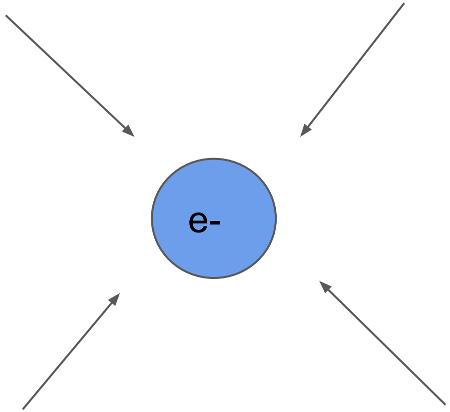
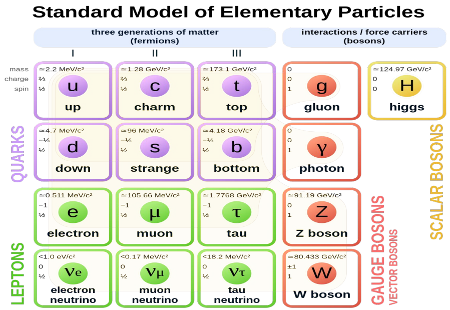
Simulating Quantum Field Theories with Neural Network Representation

Di Luo
IAIFI Fellow, MIT

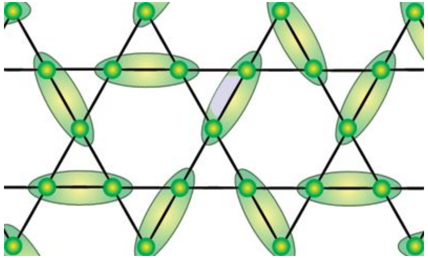
Motivations: Simulation of Quantum Field Theories



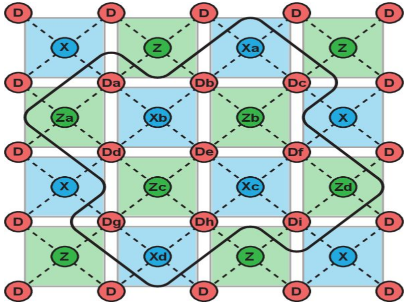
matter coupled to gauge field



High energy



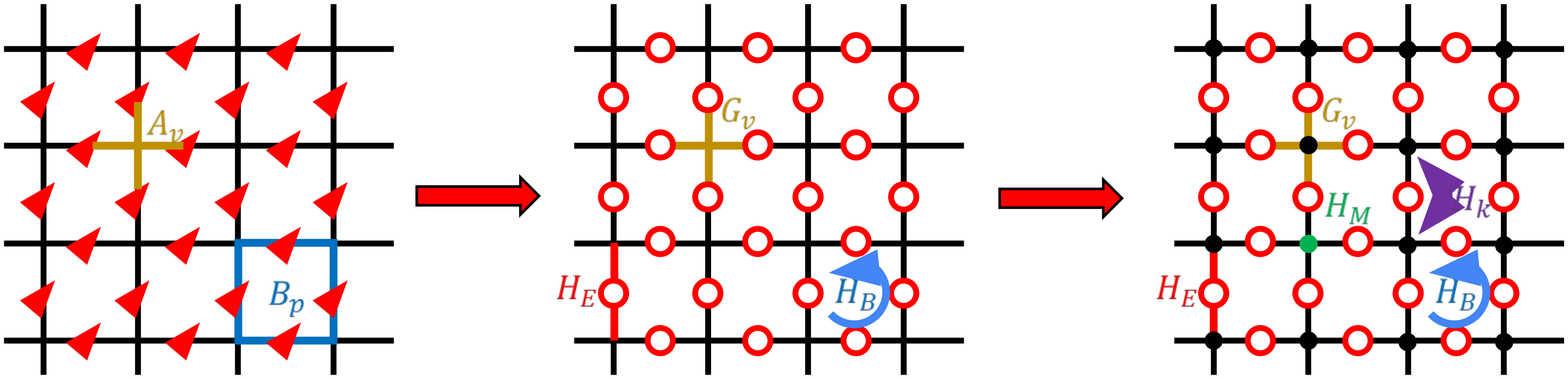
Condensed matter



Quantum error correction

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

Quantum Field Theories are Hard to Simulate

Difficulties:

- **Gauge field**: infinite degree of freedom; gauge symmetries
- **Fermions**: sign problem; antisymmetric wave function

Lagrangian formulation: challenges of sign problem

- Path integral Monte Carlo
- Flow based sampling method

Hamiltonian formulation:

- Quantum computer: limited power at early stage
- Tensor networks: cannot include infinite degree of freedom
- Neural networks quantum state: new exploration

2012.05232:
discrete gauge theory, $\mathbb{Z}_n$
Abelian & Nonabelian discrete groups

2101.07243:
- Quantum link model with fermions in 1+1D
- $\mathbb{Z}_2$ gauge theory in 2+1D
- $\mathrm{SU}(2)_3$ anyon model in 1D

2211.03198
2+1D pure $\mathrm{U}(1)$ gauge theory

2212.06835
2+1D $\mathrm{U}(1)$ gauge theory with fermions

New Exploration: Neural Quantum States

- 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, ,Phys. Rev. Research 5, 013216 arxiv.2212.06835)

- Neural Quantum Field State for continuum Quantum Field Theories

  (Phys. Rev. Lett. 131, 081601)

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: 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

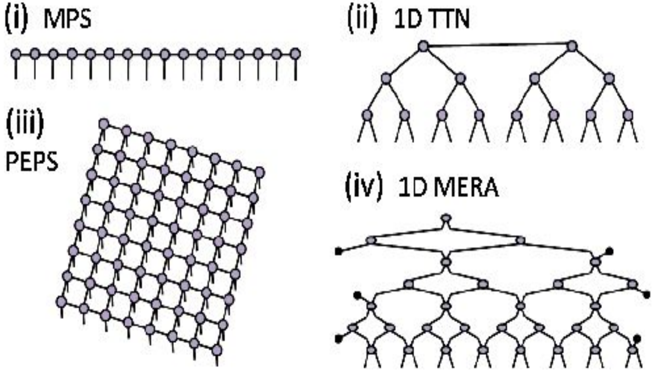
- Draw samples according to $|\psi|^2$, apply transition probability kernel
- Due to sign problem, the relative variance of the sign scales exponentially

Ongoing Efforts: Tensor Network

Tensor network: tensor decomposition of high dimensional objects

High rank tensor

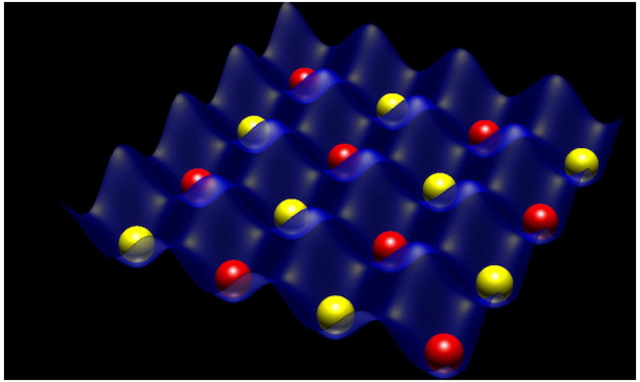
$$T_{i,j,k,l} =$$



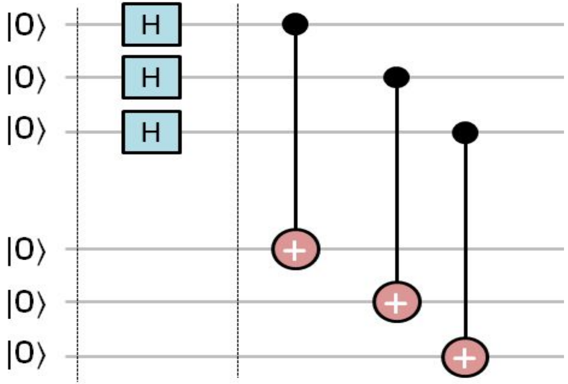
- Efficient for 1 dimensional system due to area law
- Challenges exist for two or three dimensional physics system

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

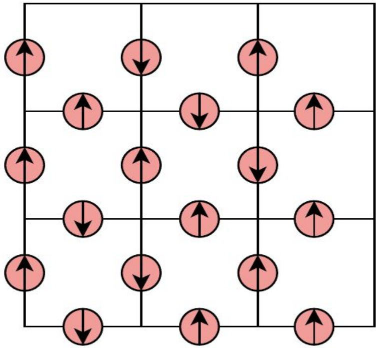
Neural Quantum States

For a n-particle (spin ½) system:

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

2^n x 2^n hermitian matrix

2^n vector

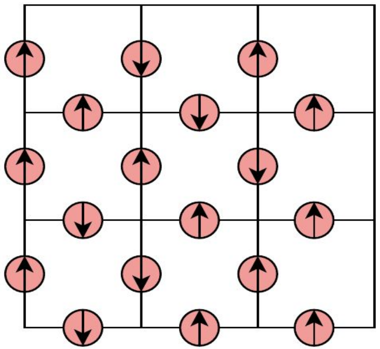


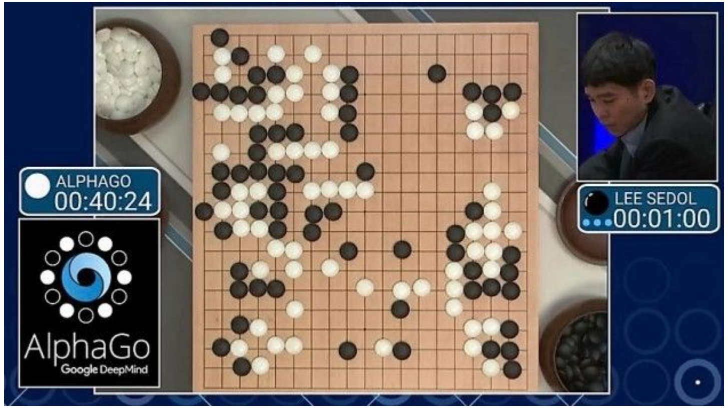
Superposition of 2^n configurations!

