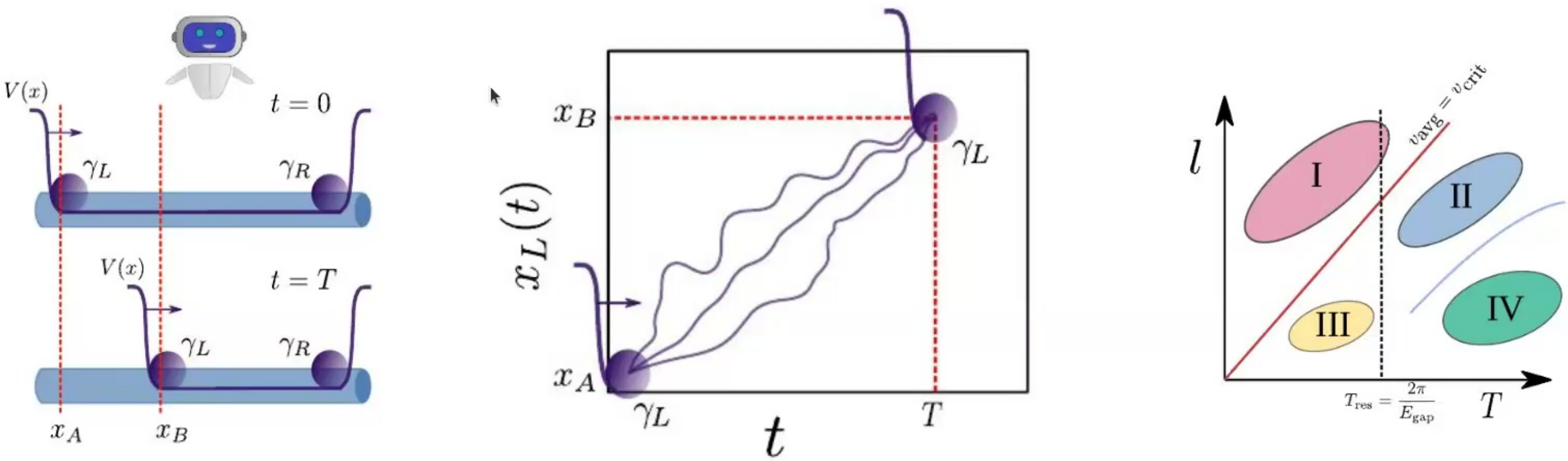




Luuk Coopmans†, Di Luo†, Graham Kells, Bryan K. Clark, Juan Carrasquilla, PRX Quantum 2, 020332

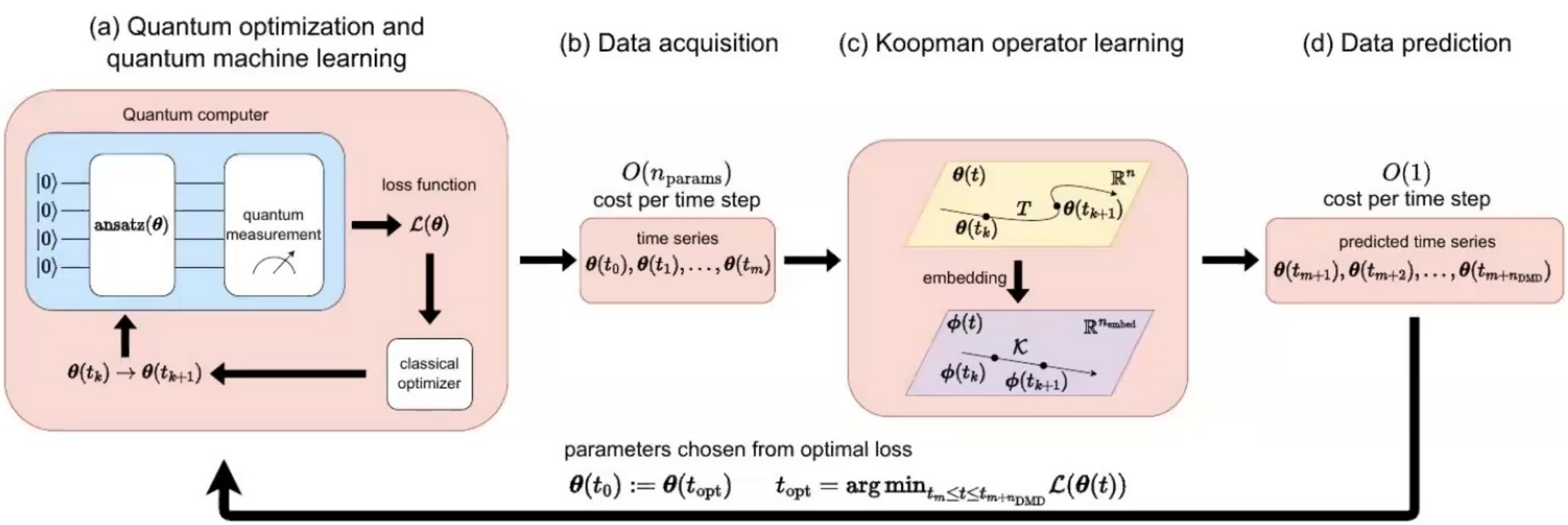
Protocol Discovery for the Quantum Control of Majoranas by Differentiable Programming and Natural Evolution Strategies

