

Title: Machine Learning Meets Quantum Science

Speakers: Di Luo

Series: Machine Learning Initiative

Date: April 06, 2023 - 3:00 PM

URL: <https://pirsa.org/23040078>

Abstract: The recent advancement of machine learning provides new opportunities for tackling challenges in quantum science, ranging from condensed matter physics, high energy physics to quantum information science. In this talk, I will first discuss a class of anti-symmetric wave functions based on neural network backflow, which is efficient for simulating strongly-correlated lattice models and artificial quantum materials. Next, I will talk about recent progress of simulating continuum quantum field theories with neural quantum field state, and lattice gauge theories such as 2+1D quantum electrodynamics with finite density dynamical fermions using gauge symmetric neural networks. I will further discuss neural network representation based on positive-value-operator and phase space measurements for quantum dynamics simulations. Finally, I will present applications of machine learning in quantum control, quantum optimization and quantum machine learning.

Zoom link: <https://pitp.zoom.us/j/93834456412?pwd=R0hxdEpxanFFRnZmTHlqZTBXRi82QT09>

Machine Learning Meets Quantum Science



Di Luo
IAIFI Fellow, MIT





AI for Quantum Many-body Physics &
Quantum Information Science

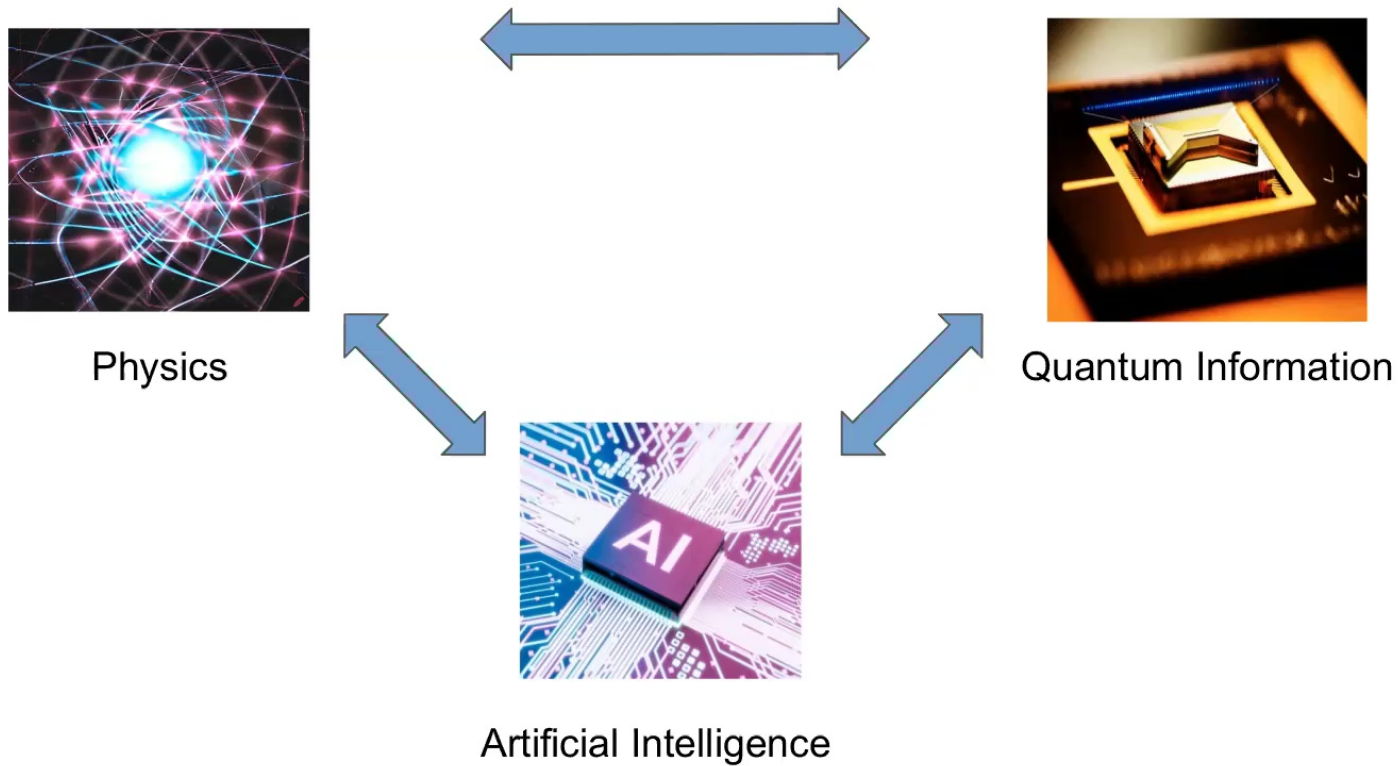
IAIFI: The NSF AI Institute for Artificial Intelligence
and Fundamental Interactions



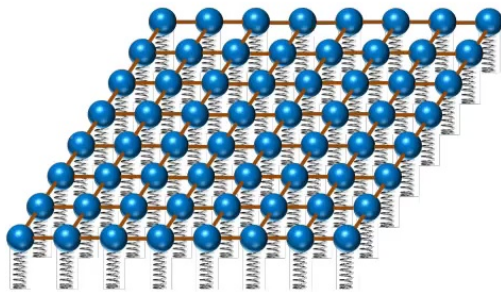
Quantum Many-body Simulation &
Quantum Information Science

C2QA: Co-design Center for Quantum Advantage

Artificial Intelligence, Quantum Information and Physics



AI for Quantum Science



High energy physics

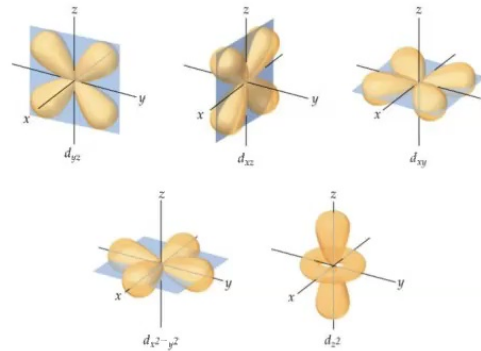
Phys. Rev. Lett. 127, 276402

arxiv: 2101.07243

arxiv: 2202.03530

arxiv. 2101.07243

arxiv. 2212.06835



Condensed matter physics

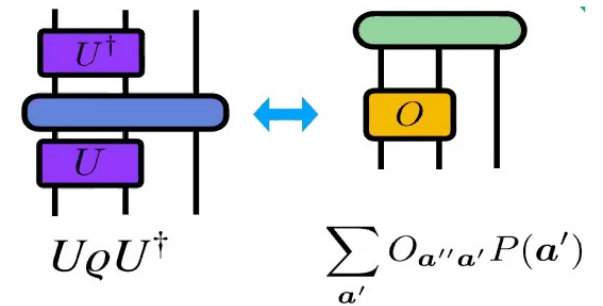
Phys. Rev. Lett. 122, 226401

arxiv: 2112.00723

arxiv. 2212.00782

Nano Lett. 2020, 20, 5, 3369–3377

arxiv.2304.01996



Quantum information science

Phys. Rev. Lett. 128, 090501

Phys. Rev. A 104, 032610

PRX Quantum 2, 020332

arxiv. 2211.01365

Physics for AI

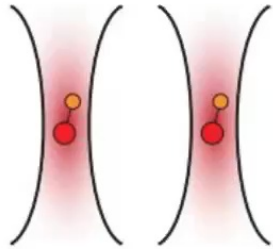
Geometry of contact: contact planning for multi-legged robots via spin models duality

Baxi Chong^{*1}, Di Luo^{*2 3 4}, Tianyu Wang^{1 5}, Gabriel B. Margolis⁶, Juntao He^{1 5},
Pulkit Agrawal^{2 6}, Marin Soljačić⁷, and Daniel I. Goldman^{1 5}

GENPHYS: FROM PHYSICAL PROCESSES TO GENERATIVE MODELS

Ziming Liu, Di Luo, Yilun Xu, Tommi Jaakkola, Max Tegmark
Massachusetts Institute of Technology
{zmliu, diluo, ylxu, jaakkola, tegmark}@mit.edu

QI for Physics: Quantum Simulations and Quantum Information Science



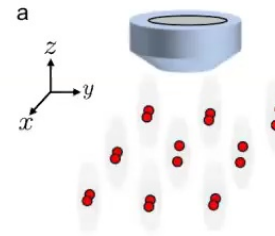
Dipolar molecule

Framework for simulating gauge theories with dipolar spin systems, Phys. Rev. A 102, 032617 (2020)



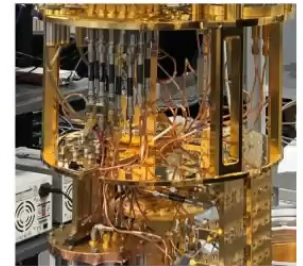
Rydberg atoms

Simulating Quantum Mechanics with a θ -term and an 't Hooft Anomaly on a Synthetic Dimension, Phys. Rev. D 105, 074505 (2022)



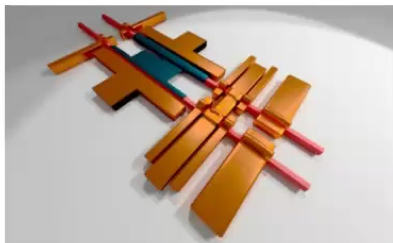
Fermion Pair

Quantum Computation and Simulation using Fermion-Pair Registers



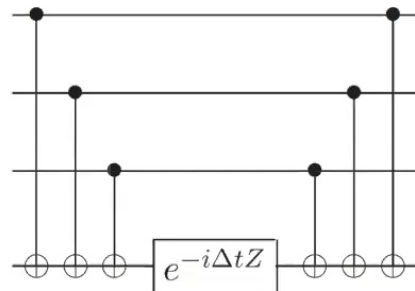
Bosonic mode

Bosonic Mode Quantum Simulations for Many-body Physics



Topological braiding

PRX Quantum 2, 020332



Digital circuit

Quantum tomography
Quantum simulations

arxiv.2110.02965
arxiv.2211.01365

.....

Quantum Many-body Physics Simulation

Spectrum calculation

$$H|\psi\rangle = E|\psi\rangle$$

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

ChatGPT: Large Language Model



ChatGPT: Optimizing Language Models for Dialogue

We've trained a model called ChatGPT which interacts in a conversational way. The dialogue format makes it possible for ChatGPT to answer followup questions, admit its mistakes, challenge incorrect premises, and reject inappropriate requests. ChatGPT is a sibling model to [InstructGPT](#), which is trained to follow an instruction in a prompt and provide a detailed response.



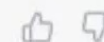
Motivations



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.



Ongoing Efforts: Quantum Monte Carlo

Quantum monte carlo: sample high dimension objects

$$e^{-\tau H}|\psi\rangle \approx \prod^N (I - \frac{\tau}{N}H)|\psi\rangle$$


Transition probability with signs

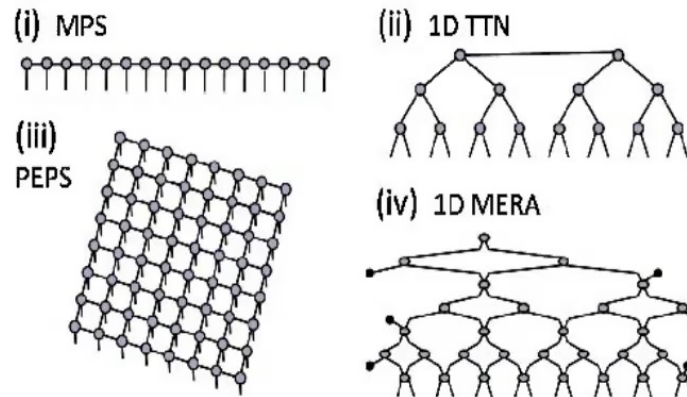
- Draw samples according to $|\psi|^2$, apply transition probability kernel
- Due to sign problem, the relative variance of the sign scales exponentially

Ongoing Efforts: Tensor Network

Tensor network: tensor decomposition of high dimensional objects

High rank tensor

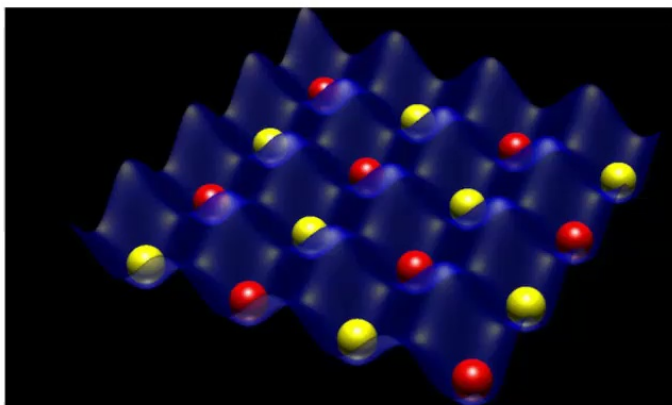
$$T_{i,j,k,l} =$$



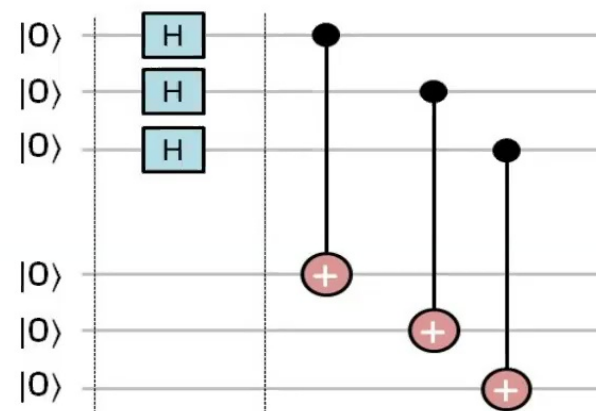
- Efficient for 1 dimensional system due to area law
- Challenges exist for two or three dimensional physics system