Neural Quantum States

For a n-particle system:

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



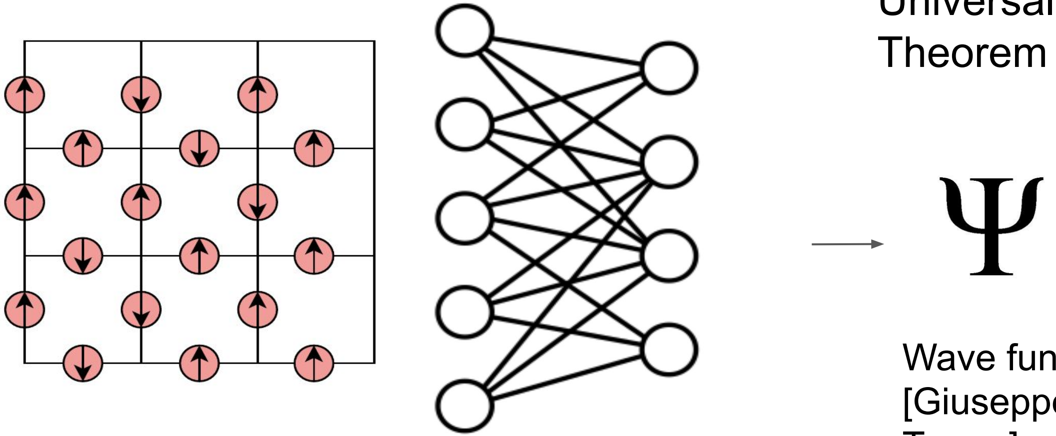


Superposition of 2^n configurations!

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

Neural Quantum States

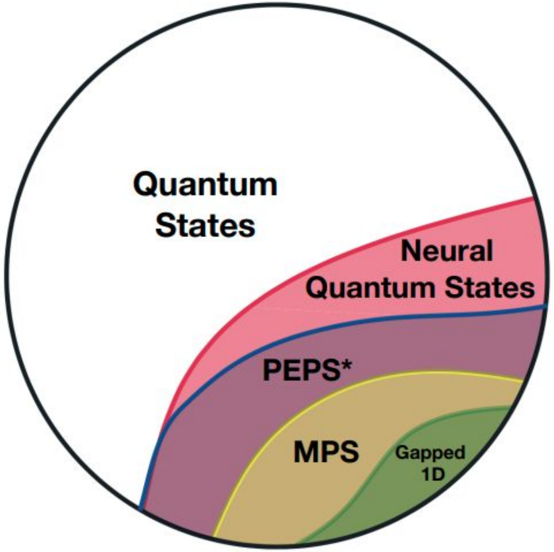
Neural network: low dimensional representation of high dimensional objects



Universal Approximation Theorem [Cybenko]

Wave function amplitude [Giuseppe Carleo, Matthias Troyer]

Neural Quantum States



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

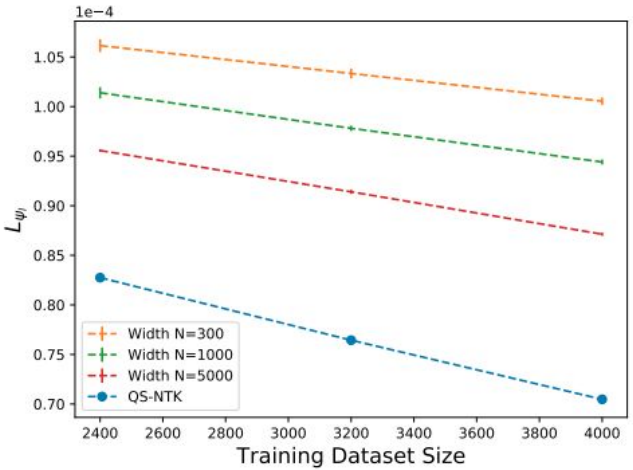
Neural Network Quantum State:

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

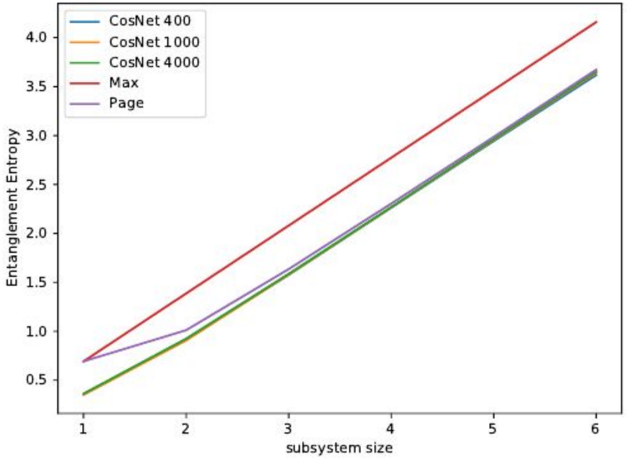
Neural Quantum States

Di Luo, James Halverson, Mach. Learn.: Sci. Technol. 4 025038

Infinite Neural Network Quantum State: Entanglement and Training Dynamics



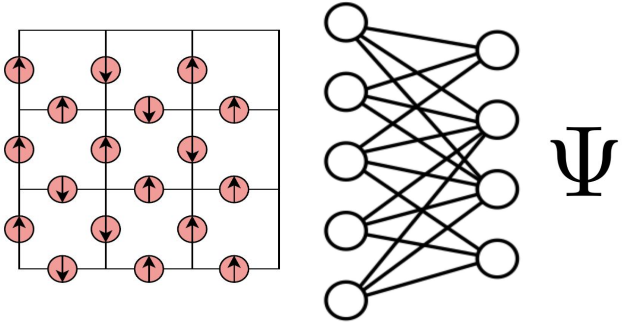
Quantum State Neural Tangent Kernel



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

Volume law entanglement engineering of CosNet

Neural Quantum States



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Giuseppe Carleo[1,*], Matthias Troyer[1,2]

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Xun Gao & Lu-Ming Duan

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

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

Phys. Rev. X **7**, 021021 – Published 11 May 2017

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

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

Motivations: Simulation of Quantum Field Theories

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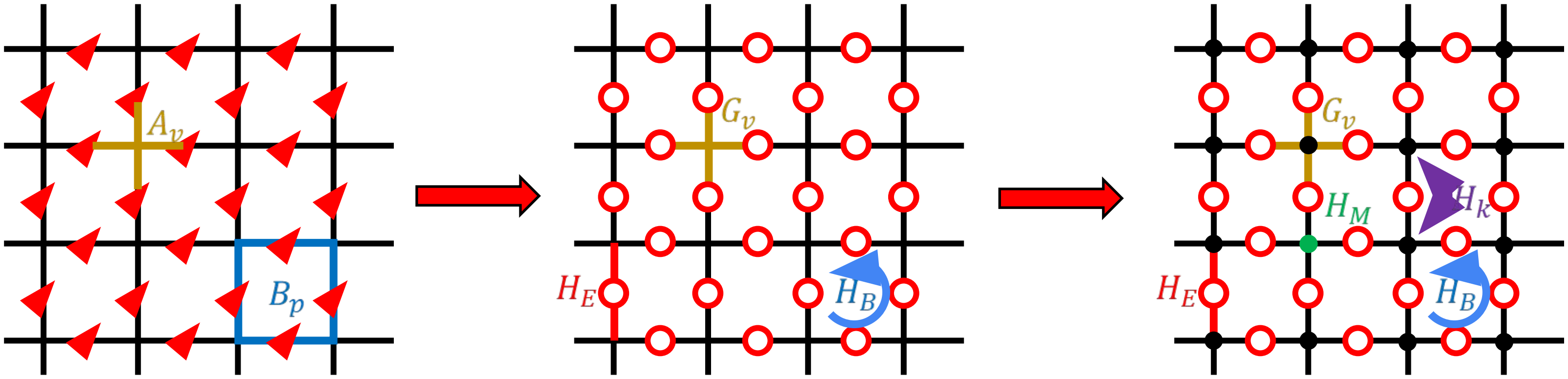

$\mathbb{Z}_2$ gauge theory
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Continuous gauge theory
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Gauge field fermion interaction
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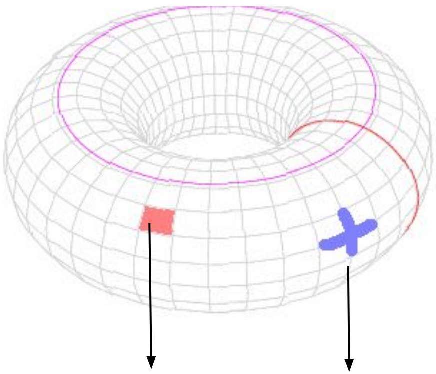
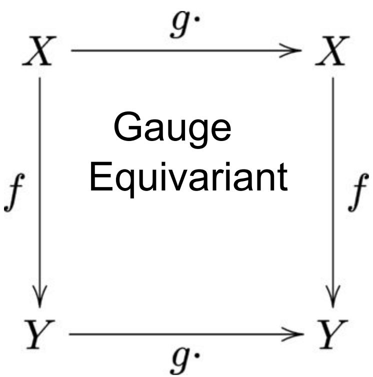
Gauge Equivariant Neural Network for Quantum Lattice Gauge Theories

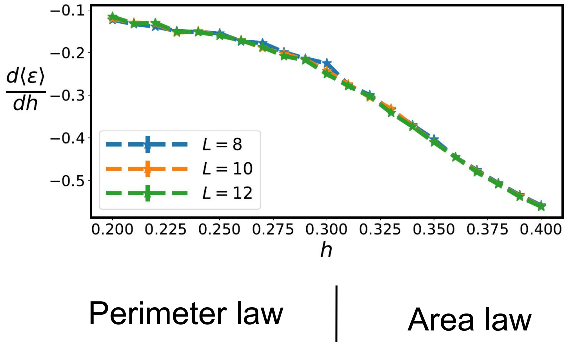
--- Develop gauge equivariant neural network for simulating quantum lattice gauge models
--- Exact representation for Toric code, Kitaev D(G) model, Fracton ground states and applications to transverse field Toric code phase transition

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



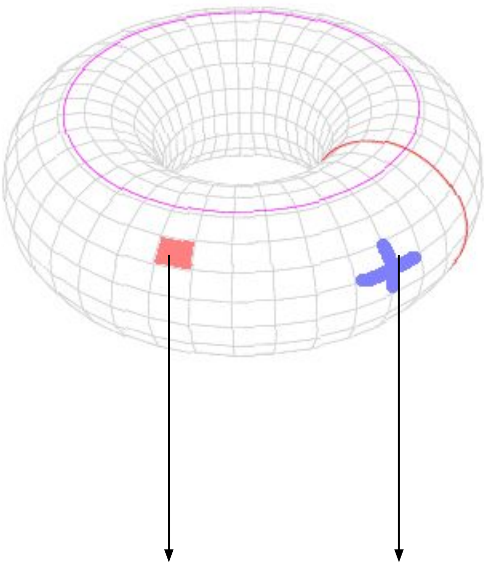
$$W_f := \prod_{e \in f} Z_e \qquad G_v := \prod_{e \ni v} X_e$$





Phys. Rev. Lett. **127**, 276402

Gauge Equivariant Neural Quantum States



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

Toric code Hamiltonian $\hat{H} = -J \sum_f W_f - \Delta \sum_{v \in V} G_v$

(AY Kitaev, 2003)

Gauge symmetry $[G_v, \hat{H}]$ = 0

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

Q: How to construct neural network representation for wave functions with gauge symmetry?