--- Differential programming for new quantum control protocol



Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

QuACK: Accelerating Gradient-Based Quantum Optimization with Koopman Operator Learning



Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

Gradient Based Optimization

Optimization is important!

Q: What is the cost of gradient based optimization? How does it scale?

Classically, the backward propagation has the same computation complexity as forward evaluation

O(gradients per step) ~ O(1) ***Efficient***

Quantumly, the large scale gradient optimization is costly

$$\nabla_\theta \, \text{Quantum Circuit}\,(\theta) = \text{Quantum Circuit}\,(\theta + s) - \text{Quantum Circuit}\,(\theta - s)$$

O(gradients per step) ~ O(# of parameters) * O(# of shot per parameter) ***Expensive***

Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

Koopman Operator Learning

Can we predict future optimization trajectory to skip some gradient calculation?

HAMILTONIAN SYSTEMS AND TRANSFORMATIONS IN HILBERT SPACE

BY B. O. KOOPMAN

DEPARTMENT OF MATHEMATICS, COLUMBIA UNIVERSITY

Communicated March 23, 1931

In recent years the theory of Hilbert space and its linear transformations has come into prominence.[1] It has been recognized to an increasing extent that many of the most important departments of mathematical physics can be subsumed under this theory. In classical physics, for example in those phenomena which are governed by linear conditions—

Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

Koopman Operator Learning

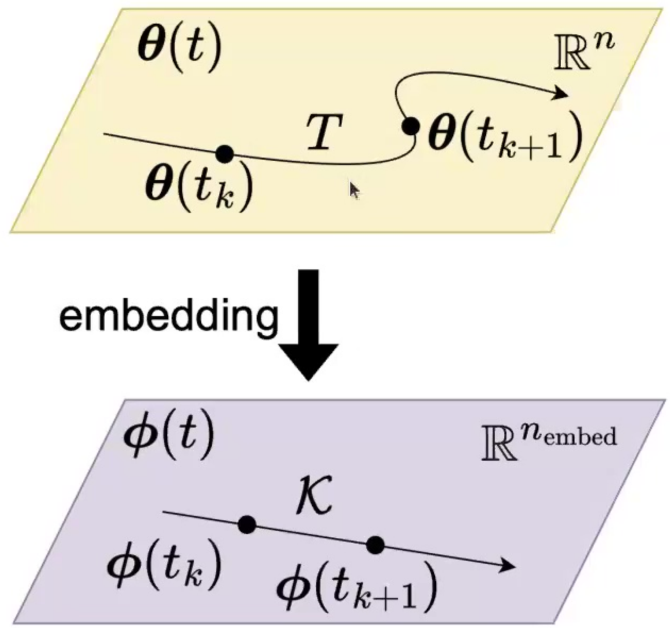
A (nonlinear) dynamical system with discrete-time evolution

$$x(t+1) = T(x(t))$$

From Koopman operator theory, an embedding g exists

$$\mathcal{K}g(x(t)) = g(T(x(t))) = g(x(t+1))$$

K is the Koopman operator and is linear,
but g can be very high-dimensional.



Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

Quantum Fisher Information and Natural Gradient

Koopman operator theory ~ Quantum imaginary time evolution ~ Quantum natural gradient

Quantum imaginary time evolution

$$\frac{d\psi_{\boldsymbol{\theta}}(t)}{dt} = -\mathbb{P}_{\psi_{\boldsymbol{\theta}}}\mathcal{H}\psi_{\boldsymbol{\theta}}(t)$$

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}}\langle\psi_{\boldsymbol{\theta}}, \mathcal{H}\psi_{\boldsymbol{\theta}}\rangle$$

Lucas Hackl, el at, *SciPost Phys.* 9, 048 (2020)

Quantum natural gradient

$$\frac{d}{dt}\boldsymbol{\theta}(t) = -\eta F^{-1}\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}(t))$$

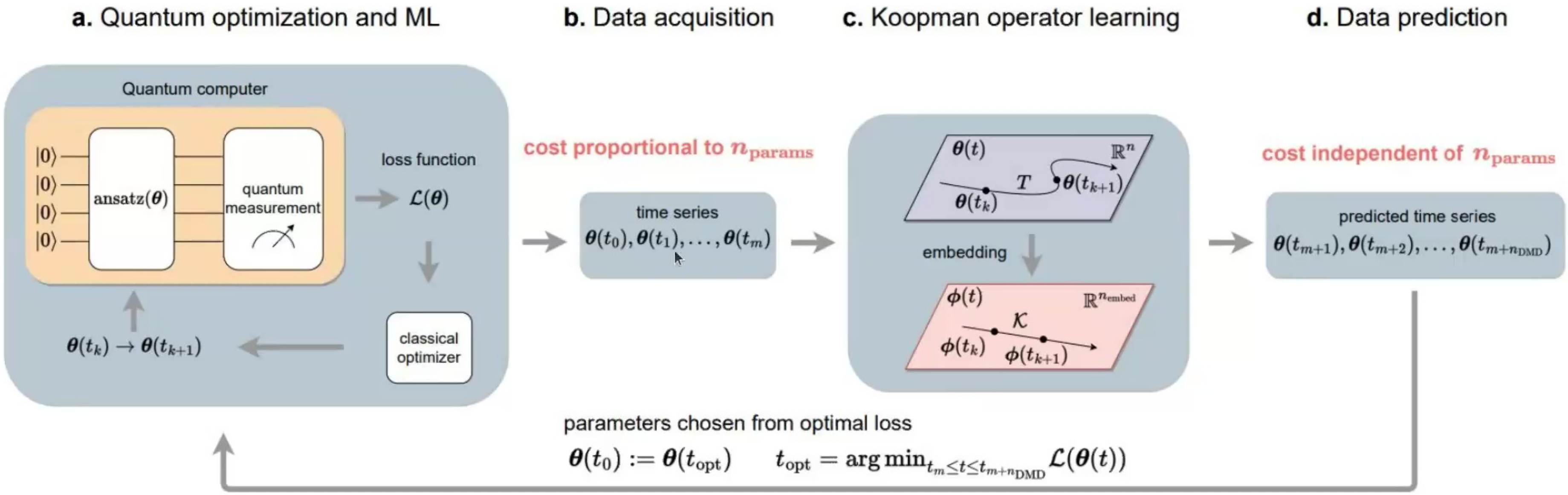
Quantum Fisher information

$$F_{ij} = \left\langle \frac{\partial\psi_{\boldsymbol{\theta}}}{\partial\theta_i}, \frac{\partial\psi_{\boldsymbol{\theta}}}{\partial\theta_j} \right\rangle - \left\langle \frac{\partial\psi_{\boldsymbol{\theta}}}{\partial\theta_i}, \partial\psi_{\boldsymbol{\theta}} \right\rangle \left\langle \psi_{\boldsymbol{\theta}}, \frac{\partial\psi_{\boldsymbol{\theta}}}{\partial\theta_j} \right\rangle$$

Linearization could happen in quantum natural gradient and overparameterization theory

Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

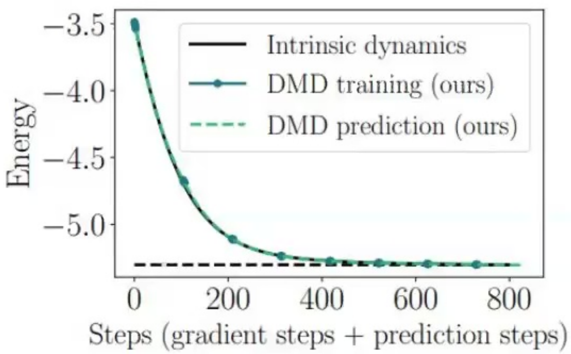
QuACK: Quantum-circuit Alternating Controlled Koopman Operator Learning