Ongoing Efforts: Quantum Computation

Quantum computation: naturally represents and operates on quantum objects



Analog quantum computation



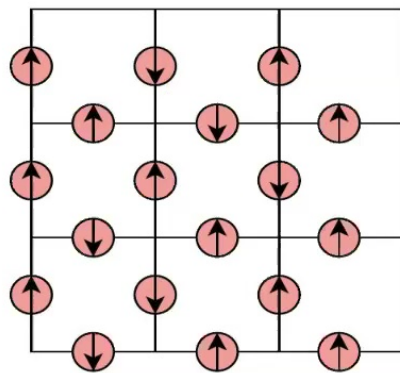
Digital quantum computation

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

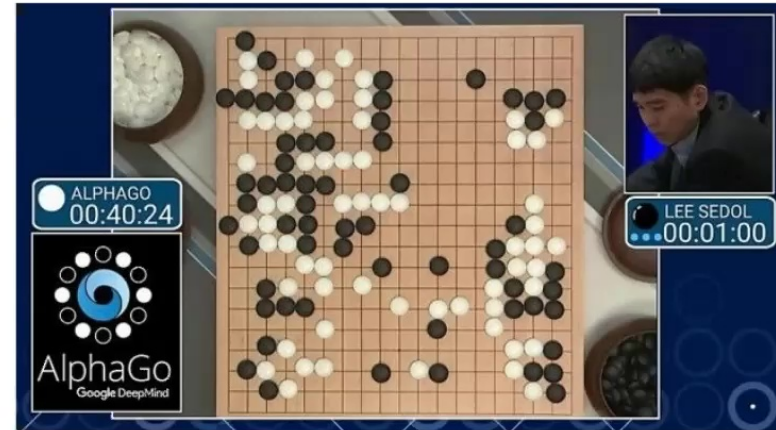
Neural Quantum States

For a n-particle (spin $\frac{1}{2}$) system:

$$2^n \times 2^n \text{ hermitian matrix} \leftarrow H|\psi\rangle = E|\psi\rangle$$



2^n vector

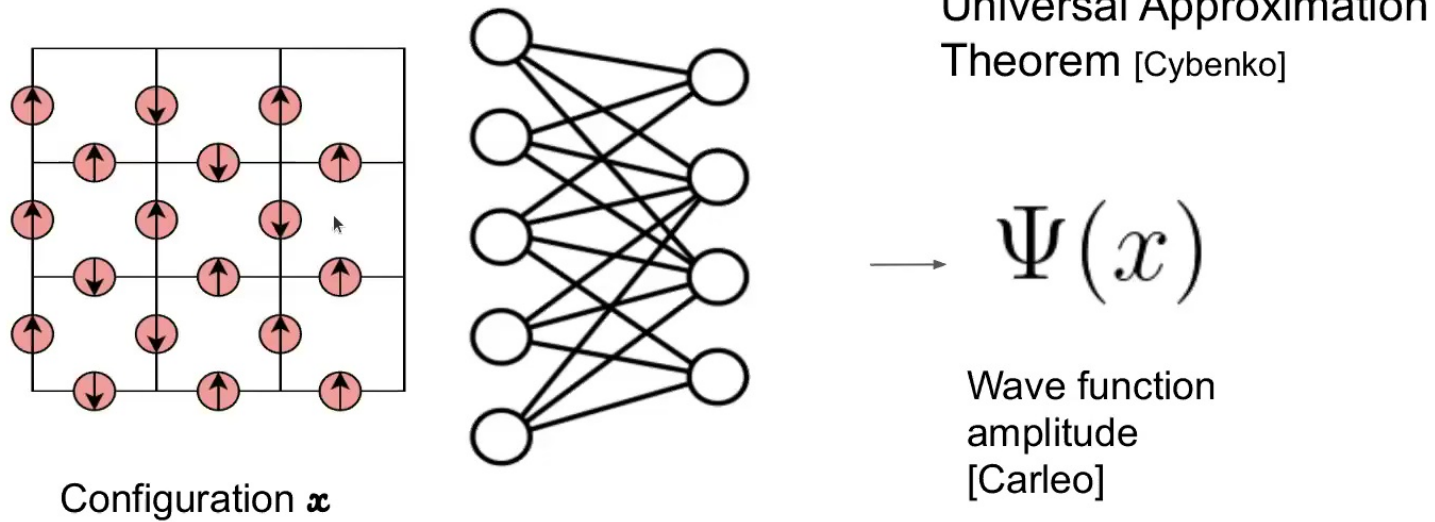


Superposition of 2^n configurations!

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

Neural Quantum States

Neural network: low dimensional representation of high dimensional objects



Variational Monte Carlo

Variational principle:

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

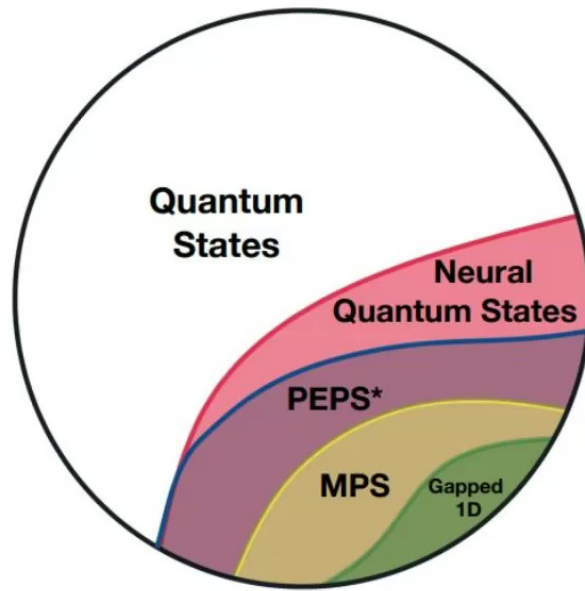
$$\partial_{\theta} E(\theta) = \frac{1}{N} \sum_{x \sim |\psi_{\theta}(x)|^2} [(E_L(x) - \langle E_L \rangle) \nabla_{\theta} \log \psi_{\theta}(x)]$$

Sampling without
sign problem

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

Parameterized
wave function

Neural Quantum States



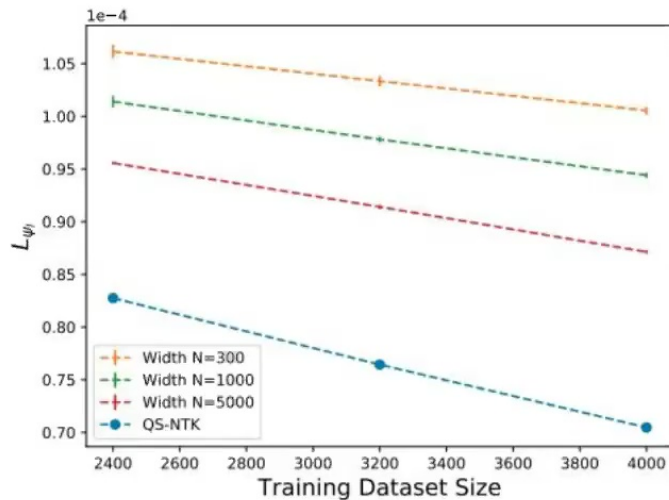
Or Sharir, Amnon Shashua, Giuseppe Carleo
<https://arxiv.org/abs/2103.10293>

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

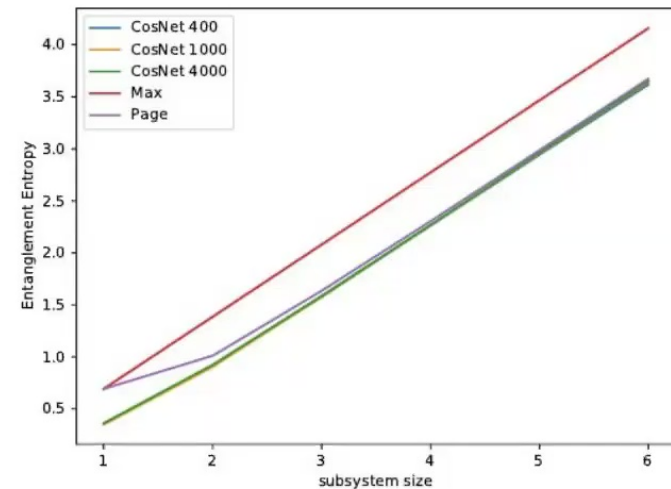
Neural Quantum States

Infinite Neural Network Quantum State: Entanglement and Training Dynamics



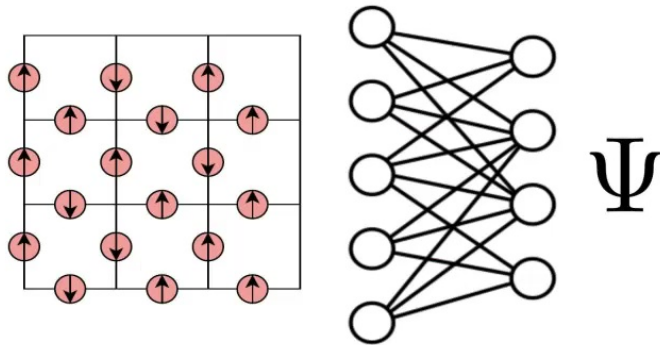
Quantum State Neural Tangent Kernel

Theorem. Quantum state supervised learning training is guaranteed to converge in infinite width limit.



Volume law entanglement engineering of CosNet

Neural Quantum States



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Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo^{1,*}, Matthias Troyer^{1,2}

Efficient representation of quantum many-body states with deep neural networks

Xun Gao & Lu-Ming Duan

Nature Communications **8**, Article number: 662 (2017) | Cite this article

Quantum Entanglement in Neural Network States

Dong-Ling Deng, Xiaopeng Li, and S. Das Sarma
Phys. Rev. X **7**, 021021 – Published 11 May 2017

Neural-network quantum state tomography

Giacomo Torlai, Guglielmo Mazzola, Juan Carrasquilla, Matthias Troyer, Roger Melko & Giuseppe Carleo



Nature Physics **14**, 447–450 (2018) | Cite this article

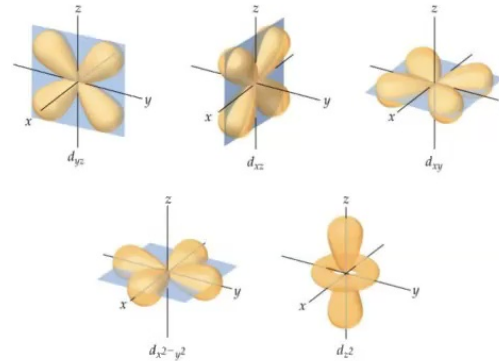
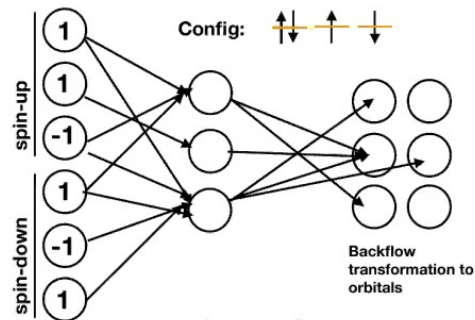
AI for Quantum: Quantum Many-body Physics

I. Strongly Correlated Systems

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

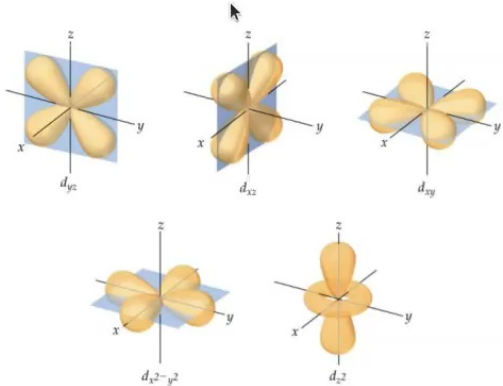
--- Develop anti-symmetry neural network for fermionic simulations

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



Neural Network Backflow

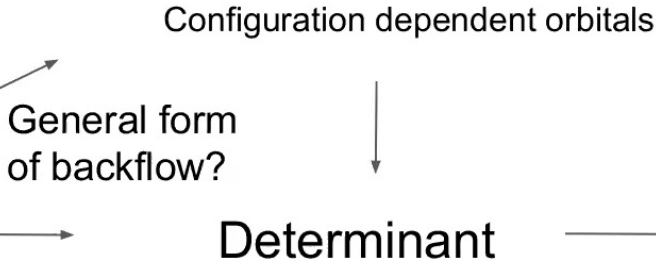
Jastrow
 +
 Backflow
 Slater Determinant