$$\psi(G_v x) = \psi(x)$$

Gauge Equivariant Neural Quantum States

- Invariant function

$$\psi(G_v x) = \psi(x)$$

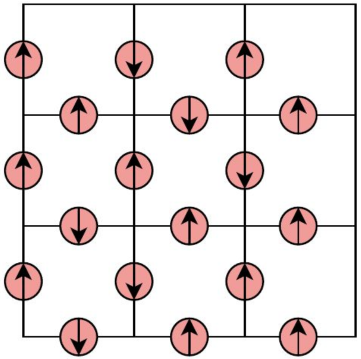
- Equivariant function

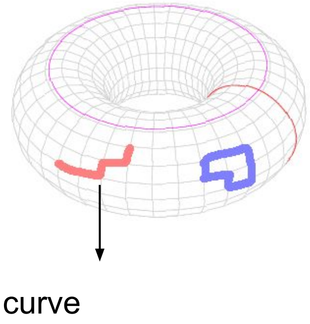
$$f(x) = f_L \circ \cdots \circ f_1(x)$$
$$f_i(G_v x) = G_v f_i(x)$$

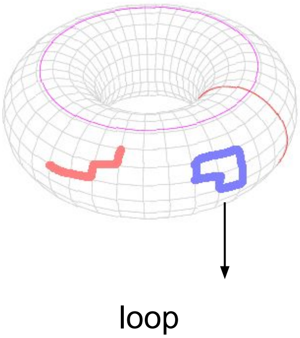
Phys. Rev. Lett. **127**, 276402

Gauge Equivariant Neural Quantum States

Configuration as 2 channel image → Z_2 equivariant layer → Z_2 invariant layer

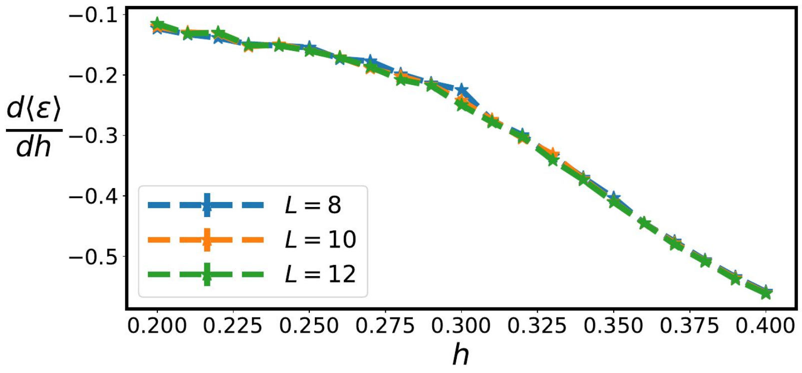


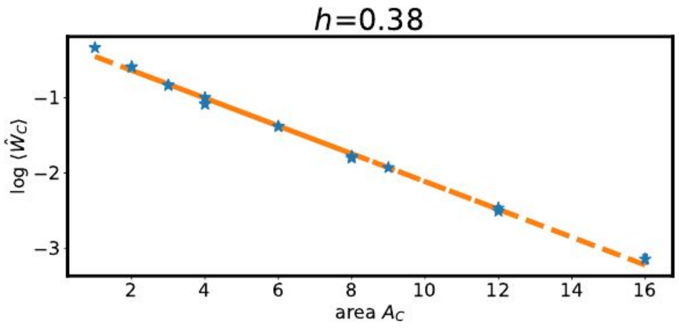


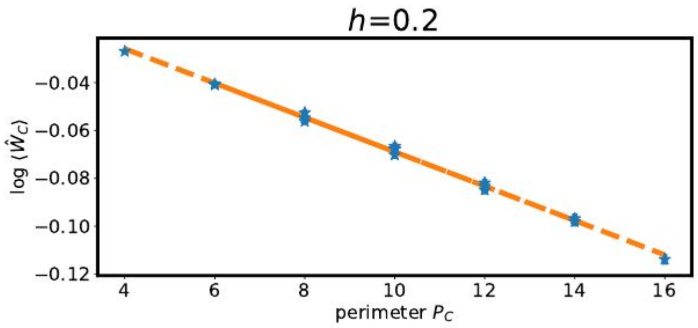


Gauge Equivariant Neural Quantum States

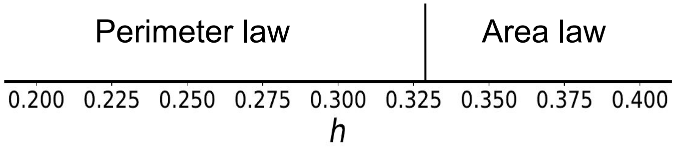
Study Area-law to Perimeter-law transition on Toric code with transverse field







Order parameter: $\hat{W}_C := \prod_{e\in C} Z_e$



(J Vidal, et al. 2009)

Gauge Equivariant Neural Quantum States

Theorem. There exists exact representation of the gauge equivariant neural network for grounds states of the following models:

- 2D Toric code
- 3D Toric code
- Kitave D(G) model with any discrete group G
- X-cube Fracton

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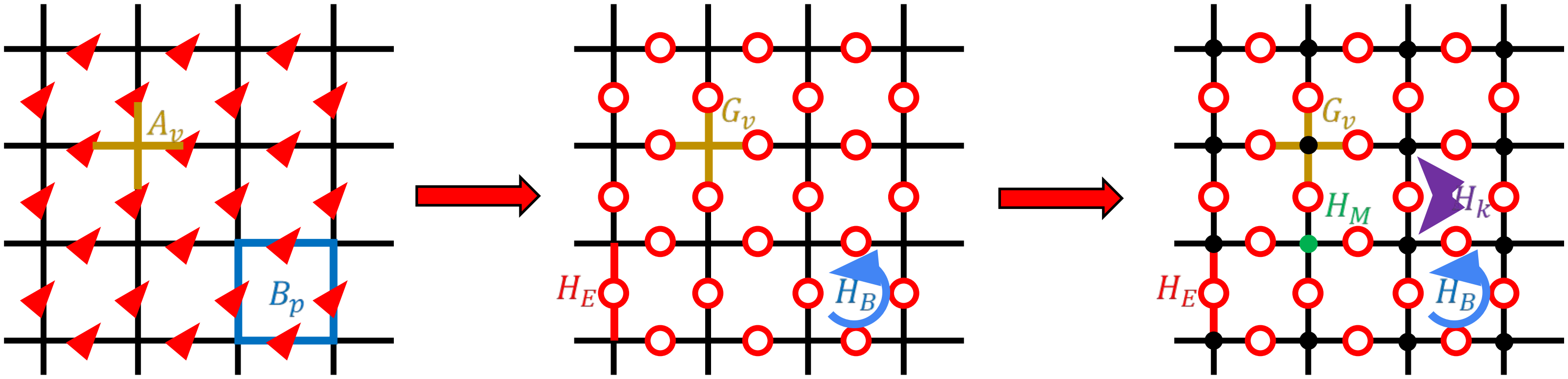


$\mathbb{Z}_2$ gauge theory
A_v: Gauss's law

Continuous gauge theory
Infinite degree of freedom

Gauge field fermion interaction
Fermionic sign problem

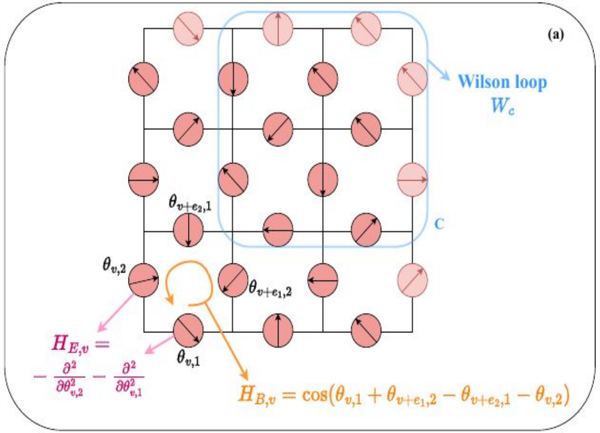
Di Luo†, Shunyue Yuan†, James Stokes, Bryan Clark. arxiv. 2211.03198

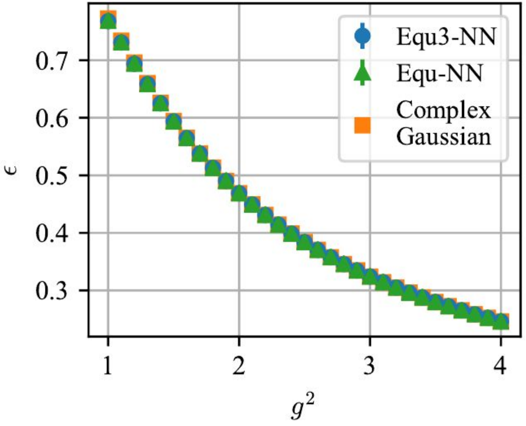
Gauge Equivariant Neural Network for 2+1D U(1) Gauge Theory Simulations in Hamiltonian Formulation

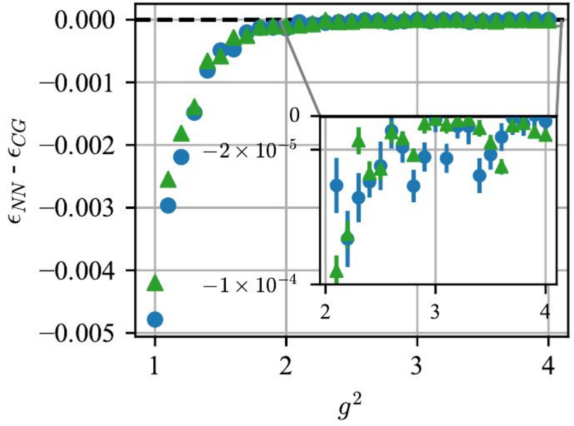
--- *Develop gauge equivariant neural network for simulating continuous-variable quantum lattice gauge models*