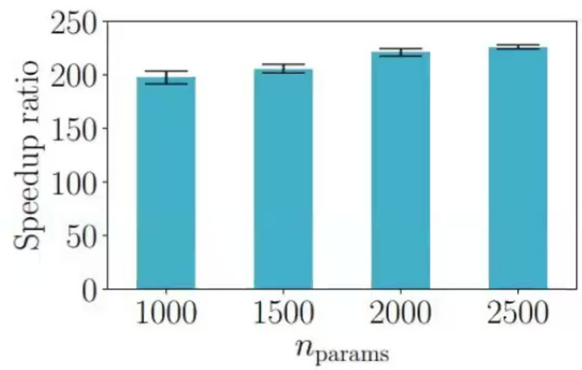
Theorem *In each iteration of QuACK, the optimal parameters $\boldsymbol{\theta}(t_{\text{opt}})$ yield an equivalent or lower loss than the m-step gradient-based optimizer.*

Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

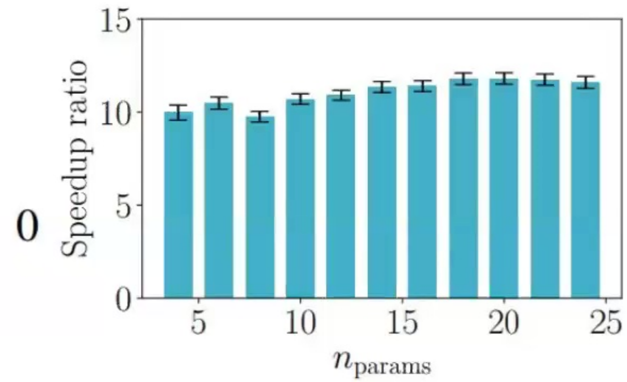
Koopman Operator Theory for Quantum



(a) Quantum natural gradients.



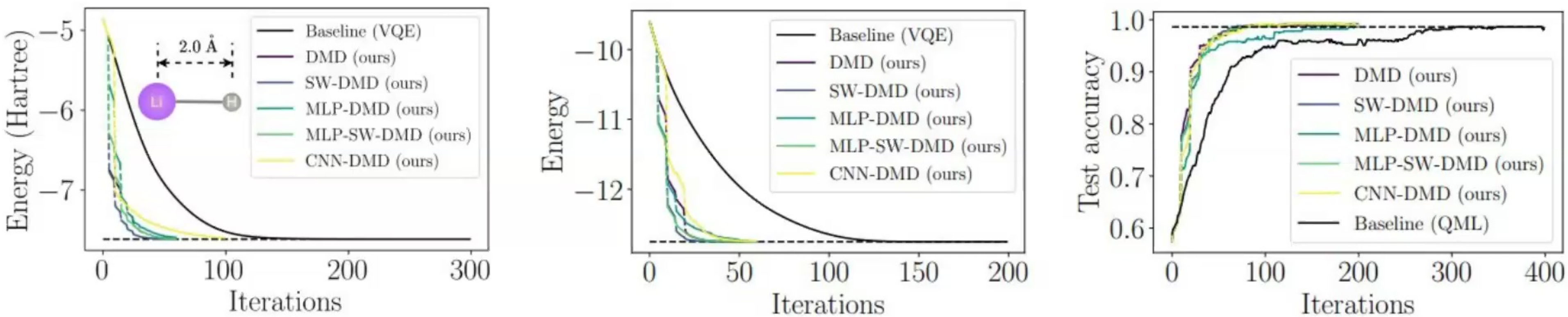
(b) Overparameterization.



(c) Smooth optimization regimes.

Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić, arxiv. 2211.01365

Koopman Operator Theory for Quantum



(a) LiH molecule. (b) Quantum Ising model. (c) Quantum machine learning.

Summary and Outlook

- New opportunities from machine learning for simulating quantum many-body physics and quantum information science
- Open questions to handle fermionic symmetry, gauge symmetries, continuous fields, open quantum dynamics
- Study ground state phase diagram, finite temperature physics, and real-time dynamics of quantum many-body systems