Pro: include correlation effect

Con: hard to figure out good configuration dependent orbitals

Backflow transformation
 [Feynman],
 [Sorella]
 \mathbf{r}



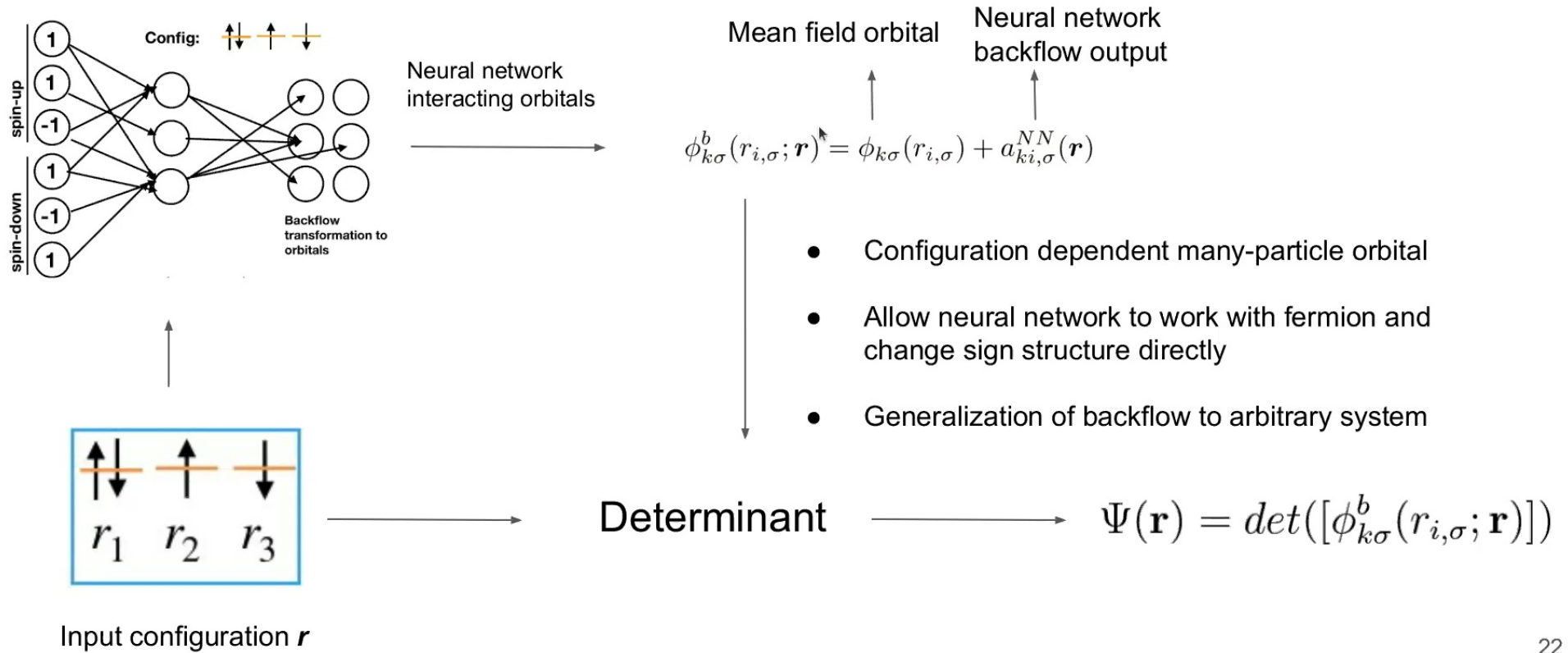
Mean field solution

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

↓ ?

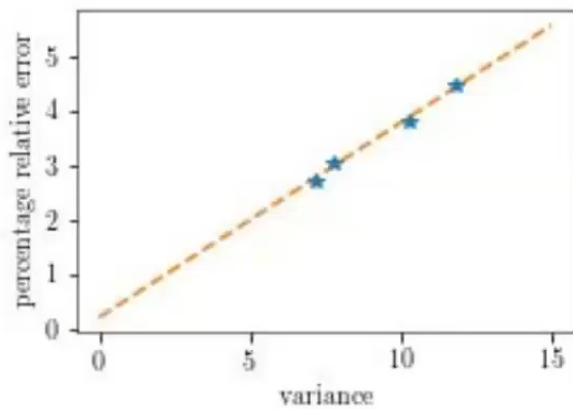
$$\Psi(\mathbf{r}) = \det([\phi_{k\sigma}^b(r_{i,\sigma}; \mathbf{r})])$$

Neural Network Backflow

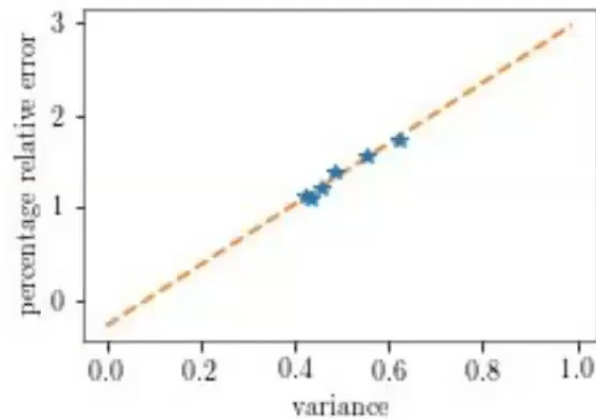


Neural Network Backflow

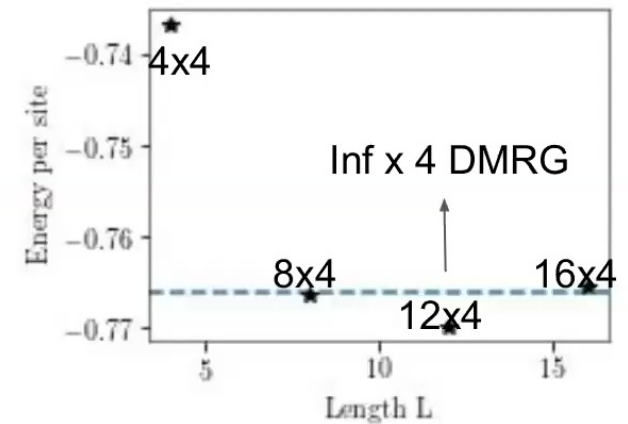
Generalization of backflow to arbitrary lattice systems with complicated sign structure.



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



4x4x3 Kagome
 Variance extrapolation
 error=0.286%



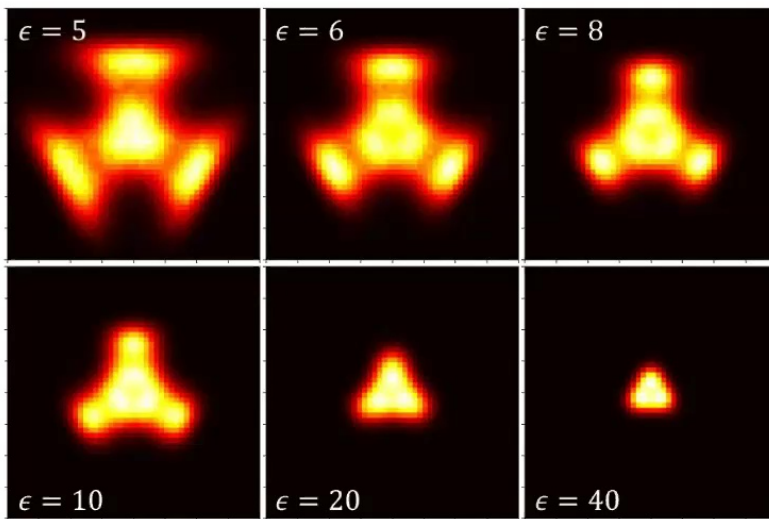
Hubbard model,
 $U/t=8$, $n=0.875$,
 finite size study

Neural Network Backflow

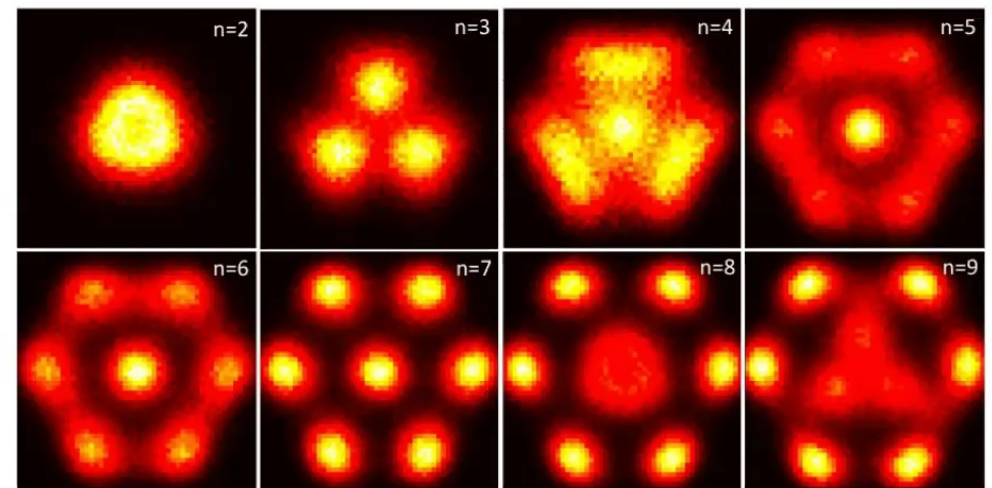
- Anti-symmetric neural network
- Change sign structure directly and generalization to arbitrary lattices
- Theoretically exact and lower bound for existing backflow methods, generalization of Slater-Jastrow-Backflow hierarchy
- Generalization to Autoregressive Neural TensorNet (arxiv.2304.01996)
- Further advancement in quantum chemistry: FermiNet, PauliNet