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

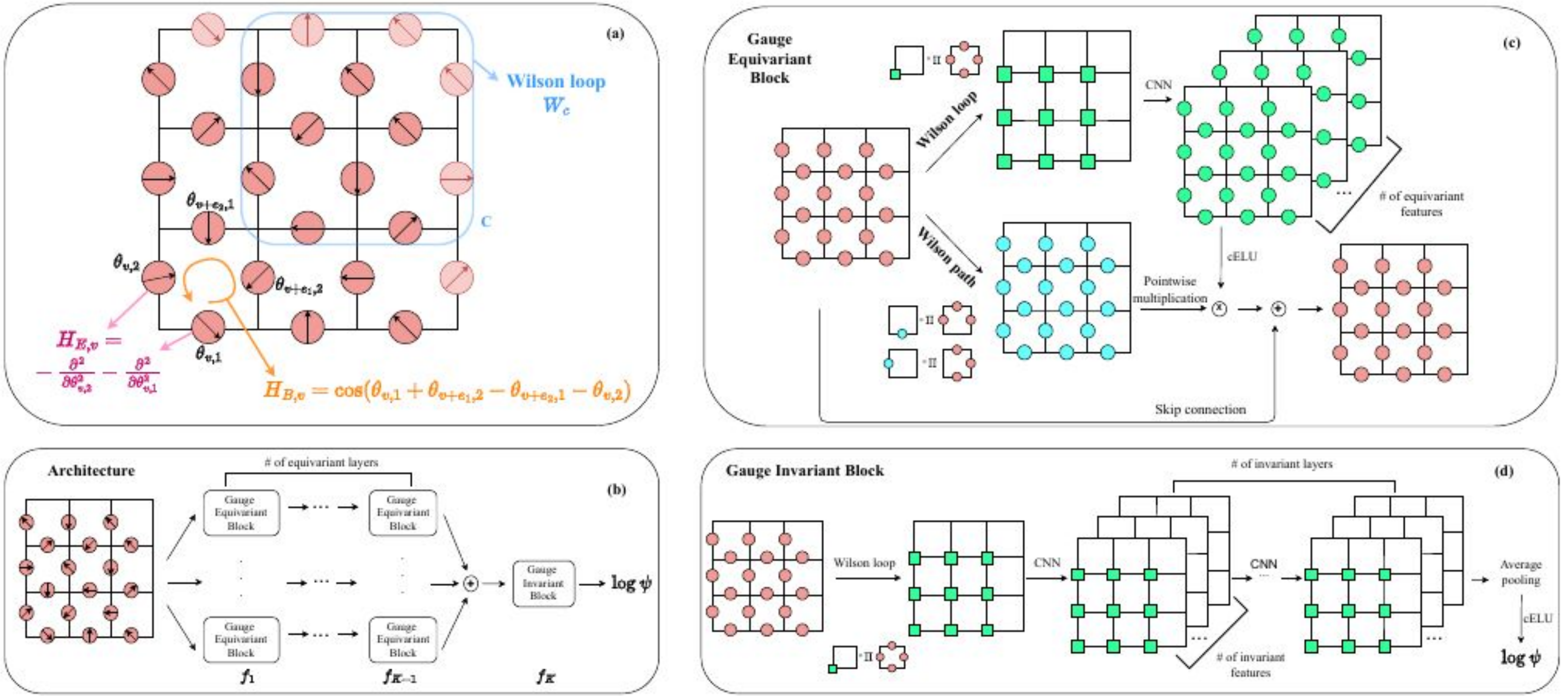
$$\Psi(\cdots,\theta_{v,\delta},\cdots)=\Psi(\cdots,\theta_{v,\delta}+\alpha_{v+e_\delta}-\alpha_v,\cdots)$$







Gauge Equivariant Neural Quantum States: 2+1D U(1) Theory



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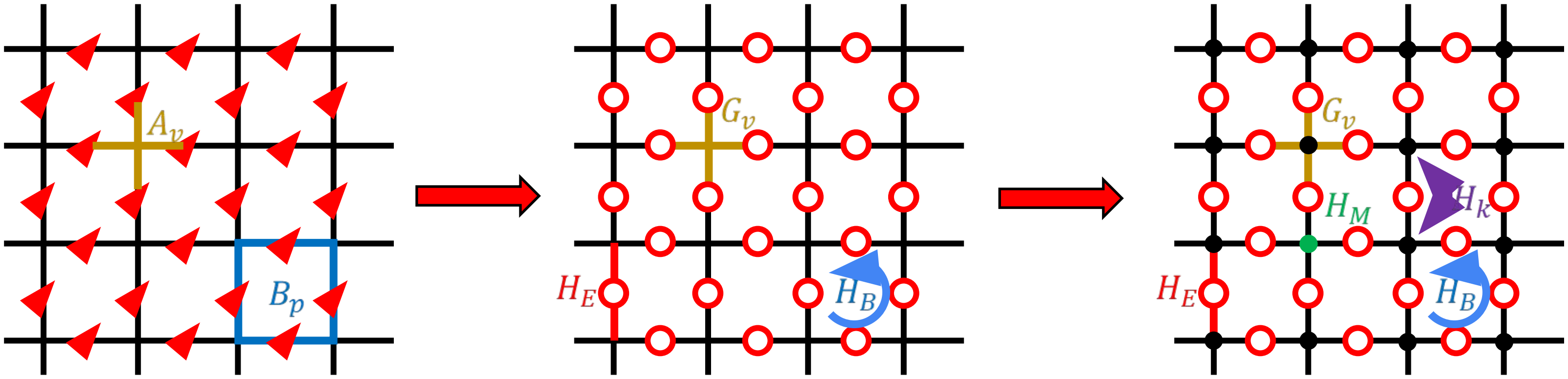


$\mathbb{Z}_2$ gauge theory
A_v: Gauss's law

Continuous gauge theory
Infinite degree of freedom

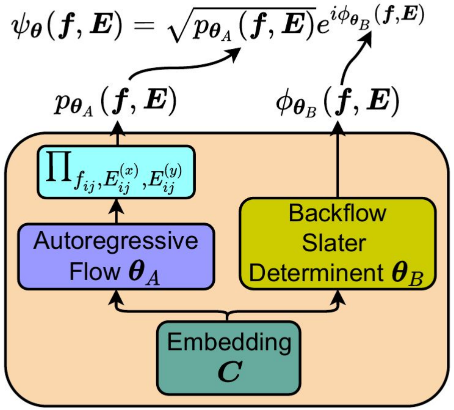
Gauge field fermion interaction
Fermionic sign problem

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

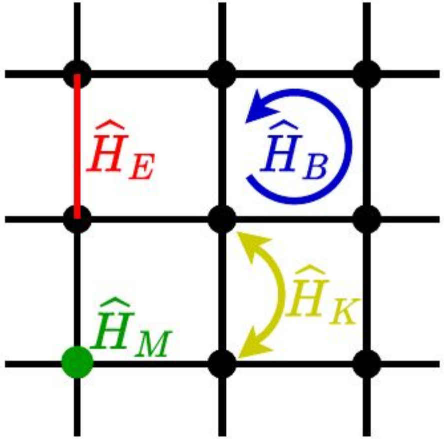
Simulating 2+1D Lattice Quantum Electrodynamics at Finite Density with Neural Flow Wavefunctions

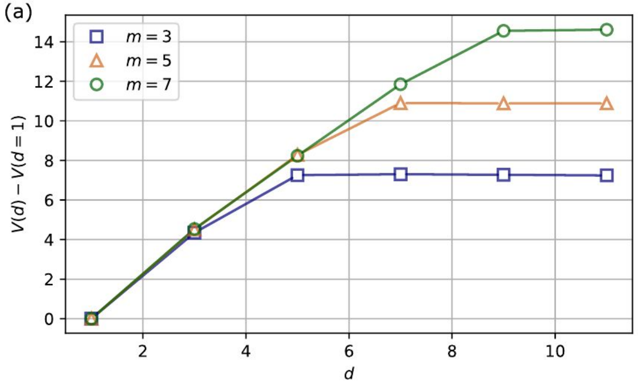
--- Develop Gauge-Fermion FlowNet, which represents U(1) gauge field without cutoff, obey Gauss's law, samples without auto-correlation time and variationally simulates model with sign problems.

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



Gauge-Fermion FlowNet





Simulate 2+1D QED at Finite Density

PHYSICAL REVIEW X **10**, 041040 (2020)

Two-Dimensional Quantum-Link Lattice Quantum Electrodynamics at Finite Density

Timo Felser,[1,2,3] Pietro Silvi,[4,5] Mario Collura,[1,2,6] and Simone Montangero[2,3]

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[2]*Dipartimento di Fisica e Astronomia "G. Galilei," Università di Padova, I-35131 Padova, Italy*
[3]*Istituto Nazionale di Fisica Nucleare (INFN), Sezione di Padova, I-35131 Padova, Italy*
[4]*Center for Quantum Physics, and Institute for Experimental Physics, University of Innsbruck, A-6020 Innsbruck, Austria*
[5]*Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, A-6020 Innsbruck, Austria*
[6]*SISSA-International School for Advanced Studies, I-34136 Trieste, Italy*

(Received 13 January 2020; revised 13 July 2020; accepted 21 September 2020; published 25 November 2020)

We present an unconstrained tree-tensor-network approach to the study of lattice gauge theories in two spatial dimensions, showing how to perform numerical simulations of theories in the presence of fermionic matter and four-body magnetic terms, at zero and finite density, with periodic and open boundary conditions. We exploit the quantum-link representation of the gauge fields and demonstrate that a fermionic rishon representation of the quantum links allows us to efficiently handle the fermionic matter while finite densities are naturally enclosed in the tensor network description. We explicitly perform calculations for quantum electrodynamics in the spin-one quantum-link representation on lattice sizes of up to 16×16 sites, detecting and characterizing different quantum regimes. In particular, at finite density, we detect signatures of a phase separation as a function of the bare mass values at different filling densities. The presented approach can be extended straightforwardly to three spatial dimensions.

DOI: 10.1103/PhysRevX.10.041040 Subject Areas: Computational Physics, Particles and Fields, Quantum Physics

- Tensor network study on 2+1D quantum link model with spin 1 representation of gauge field

Simulate 2+1D QED at Finite Density

PHYSICAL REVIEW X **9**, 021022 (2019)

Monte Carlo Study of Lattice Compact Quantum Electrodynamics with Fermionic Matter: The Parent State of Quantum Phases

Xiao Yan Xu,[1,*] Yang Qi,[2–4,†] Long Zhang,[5] Fakher F. Assaad,[6] Cenke Xu,[7] and Zi Yang Meng[8,9,10,11,‡]

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[11]*Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China*

(Received 1 August 2018; revised manuscript received 19 March 2019; published 2 May 2019)

The interplay between lattice gauge theories and fermionic matter accounts for fundamental physical phenomena ranging from the deconfinement of quarks in particle physics to quantum spin liquid with fractionalized anyons and emergent gauge structures in condensed matter physics. However, except for certain limits (for instance, a large number of flavors of matter fields), analytical methods can provide few concrete results. Here we show that the problem of compact U(1) lattice gauge theory coupled to fermionic matter in $(2+1)$D is possible to access via sign-problem-free quantum Monte Carlo simulations. One can hence map out the phase diagram as a function of fermion flavors and the strength of gauge fluctuations. By increasing the coupling constant of the gauge field, gauge confinement in the form of various spontaneous-symmetry-breaking phases such as the valence-bond solid (VBS) and Néel antiferromagnet emerge. Deconfined phases with algebraic spin and VBS correlation functions are also observed. Such deconfined phases are incarnations of exotic states of matter, i.e., the algebraic spin liquid, which is generally viewed as the parent state of various quantum phases. The phase transitions between the deconfined and confined phases, as well as that between the different confined phases provide various manifestations of deconfined quantum criticality. In particular, for four flavors $N_f = 4$, our data suggest a continuous quantum phase transition between the VBS and Néel order. We also provide preliminary theoretical analysis for these quantum phase transitions.

- Monte Carlo study with even species of fermions without sign problem

Simulate 2+1D QED at Finite Density

PRX QUANTUM **2**, 030334 (2021)

Editors' Suggestion

Simulating 2D Effects in Lattice Gauge Theories on a Quantum Computer

Danny Paulson,[1,2,†] Luca Dellantonio,[1,2,†] Jan F. Haase,[1,2,3,†] Alessio Celi,[4,5,6] Angus Kan,[1,2] Andrew Jena,[1,7] Christian Kokail,[5,6] Rick van Bijnen,[5,6] Karl Jansen,[8] Peter Zoller,[5,6] and Christine A. Muschik[1,2,9,*]

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[7] *Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*
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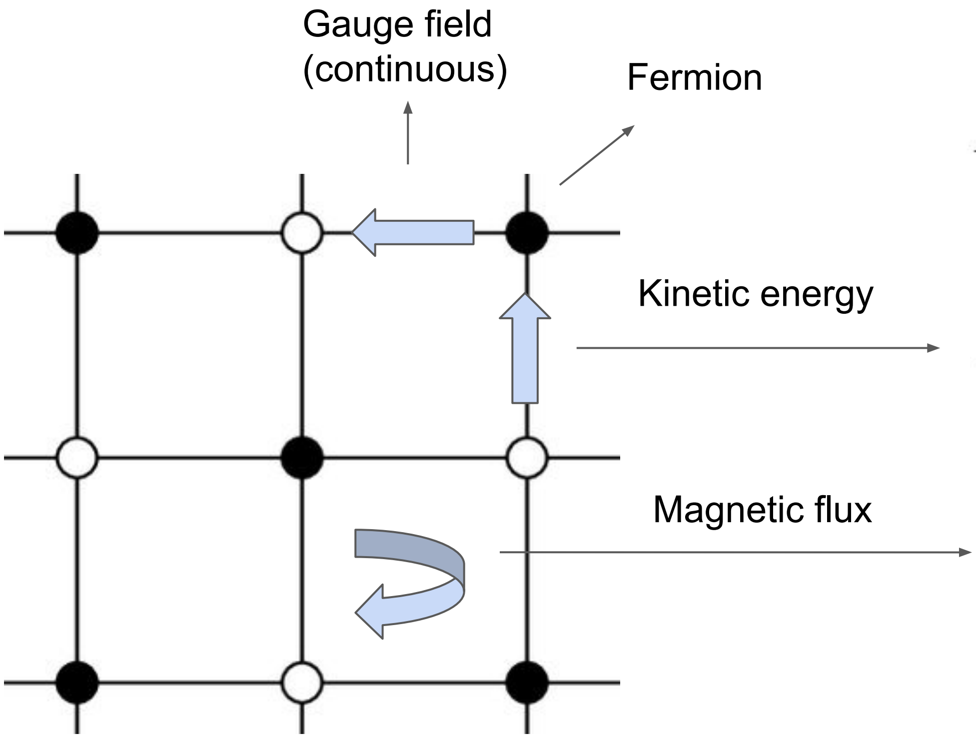
Quantum computing is in its greatest upswing, with so-called noisy-intermediate-scale-quantum devices heralding the computational power to be expected in the near future. While the field is progressing toward quantum advantage, quantum computers already have the potential to tackle classically intractable problems. Here, we consider gauge theories describing fundamental-particle interactions. On the way to their full-fledged quantum simulations, the challenge of limited resources on near-term quantum devices has to be overcome. We propose an experimental quantum simulation scheme to study ground-state properties in two-dimensional quantum electrodynamics (2D QED) using existing quantum technology. Our protocols can be adapted to larger lattices and offer the perspective to connect the lattice simulation to low-energy observable quantities, e.g., the hadron spectrum, in the continuum theory. By including both dynamical matter and a nonminimal gauge-field truncation, we provide the novel opportunity to observe 2D effects on present-day quantum hardware. More specifically, we present two variational-quantum-eigensolver- (VQE) based protocols for the study of magnetic field effects and for taking an important first step toward computing the running coupling of QED. For both instances, we include variational quantum circuits for qubit-based hardware. We simulate the proposed VQE experiments classically to calculate the required measurement budget under realistic conditions. While this feasibility analysis is done for trapped ions, our approach can be directly adapted to other platforms. The techniques presented here, combined with advancements in quantum hardware, pave the way for reaching beyond the capabilities of classical simulations.

- Proposal on simulating 2+1D QED on quantum computer with gauge field cutoff
- Interesting phenomena on 1 plaquette

2+1D QED with Finite Density Dynamical Fermions



$$\hat{H} = \hat{H}_E + \hat{H}_B + \hat{H}_M + \hat{H}_K$$

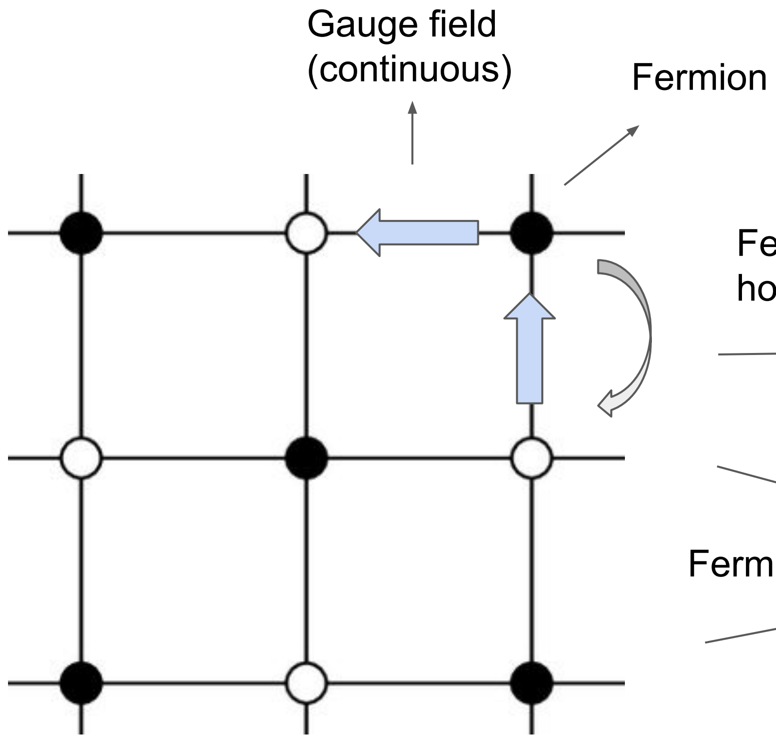
$$\hat{H}_E = \frac{g_E^2}{2} \sum_{i,j} \left[\left(\hat{E}_{i,j}^{(x)} \right)^2 + \left(\hat{E}_{i,j}^{(y)} \right)^2 \right]$$

$$\hat{H}_B = -\frac{g_B^2}{2} \sum_{i,j} \left(\hat{P}_{i,j} + \hat{P}_{i,j}^{\dagger} \right)$$

$$\hat{P}_{i,j} = \hat{U}_{i,j}^{(x)} \hat{U}_{i+1,j}^{(y)} \left(\hat{U}_{i,j+1}^{(x)} \right)^{\dagger} \left(\hat{U}_{i,j}^{(y)} \right)^{\dagger}.$$

$$[\hat{E}_{i,j}^{(w)}, \hat{U}_{i',j'}^{(w')}] = -\delta_{i,i'} \delta_{j,j'} \delta_{w,w'} \hat{U}_{i',j'}^{(w')}$$

2+1D QED with Finite Density Dynamical Fermions



$$\hat{H} = \hat{H}_E + \hat{H}_B + \hat{H}_M + \hat{H}_K$$

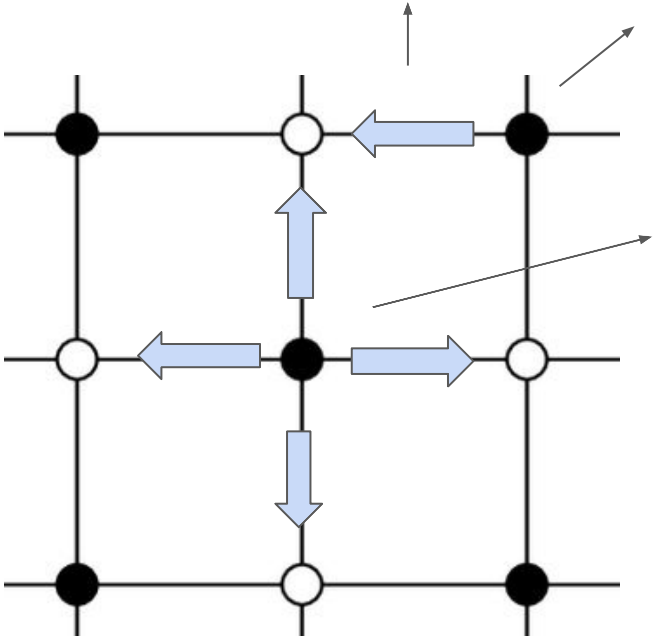
Fermion hopping

$$\hat{H}_K = -\kappa \sum_{i,j} \Big[\hat{\psi}^\dagger_{i,j} \left(\hat{U}^{(x)}_{i,j}\right)^\dagger \hat{\psi}_{i+1,j} + \hat{\psi}^\dagger_{i,j} \left(\hat{U}^{(y)}_{i,j}\right)^\dagger \hat{\psi}_{i,j+1} + \text{H.C.} \Big]$$

Fermion mass

$$\hat{H}_M = m \sum_{i,j} \left\{ \frac{1}{2}\left[(-1)^{i+j} + 1\right] \hat{\psi}^\dagger_{i,j} \hat{\psi}_{i,j} - \frac{1}{2}\left[(-1)^{i+j} - 1\right] \hat{\psi}_{i,j} \hat{\psi}^\dagger_{i,j} \right\},$$