Neural Network Backflow

Artificial intelligence for artificial materials: moiré atom

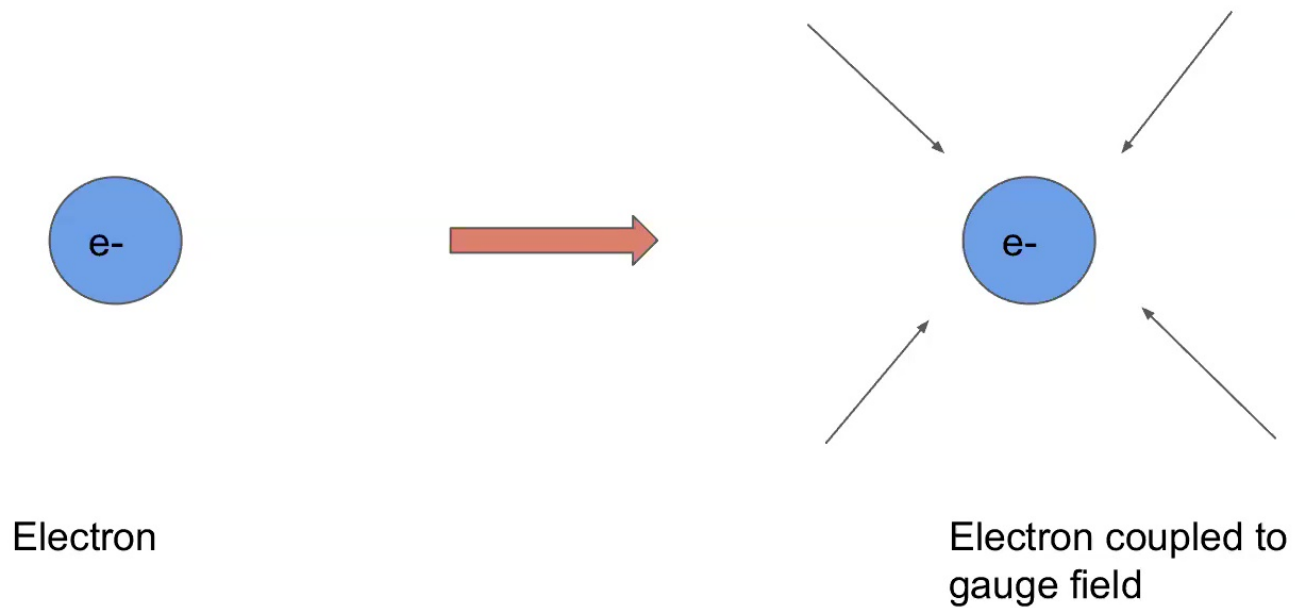


From Schrödinger atom to Wigner molecule



Effect of crystal field on charge distribution

Motivations: Simulation of Gauge Theory



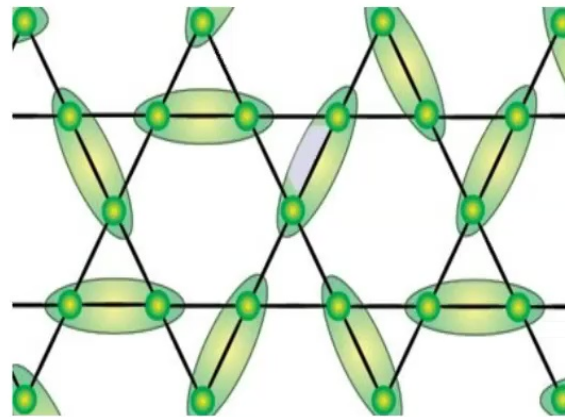
Motivations: Simulation of Gauge Theory

Standard Model of Elementary Particles

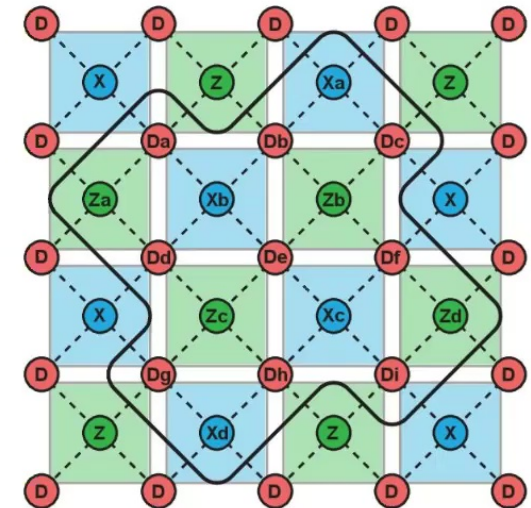
	three generations of matter (fermions)			interactions / force carriers (bosons)	
	I	II	III		
mass	$\approx 2.2 \text{ MeV}/c^2$	$\approx 1.28 \text{ GeV}/c^2$	$\approx 173.1 \text{ GeV}/c^2$	0	$\approx 124.97 \text{ GeV}/c^2$
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	0
QUARKS	u up	c charm	t top	g gluon	H higgs
	$\approx 4.7 \text{ MeV}/c^2$	$\approx 96 \text{ MeV}/c^2$	$\approx 4.18 \text{ GeV}/c^2$	0	
	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	0	
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	
	d down	s strange	b bottom	γ photon	
	$\approx 0.511 \text{ MeV}/c^2$	$\approx 105.66 \text{ MeV}/c^2$	$\approx 1.7768 \text{ GeV}/c^2$	0	
	-1	-1	-1	0	
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	
LEPTONS	e electron	μ muon	τ tau	Z Z boson	
	$< 1.0 \text{ eV}/c^2$	$< 0.17 \text{ MeV}/c^2$	$< 18.2 \text{ MeV}/c^2$	$\approx 80.433 \text{ GeV}/c^2$	
	0	0	0	± 1	
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	
	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino	W W boson	

GAUGE BOSONS
VECTOR BOSONS
SCALAR BOSONS

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

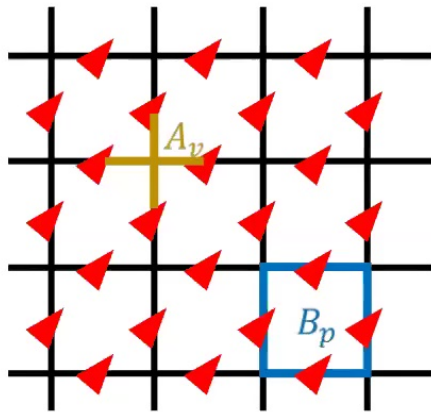
(Phys. Rev. Lett. 122, 226401, arxiv.2101.07243, arxiv. 2212.06835)

- Neural Quantum Field State for continuum Quantum Field Theories

(arxiv. 2212.00782)

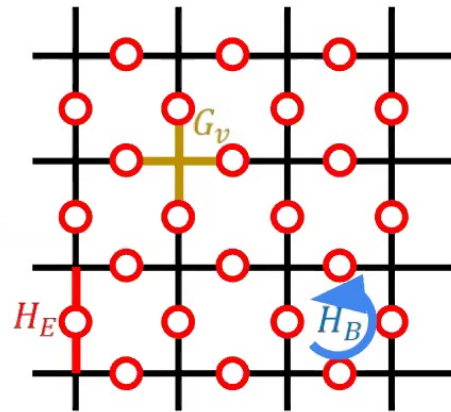
Motivations: Simulation of Quantum Field Theories

\mathbb{Z}_2 toric code model



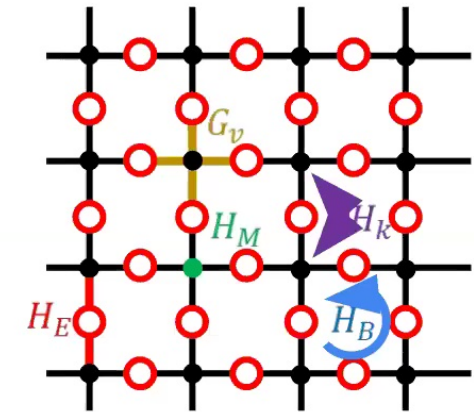
\mathbb{Z}_2 gauge theory
 A_v : Gauss's law

U(1) pure gauge theory



Continuous gauge theory
 Infinite degree of freedom

U(1) gauge theory with fermions

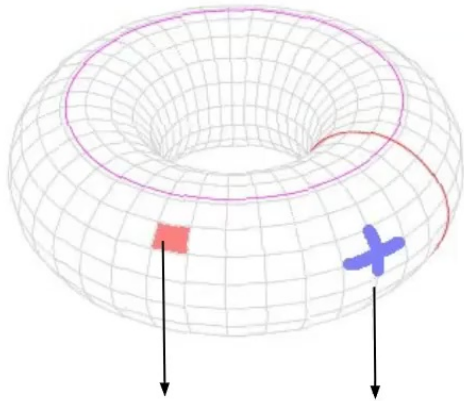


Gauge field fermion interaction
 Fermionic sign problem

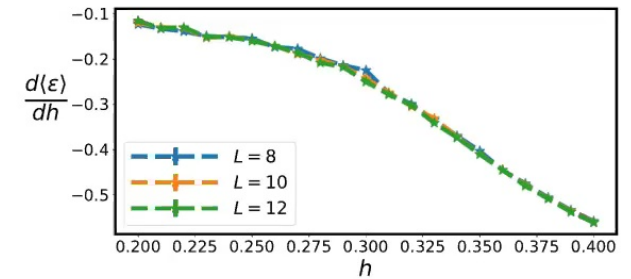
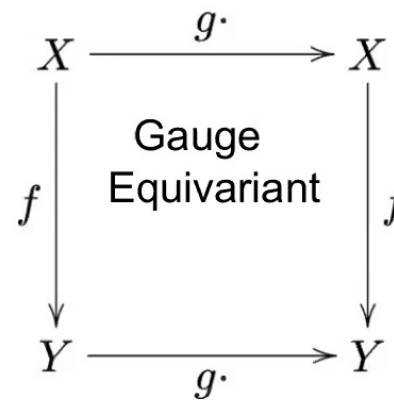
Gauge Equivariant Neural Network for Quantum Lattice Gauge Theories

--- Develop gauge equivariant neural network for simulating quantum lattice gauge models

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



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

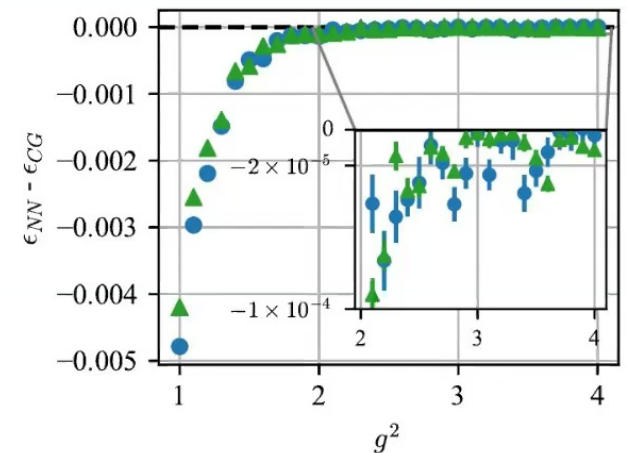
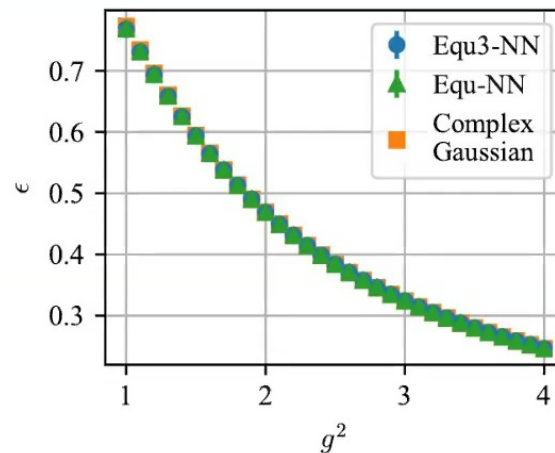
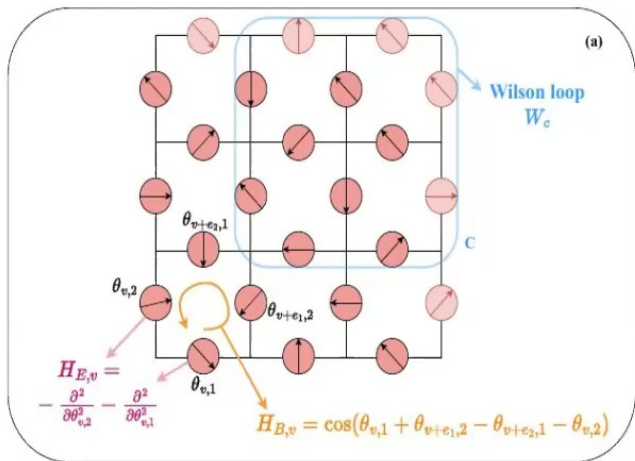


Perimeter law | Area law

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

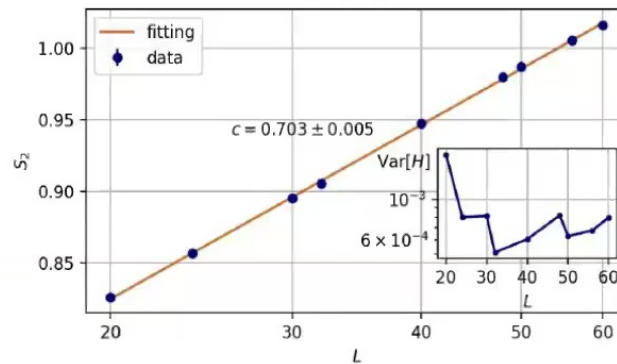
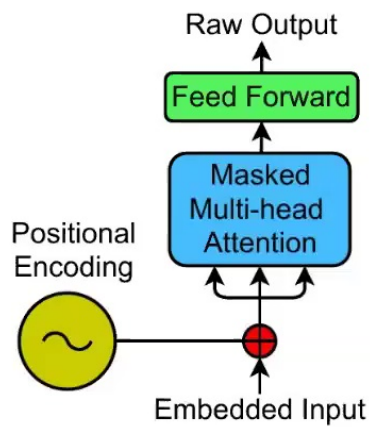
$$\Psi(\dots, \theta_{v,\delta}, \dots) = \Psi(\dots, \theta_{v,\delta} + \alpha_{v+e_\delta} - \alpha_v, \dots)$$



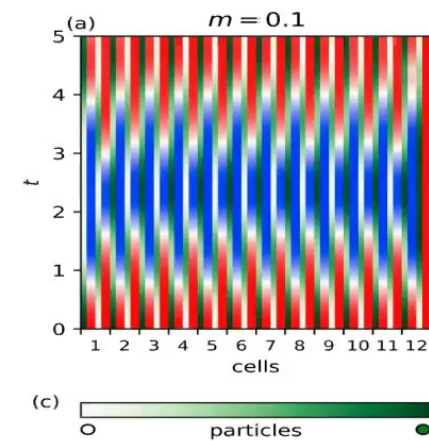
Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network for Quantum Lattice Models

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

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



Anyon central charge

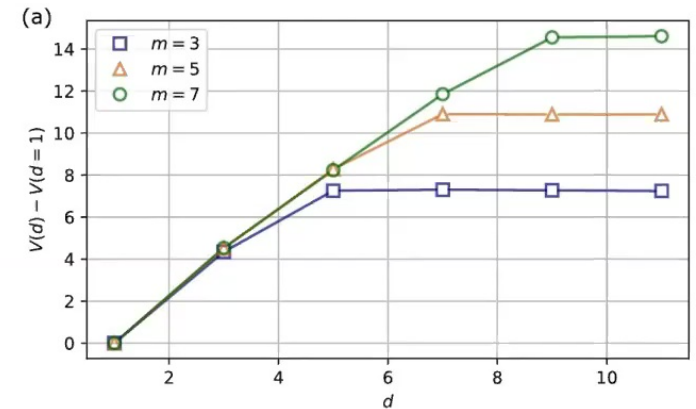
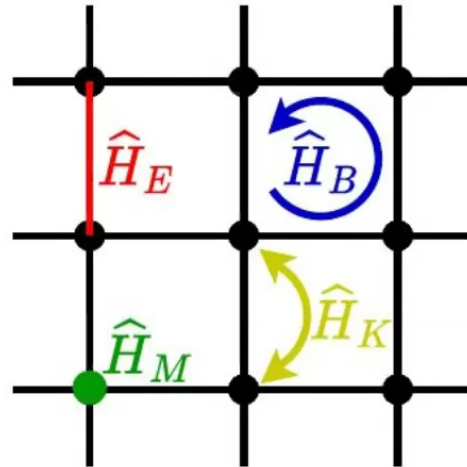
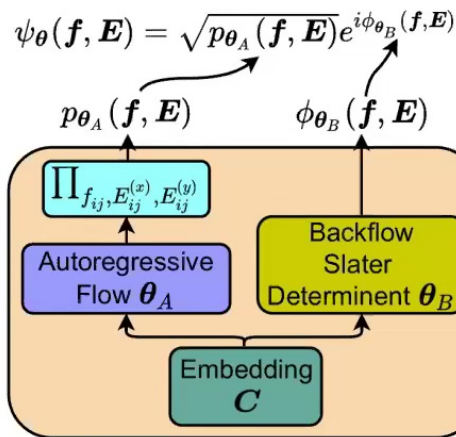


1+1-D QED dynamics

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.

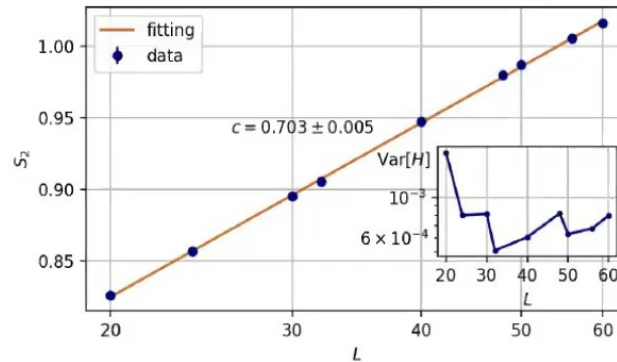
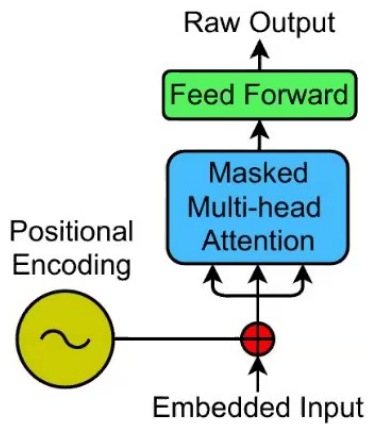
--- Simulate 2+1D QED at finite density to study string breaking, charge crystal phase transition and magnetic phase transition.



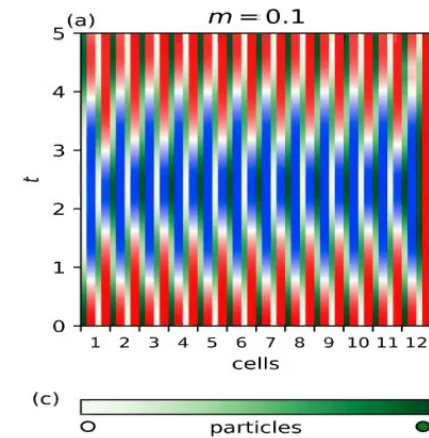
Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network for Quantum Lattice Models

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

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



Anyon central charge

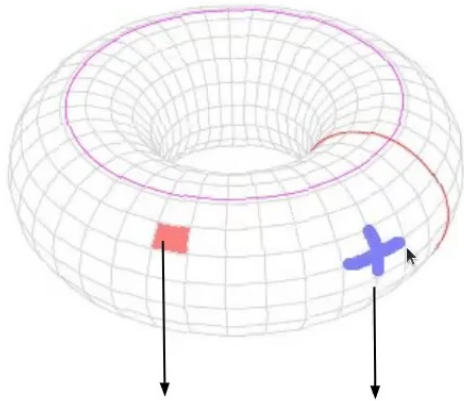


1+1-D QED dynamics

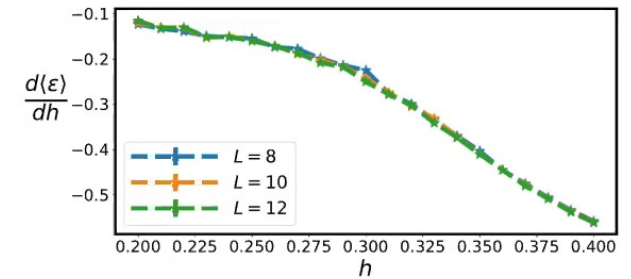
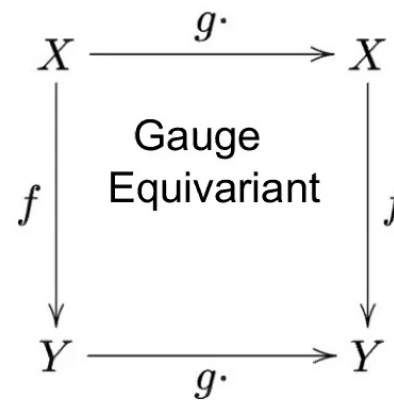
Gauge Equivariant Neural Network for Quantum Lattice Gauge Theories

--- Develop gauge equivariant neural network for simulating quantum lattice gauge models

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



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

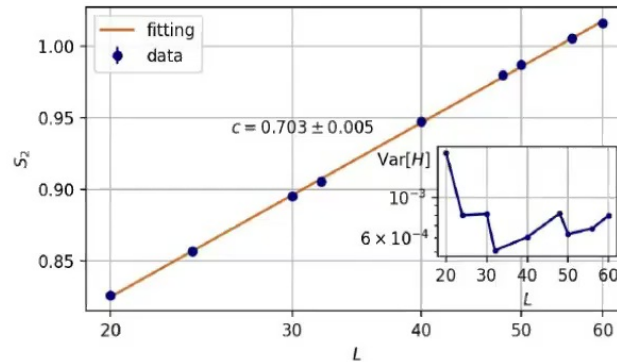
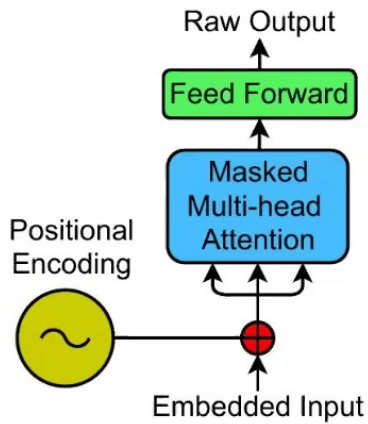


Perimeter law | Area law

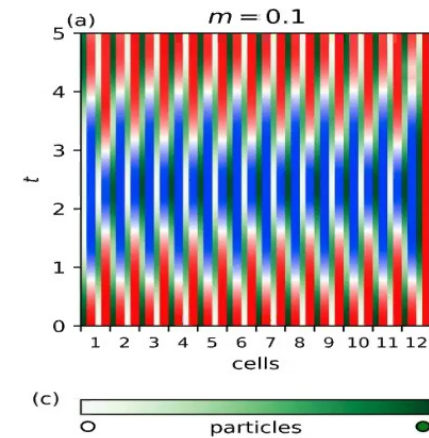
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Anyon central charge

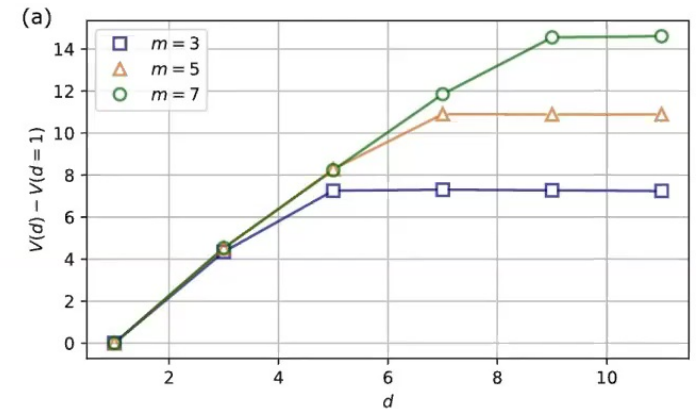
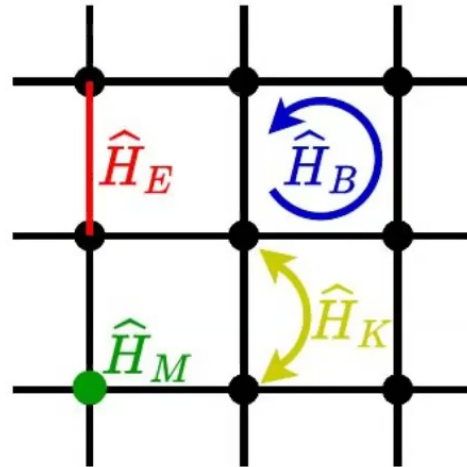
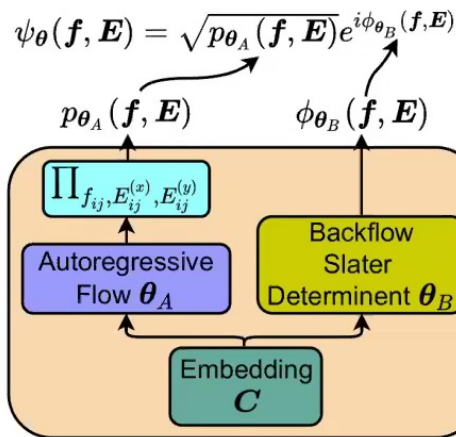


1+1-D QED dynamics

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.

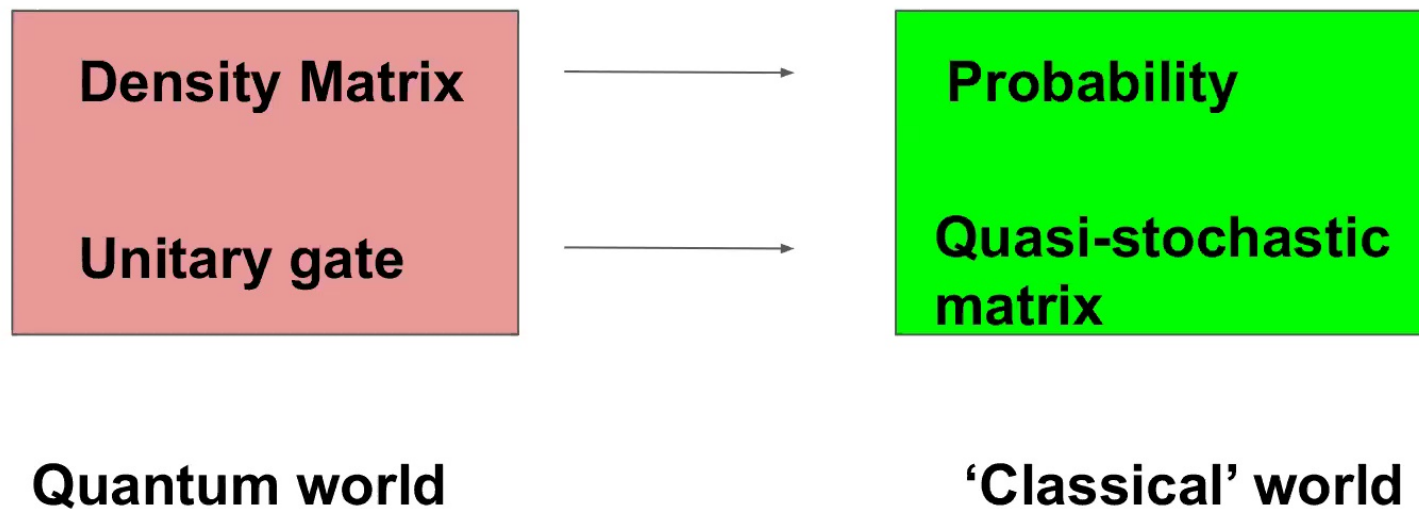


AI for Quantum: Quantum Many-body Physics

III. Real-time Quantum Dynamics

Neural POVM Simulation of Quantum Dynamics

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



Neural POVM Simulation

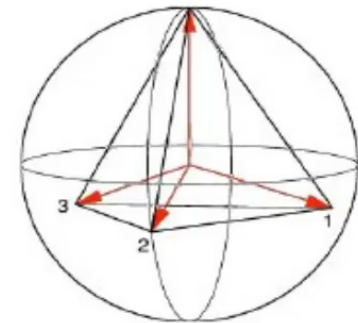
Positive Operator-Valued Measurement (POVM)