2+1D QED with Finite Density Dynamical Fermions



$$\hat{H} = \hat{H}_E + \hat{H}_B + \hat{H}_M + \hat{H}_K$$

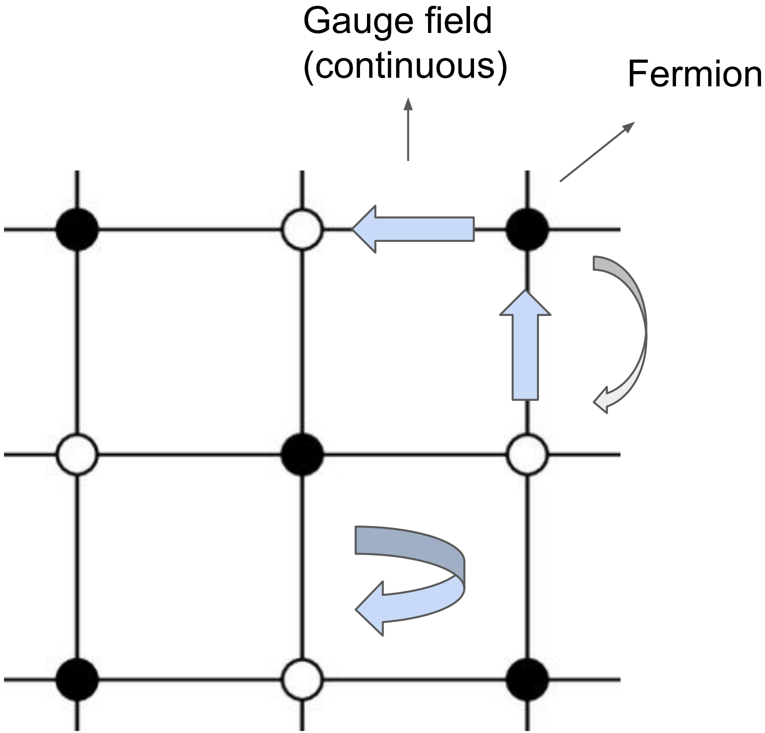
Gauss' law

$$\hat{E}^{(x)}_{i,j} + \hat{E}^{(y)}_{i,j} - \hat{E}^{(x)}_{i-1,j} - \hat{E}^{(y)}_{i,j-1} = \hat{q}_{i,j} \quad \forall (i,j)$$

$$\hat{q}_{i,j} = \hat{\psi}^{\dagger}_{i,j}\hat{\psi}_{i,j} + \frac{1}{2}\left[(-1)^{i+j} - 1\right]$$

Sign problem exist even for zero density

2+1D QED with Finite Density Dynamical Fermions



$$\hat{H} = \hat{H}_E + \hat{H}_B + \hat{H}_M + \hat{H}_K$$

$$\psi(f, E) = \psi_{density}(f, E)\psi_{backflow}(f, E)$$

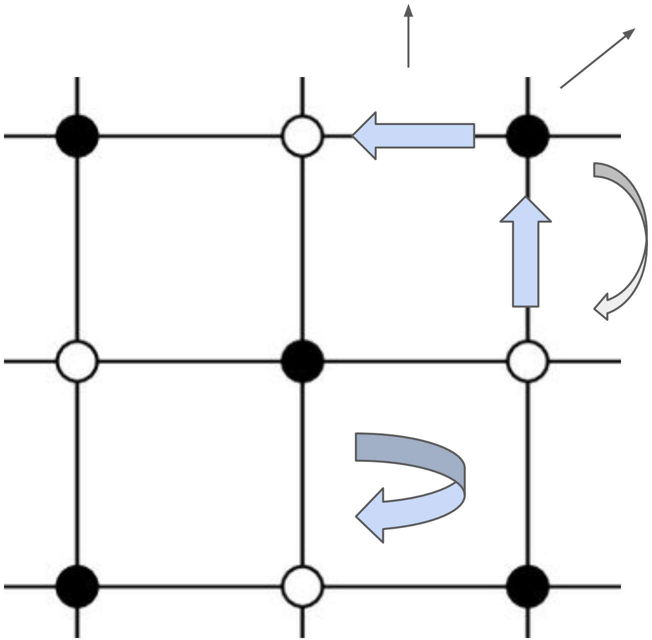
Gauge invariant network and Flow-based model

Neural network backflow

$$\begin{vmatrix} \chi^1_{\boldsymbol{\theta}_B}(i_1, j_1; \boldsymbol{C}) & \cdots & \chi^1_{\boldsymbol{\theta}_B}(i_{N_e}, j_{N_e}; \boldsymbol{C}) \\ \vdots & \ddots & \vdots \\ \chi^{N_e}_{\boldsymbol{\theta}_B}(i_1, j_1; \boldsymbol{C}) & \cdots & \chi^{N_e}_{\boldsymbol{\theta}_B}(i_{N_e}, j_{N_e}; \boldsymbol{C}) \end{vmatrix}$$

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

2+1D QED with Finite Density Dynamical Fermions



$$\hat{H} = \hat{H}_E + \hat{H}_B + \hat{H}_M + \hat{H}_K$$

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1. Neural network backflow:
   - fermionic anti-symmetry and sign problems

2. Gauge invariant autoregerssive network:
   - Sample without auto-correlation time
   - Enforce gauge symmetry with fermions

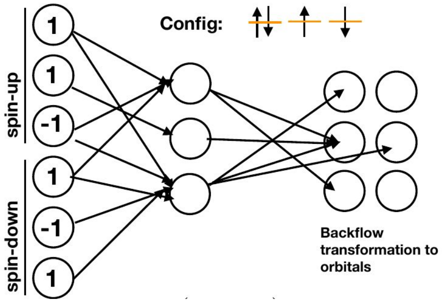
3. Discrete Flow-based model:
   - U(1) degree without cut-off

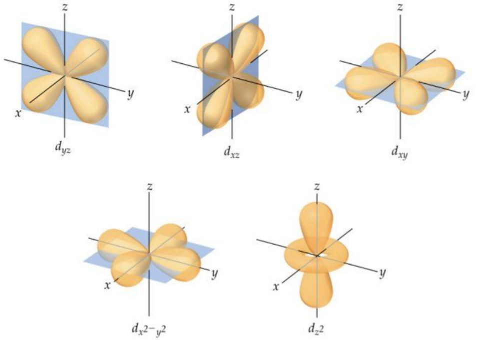
Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

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

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

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





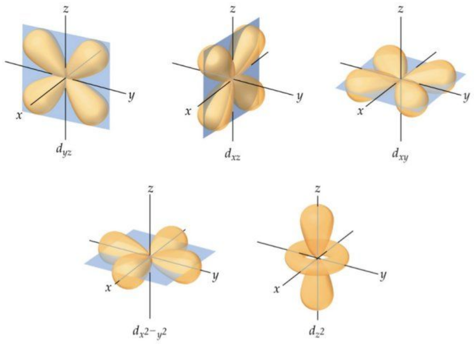
Di Luo, Bryan Clark, Phys. Rev. Lett. 122, 226401

Neural Network Backflow

Jastrow

+

Backflow
Slater Determinant



Pro: include correlation effect

Con: hard to figure out good configuration dependent orbitals

Backflow transformation

[Feynman], [Sorella]

Configuration dependent orbitals

General form of backflow?

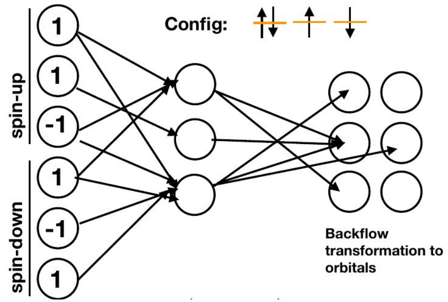
Mean field solution

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

?

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

Neural Network Backflow



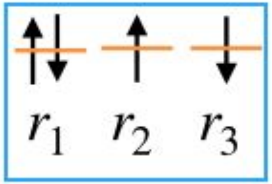
Neural network interacting orbitals

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 in arbitrary system
- Allow transformation to slater determinant and pairing functions



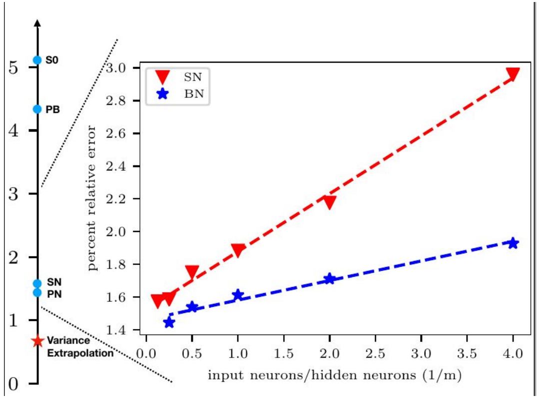
Input configuration ***r***

Determinant

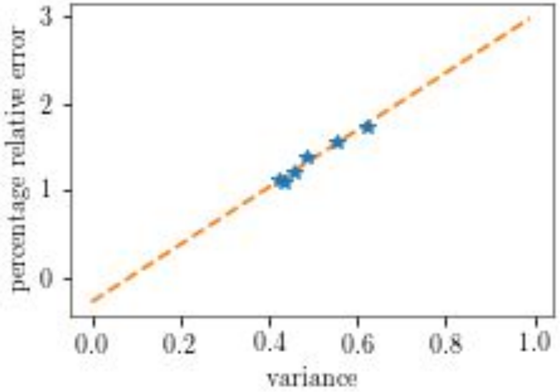
$$\Psi(\mathbf{r}) = det([\phi^b_{k\sigma}(r_{i,\sigma};\mathbf{r})])$$

Neural Network Backflow

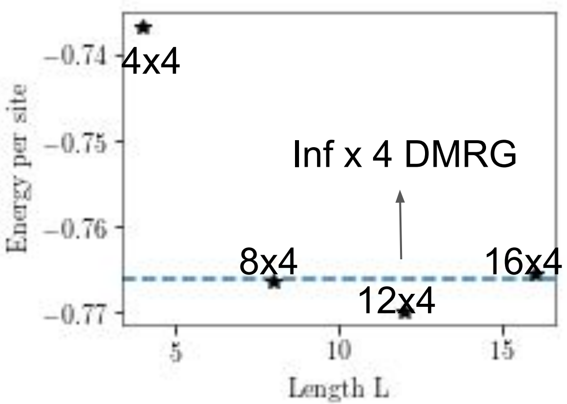
Generalization of backflow to arbitrary lattice systems with complicated sign structure.



4x4 Hubbard, U/t=8, n=0.875
Slater Det+NNB
BDG Pairing+NNB



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
- Further advancement in quantum chemistry (FermiNet, PauliNet) and nuclear physics

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

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

Neural Network Backflow

Advancement in Fermionic Simulation:

This workshop:

Markus Holzmann, David Linteau, Carlo Barbieri,
James Keeble, Javier Rozalén, Jane Kim,
Amir Azzam, David Pfau, Bryce Fore, Elad Parnes,
Mehdi Drissi, Andrea Di Donna, Alessandro Lovato,
Arnau Rios Huguet, ….

Many-body quantum physics with machine learning

Machine learning many-electron wave functions via backflow transformations

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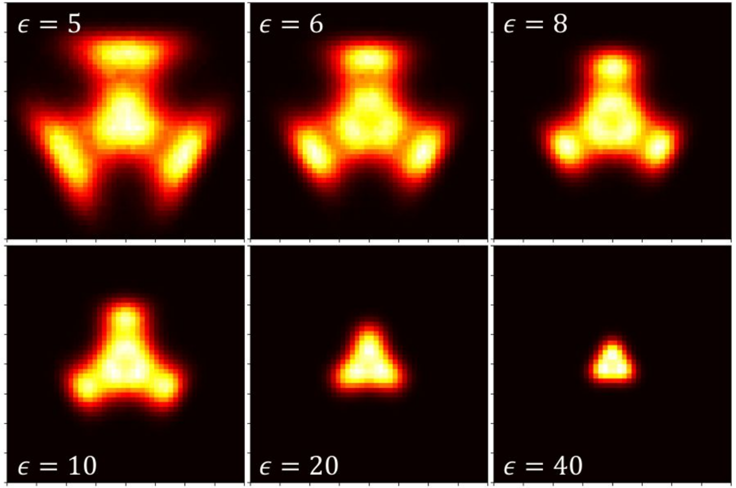
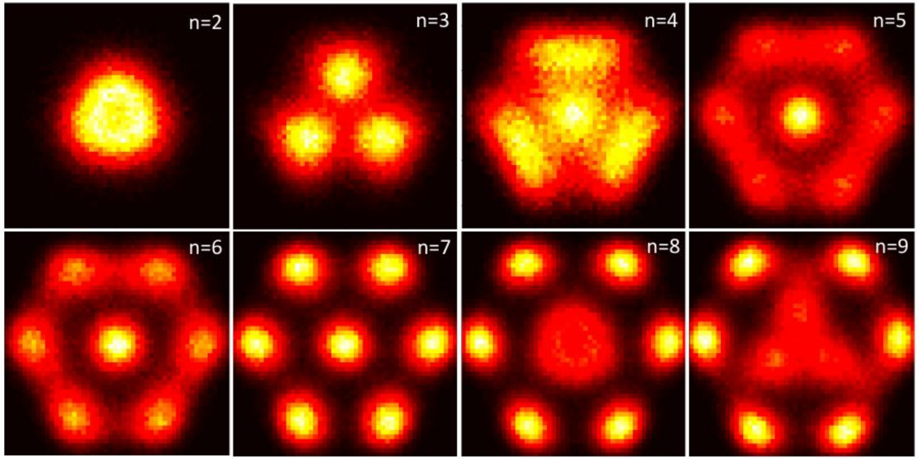
Neural Network Backflow

Artificial intelligence for artificial materials: moiré atom



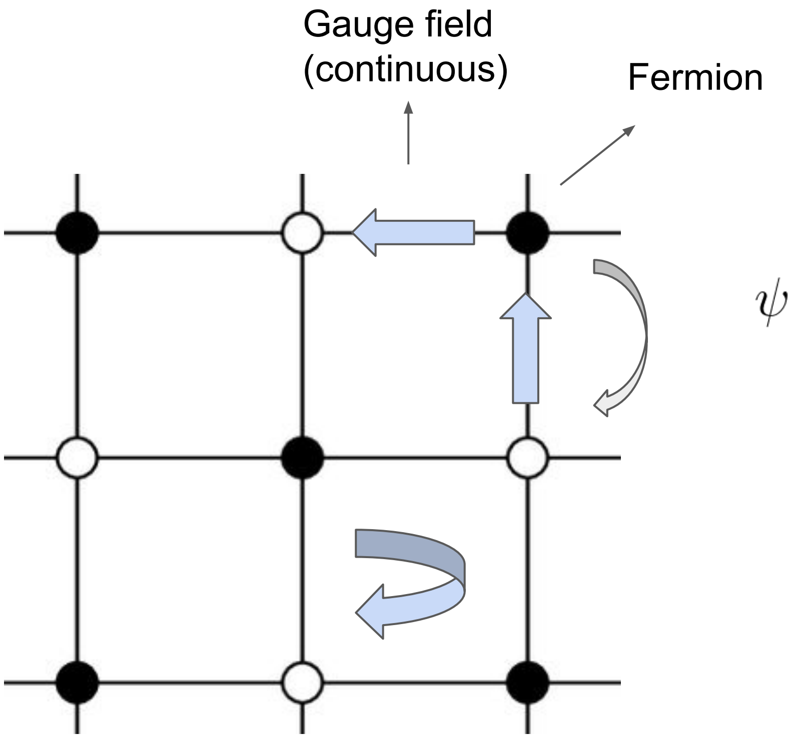
From Schrödinger atom to Wigner molecule



Effect of crystal field on charge distribution

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

2+1D QED with Finite Density Dynamical Fermions



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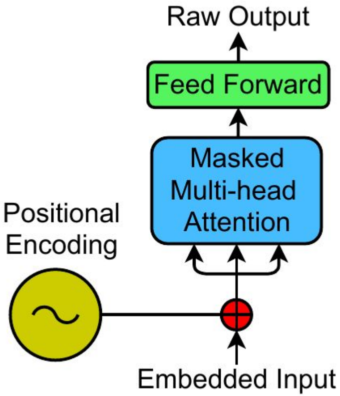
   - U(1) degree without cut-off

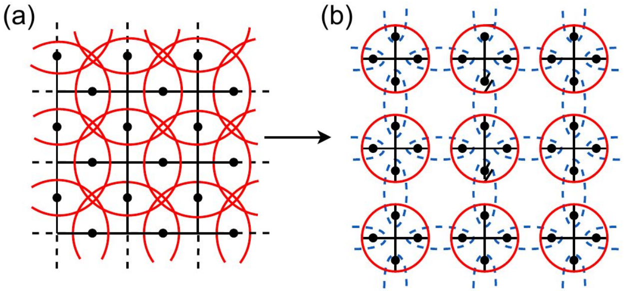
Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network for Quantum Lattice Models

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

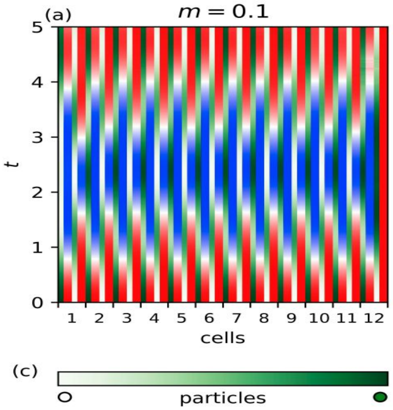
$$f(x_1, x_2, ..., x_n) = \prod_i^n f(x_i | x_{i<})$$



Transformer Autoregressive Wave function



Symmetry via Composite Particles



Di Luo†, Zhuo Chen†, Kaiwen Hu, Zhizhen Zhao, Vera Hu, Bryan Clark. Phys. Rev. Research 5, 013216

Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network

Autoregressive neural network with gauge symmetry or Anyonic symmetry

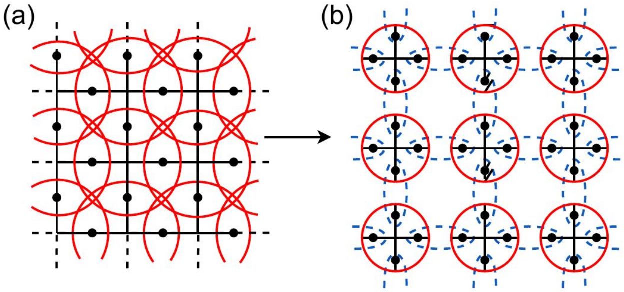
$$f(x_1, x_2, ..., x_n) = \prod_{i}^{n} f(x_i | x_{i<})$$

- Exact sampling, which is more efficient than Markov Chain Monte Carlo
- It could be constructed to obey gauge symmetries or other algebraic constraint

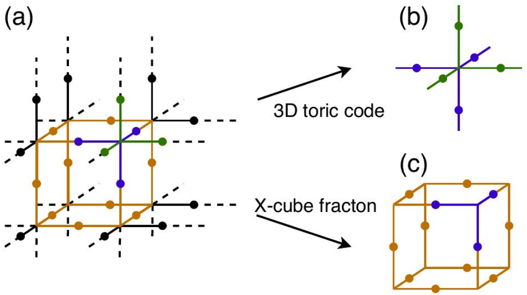
Di Luo†, Zhuo Chen†, Kaiwen Hu, Zhizhen Zhao, Vera Hu, Bryan Clark. Phys. Rev. Research 5, 013216

Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network

Applications to 2D, 3D Toric code and X-cube Fracton model



2D toric code

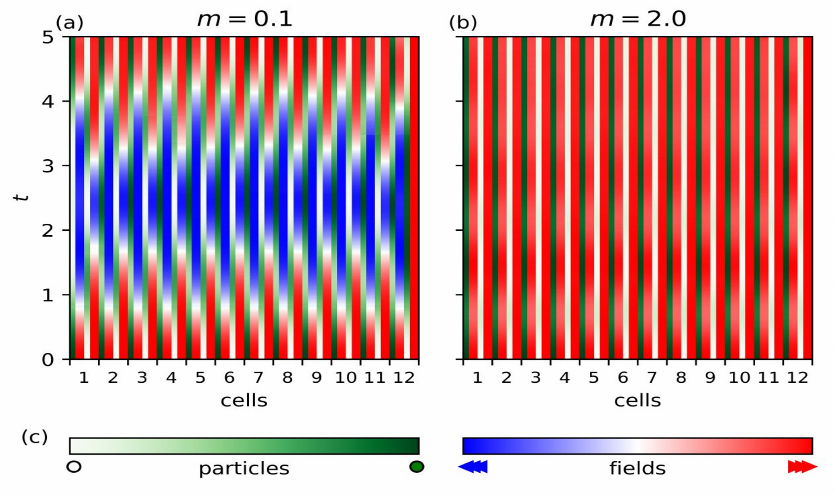


Exact representation of grounds states and excited states for:

- 2D Toric code
- 3D Toric code
- X-cube Fracton

Di Luo†, Zhuo Chen†, Kaiwen Hu, Zhizhen Zhao, Vera Hu, Bryan Clark. Phys. Rev. Research 5, 013216

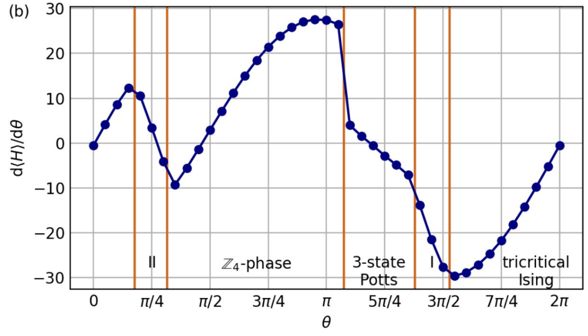
Gauge Invariant and Anyonic Symmetric Autoregressive Neural Network



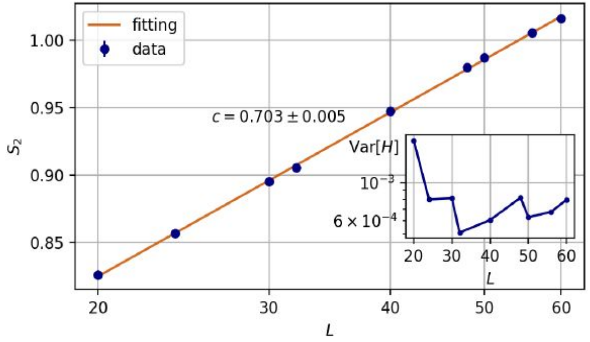
String inversion of real-time dynamics in 1+1D Quantum Link Model