Tetrahedral POVM: $P_{(i)} = \text{tr}(\rho M_{(i)})$

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

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

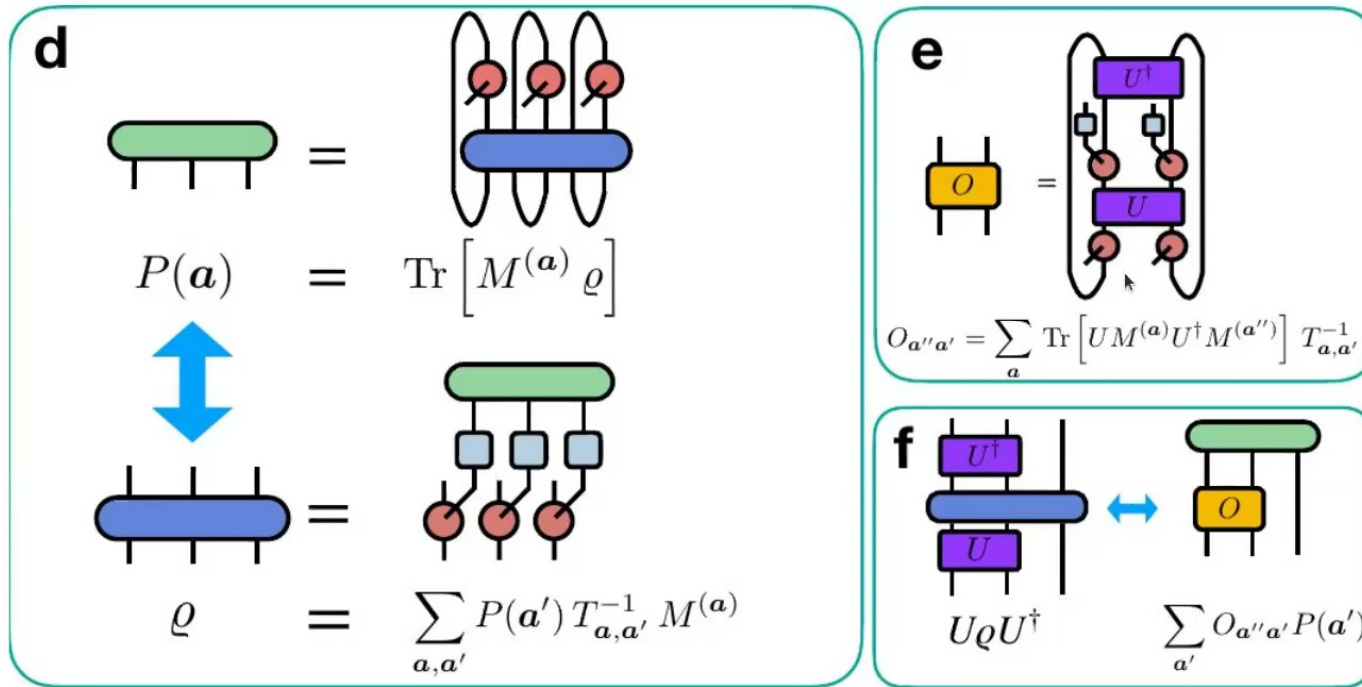
$$v_{(3)} = (-1, 1, -1) \quad v_{(4)} = (-1, -1, 1)$$



Quantum tomography

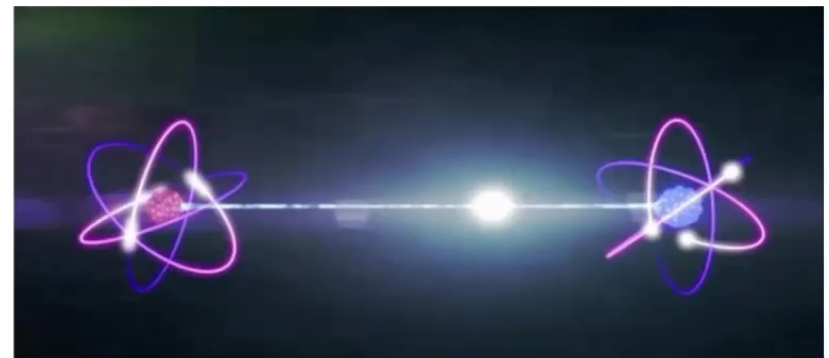
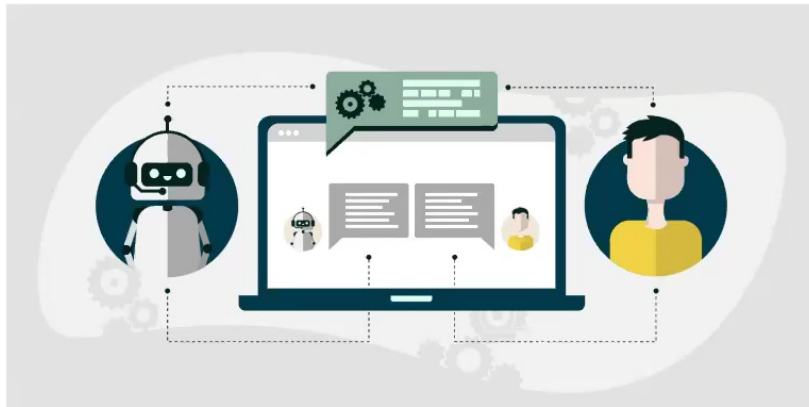
Neural POVM Simulation: Quantum Circuits

POVM simulation of quantum circuit



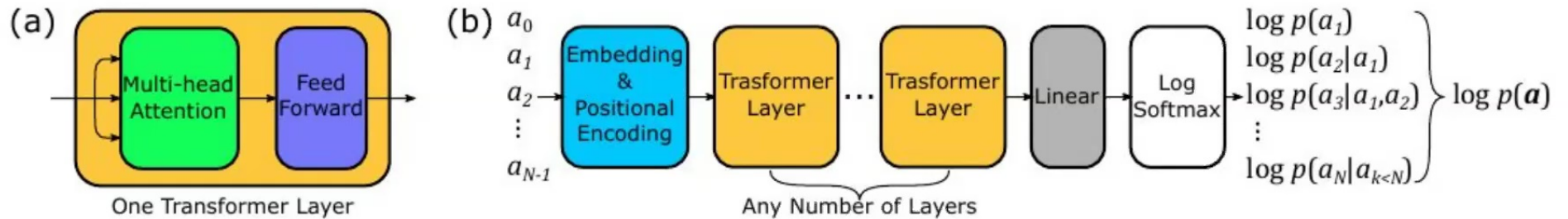
Neural POVM Simulation: Quantum Circuits

qubits as language: high dimensional distribution with long range correlation



Neural POVM Simulation: Transformer Representation

$$P_{\theta}(a_1, \dots, a_N) = \prod_{k=1}^N P_{\theta}(a_k | a_{<k}),$$



Attention is All You Need

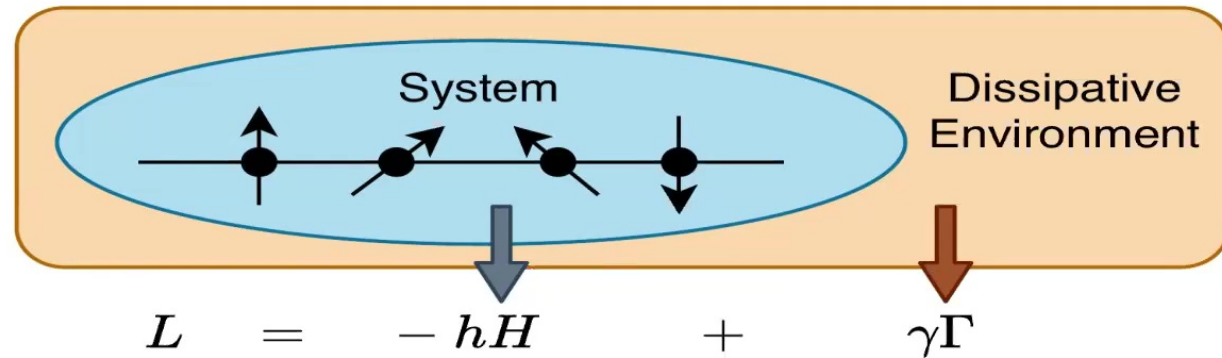
(<https://papers.nips.cc/paper/7181-attention-is-all-you-need.pdf>)

Conditional probability for exact sampling and inference

Compact representation for high dimensional distribution

Neural POVM Simulation: Open System Dynamics

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



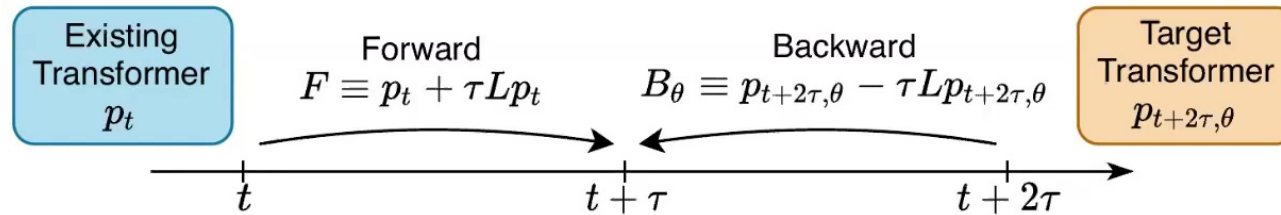
POVM formulation:
$$\dot{p}(\mathbf{a}) = \sum_{\mathbf{b}} p(\mathbf{b}) L_{\mathbf{a}}^{\mathbf{b}} = \sum_{\mathbf{b}} p(\mathbf{b}) (A_{\mathbf{a}}^{\mathbf{b}} + B_{\mathbf{a}}^{\mathbf{b}})$$

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

Neural POVM Simulation: Optimization

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

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



Steady state: minimize the derivative to be zero

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

Neural POVM Simulation: Open System Dynamics

1D Dissipative Transverse Ising Chain

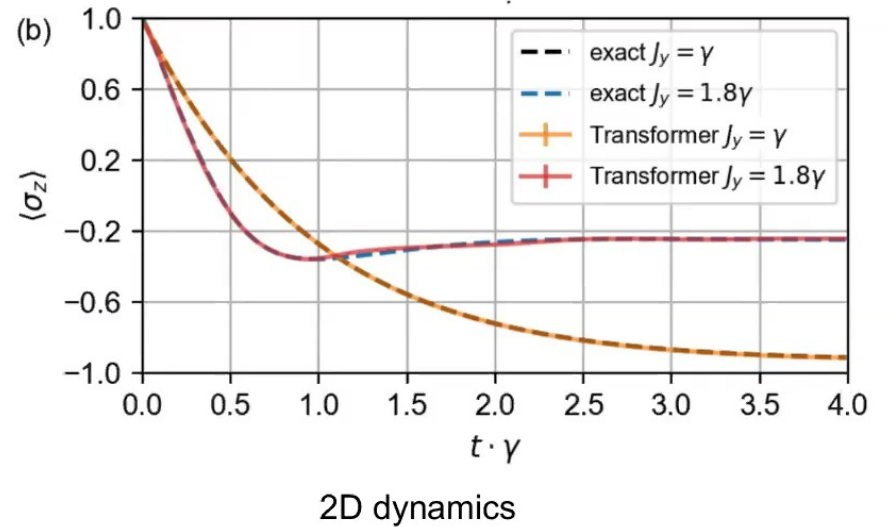
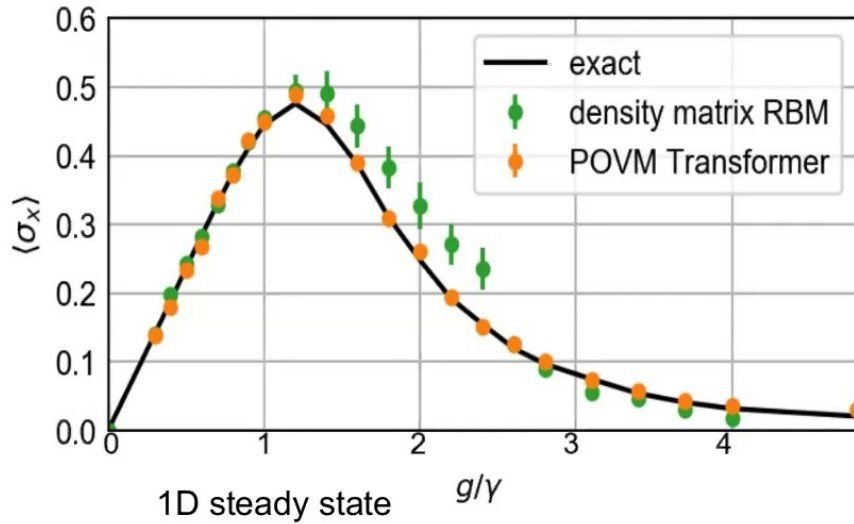
$$H = \frac{V}{4} \sum_{\langle i,j \rangle} \sigma_i^{(z)} \sigma_j^{(z)} + \frac{g}{2} \sum_k \sigma_k^{(x)}$$

Dissipative Heisenberg Chain

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

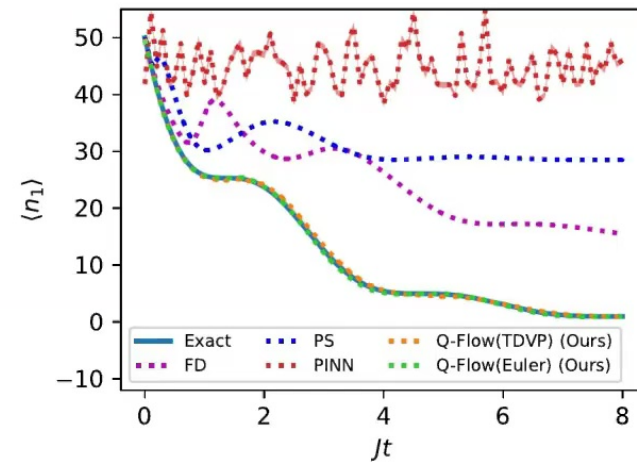
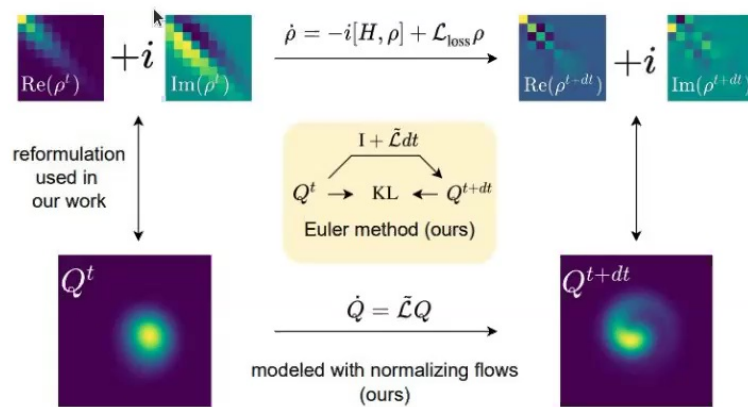
$$\Gamma_k = \sigma_k^{(-)} = \frac{1}{2} (\sigma_k^{(x)} - i\sigma_k^{(y)})$$

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



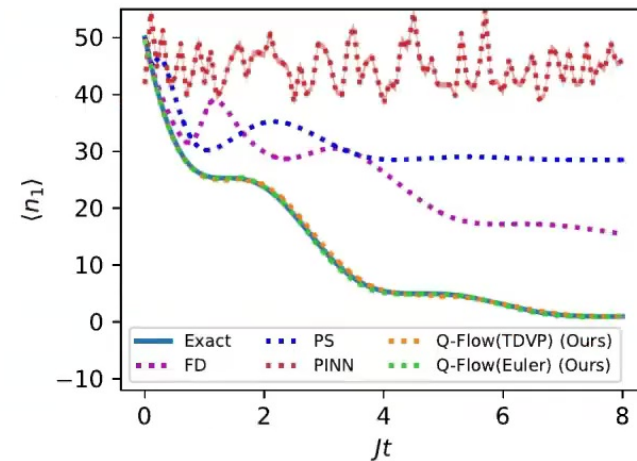
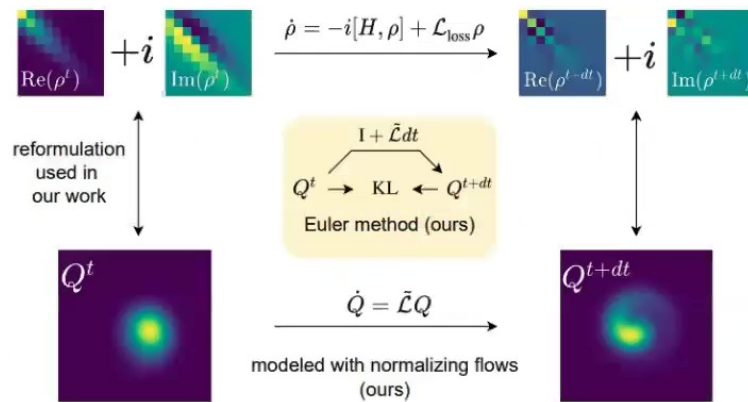
QFlow: Generative Modeling for Differential Equations of Open Quantum Dynamics with Normalizing Flows

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



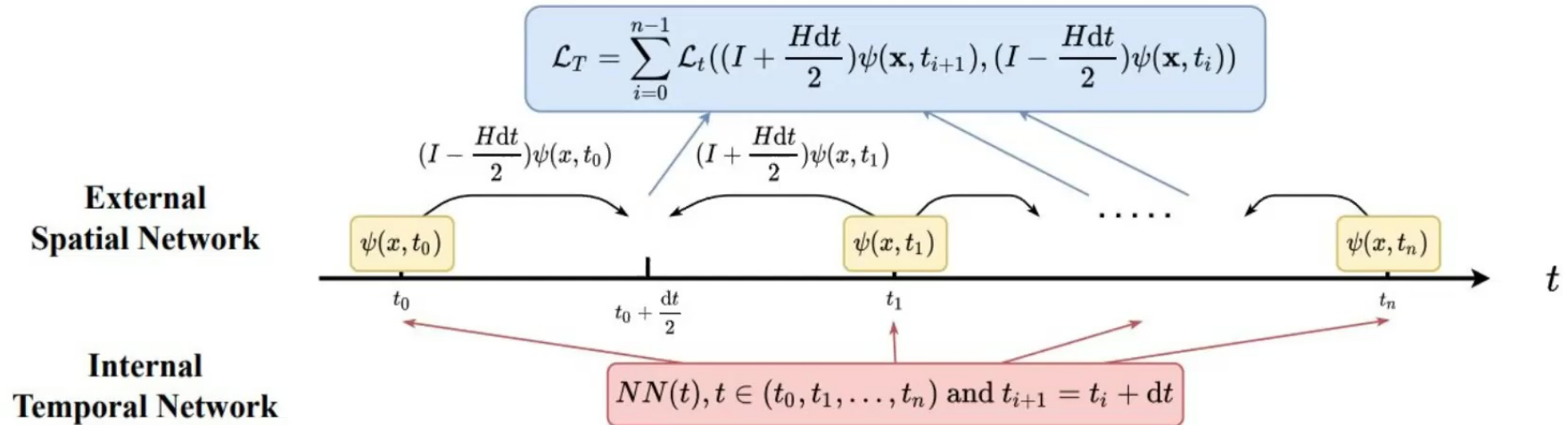
QFlow: Generative Modeling for Differential Equations of Open Quantum Dynamics with Normalizing Flows

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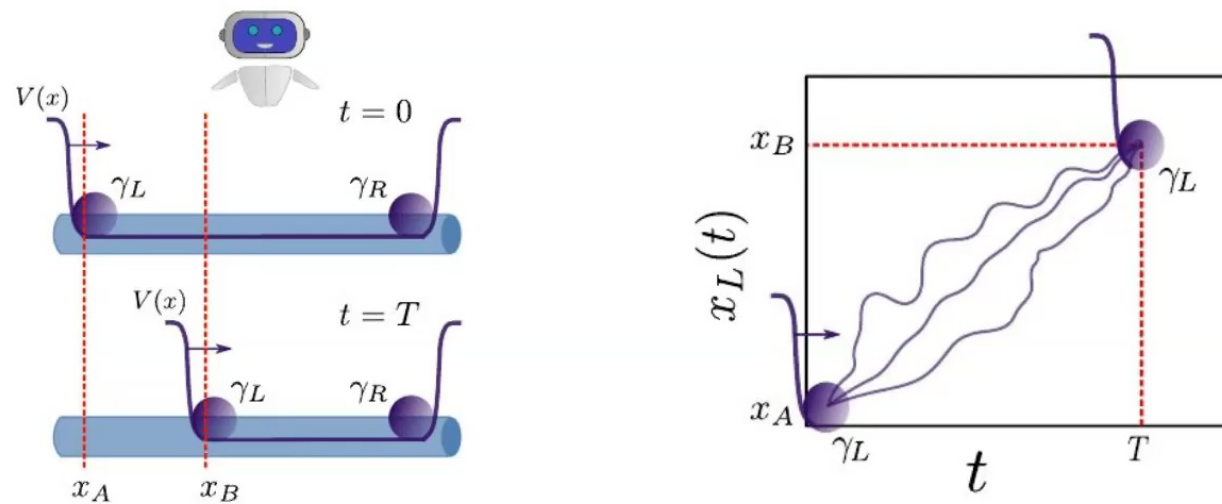
Spacetime Neural Network for High Dimensional Quantum Dynamics

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

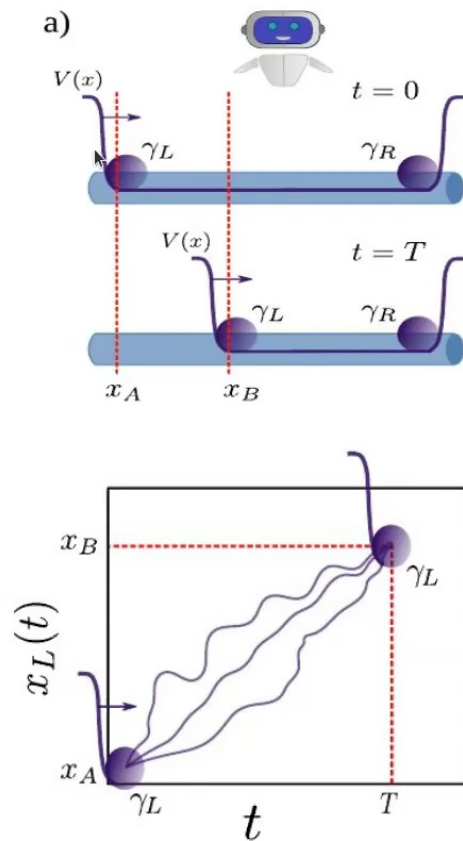


Protocol Discovery for the Quantum Control of Majoranas by Differentiable Programming and Natural Evolution Strategies

Luuk Coopmans†, Di Luo†, Graham Kells, Bryan K. Clark, Juan Carrasquilla



Differentiable Programming for Quantum Control



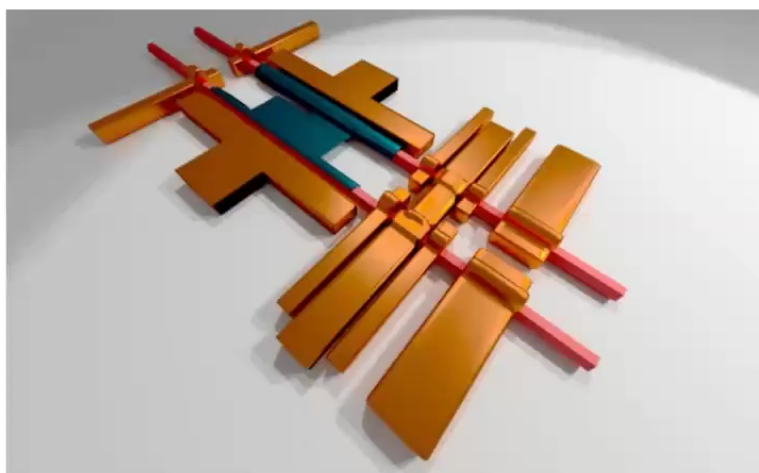
Control: $V(x,t)$

$$\mathcal{H}(t) = - \sum_{x=1}^N [\mu(x) - V(x,t)] (c_x^\dagger c_x - 1/2) - w \sum_{x=1}^{N-1} (c_x^\dagger c_{x+1} + h.c.) + \Delta \sum_{x=1}^{N-1} (c_x^\dagger c_{x+1}^\dagger + h.c.),$$

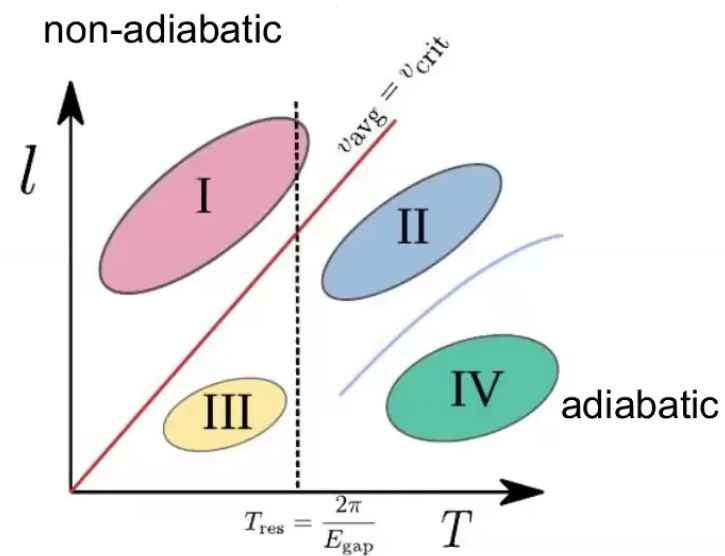
Goal: minimize

$$\mathcal{I}(T) = 1 - |\langle \psi_B | \mathcal{T} e^{-i \int_0^T \mathcal{H}(t) dt} | \psi_A \rangle|^2 \equiv 1 - \mathcal{F}(T)$$

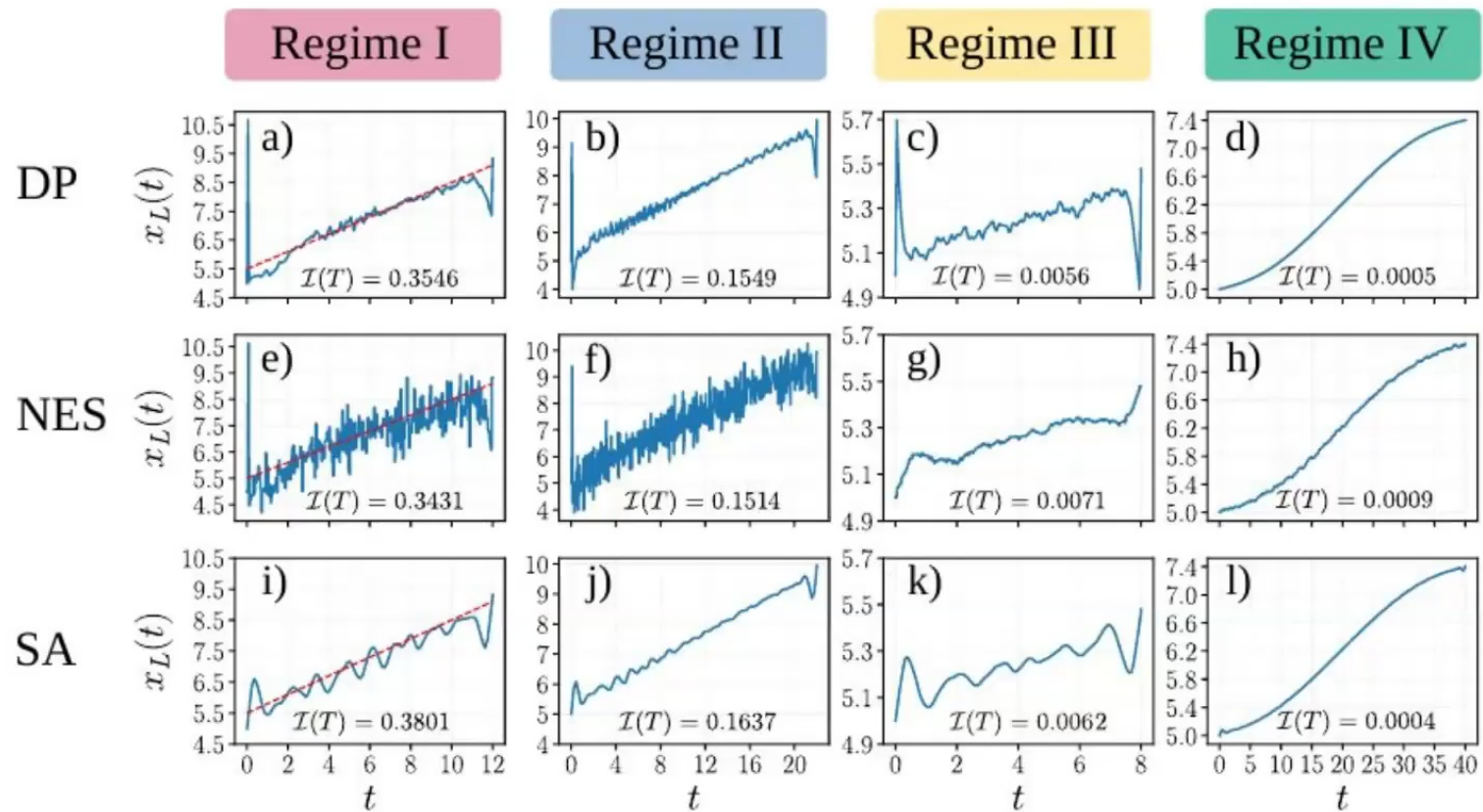
Differentiable Programming for Quantum Control



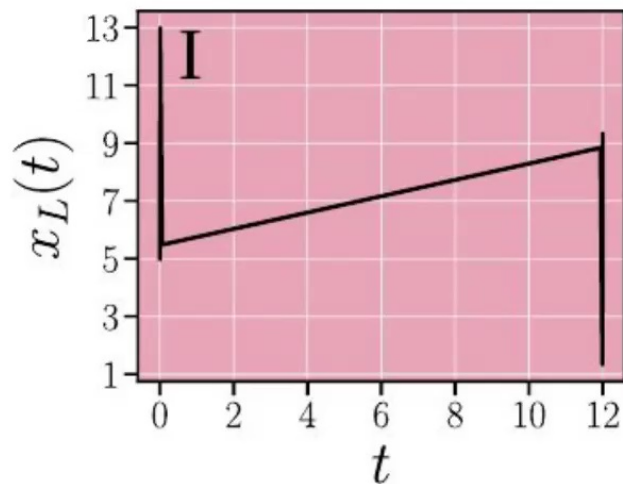
Topological quantum computation and majorana braiding



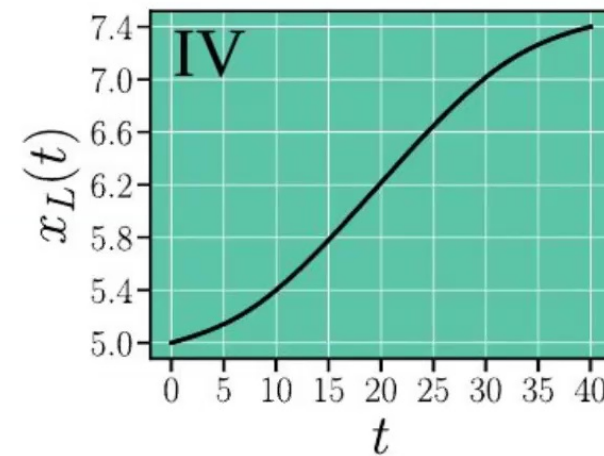
Differentiable Programming for Quantum Control



Differentiable Programming for Quantum Control



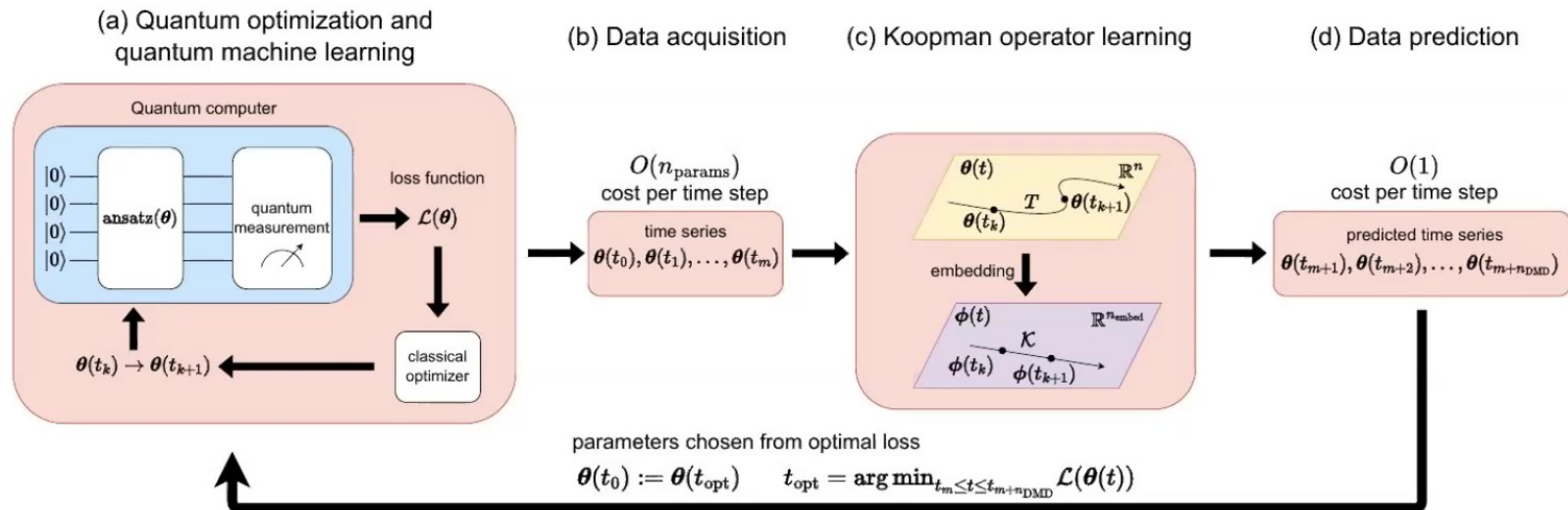
New Jump-move-jump protocol discovered
(later justified by moving frame analysis)



Rediscover of ramp-up ramp down
adiabatic protocol

Koopman Operator learning for Accelerating Quantum Optimization and Machine Learning

Di Luo†, Jiayu Shen†, Rumen Dangovski, Marin Soljačić

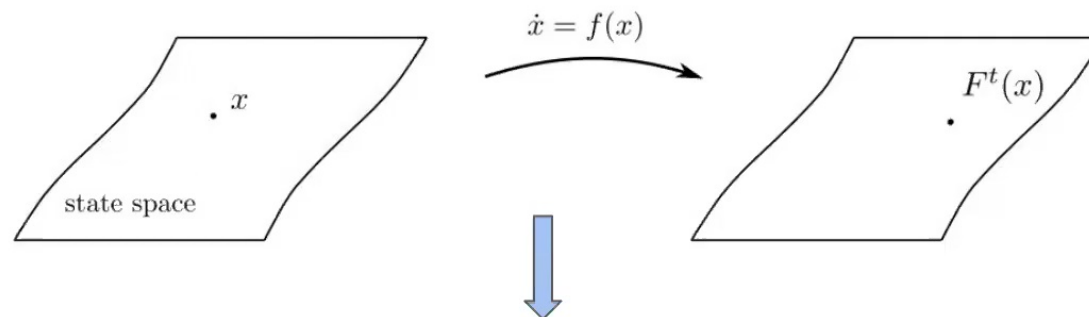


Koopman Operator Theory for Quantum

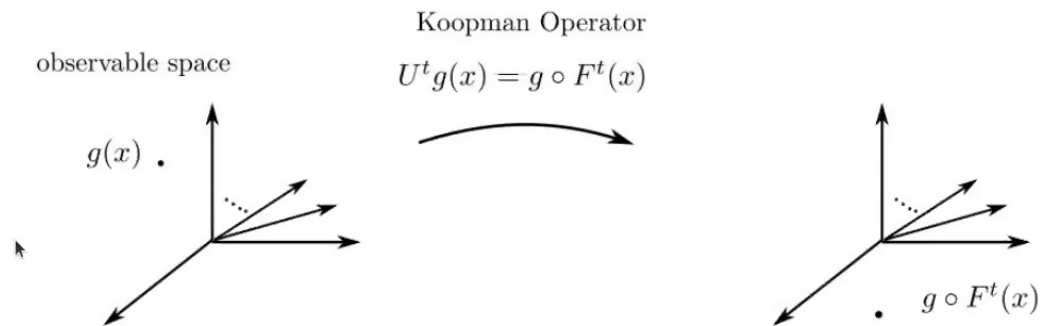
arxiv. 2211.01365

Predict quantum gradient as dynamical equation using Koopman Operator theory

Classical variable



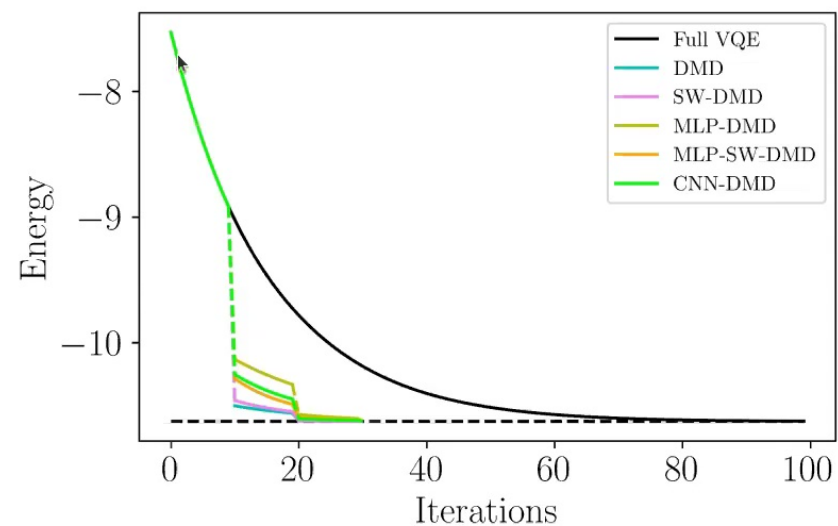
Quantum
observable
embedding



Koopman Operator Theory for Quantum

arxiv. 2211.01365

	Classical ML	VQA
Data Type	Classical	Classical or Quantum
Typical Model	Classical Neural Net	Parametrized Quantum Circuit
Forward Propagation Cost per Step	$O(1)$	$O(n_{shots})$
Backward Propagation Cost per Step	$O(1)$	$O(n_{params} \cdot n_{shots})$
QuACK Gradient Cost per Step	$O(1)$	$O(n_{shots})$



10-qubit quantum Ising model
with quantum natural gradient

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