$SU(2)_3$ Fibonacci anyons

$$\tau \otimes \tau = \tau \oplus \mathbb{1},\ \tau \otimes \mathbb{1} = \mathbb{1} \otimes \tau = \tau.$$



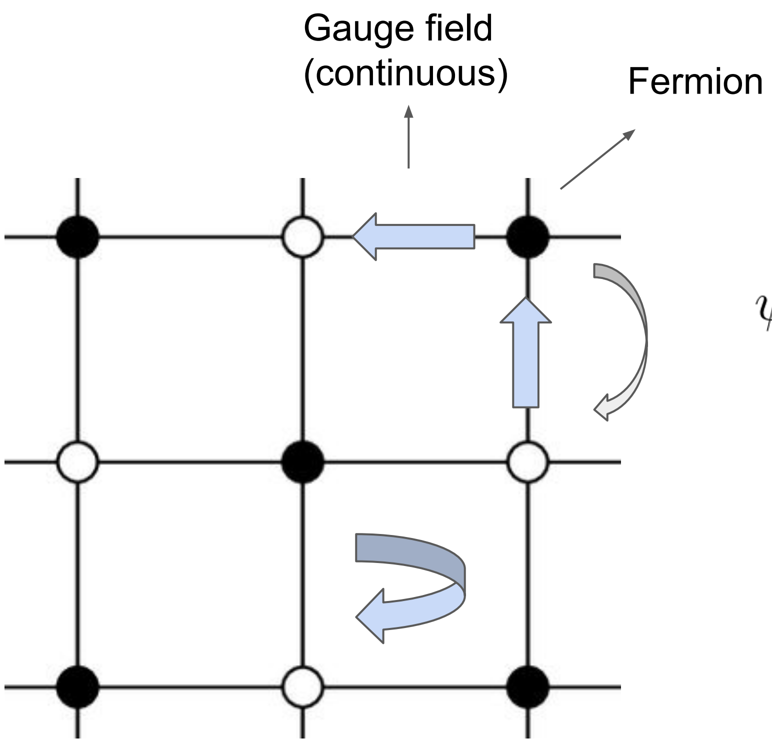
Phase diagram



Central charge

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

2+1D QED with Finite Density Dynamical Fermions



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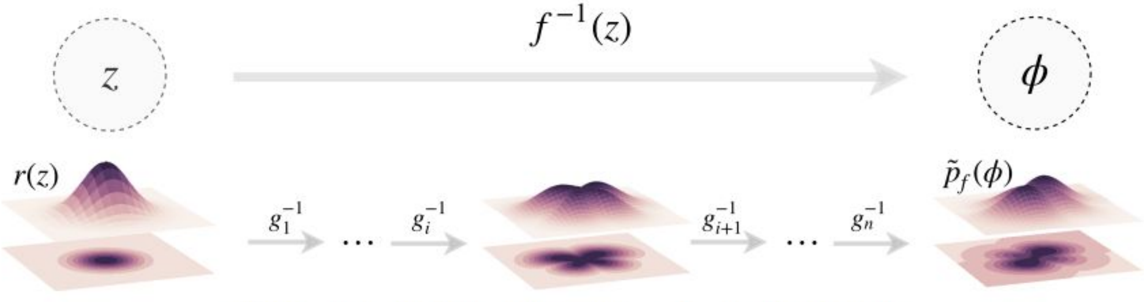
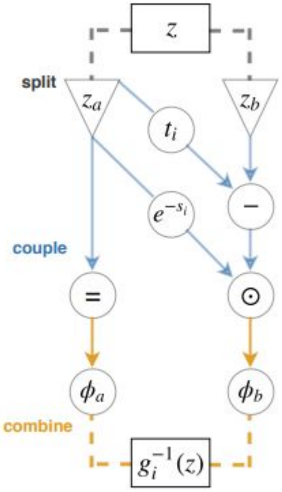
Flow-based Model

Continuous Flow



(a) Normalizing flow between prior and output distributions

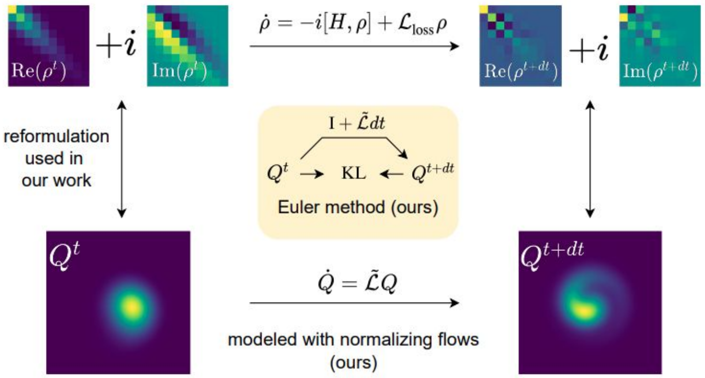


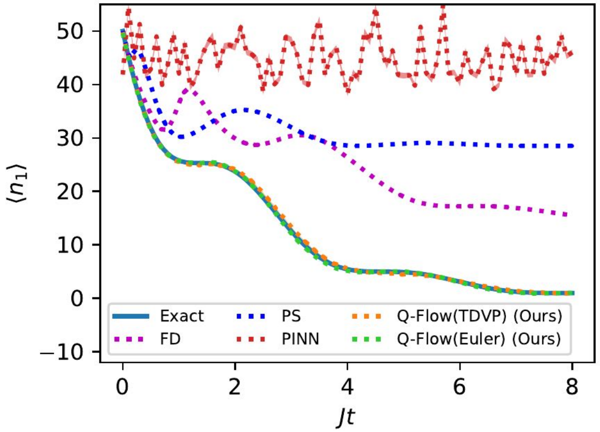
- M. S. Albergo, G. Kanwar, P. E. Shanahan, PRD 100 (3), 034515
- G Kanwar, etc, P.E. Shanahan, PRL 125 (12), 121601

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

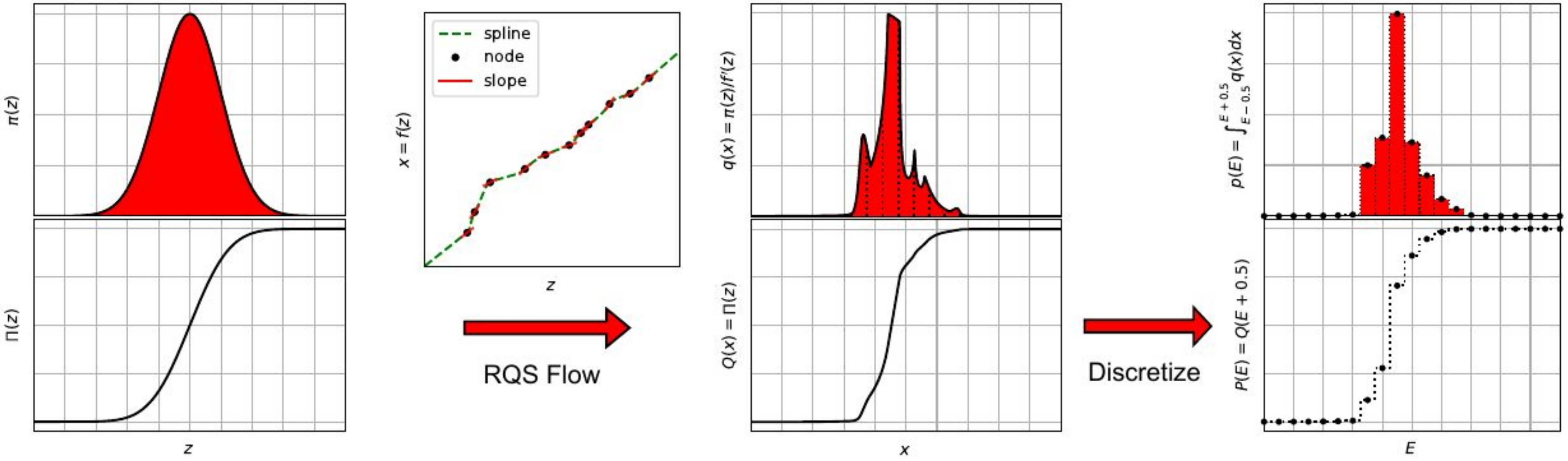




Zhuo Chen†, Di Luo†, Kaiwen Hu, Bryan Clark. arxiv. 2212.06835

Discretized Flow-based Model

Discretized Flow: represent U(1) degree freedom in *E* basis without cutoff



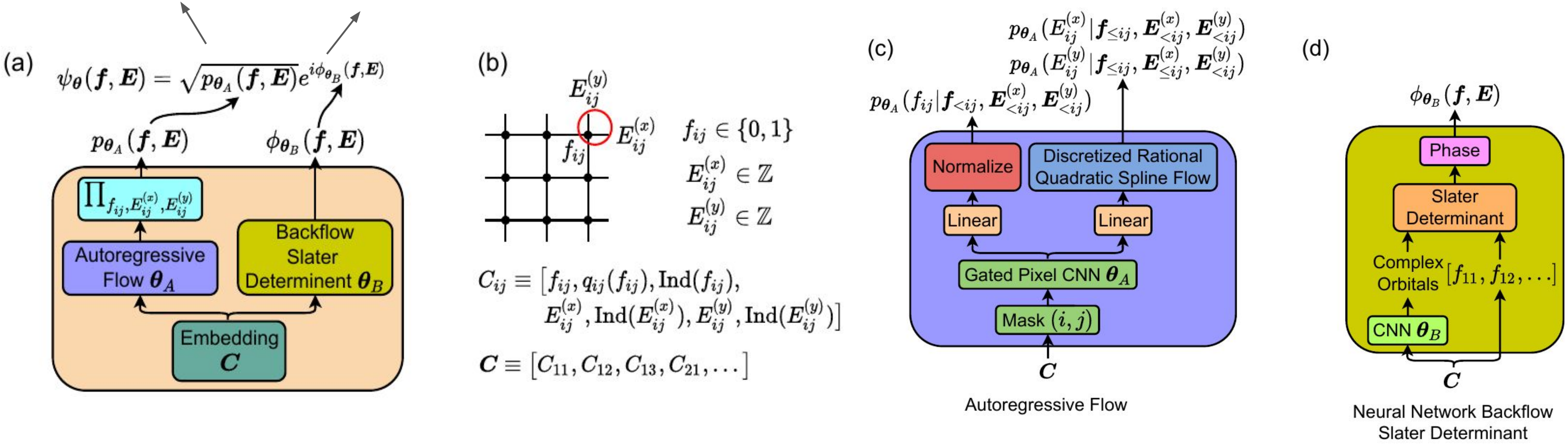
Prior | Rational quadratic spline flow | Discrete target distribution

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

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

Impose Gauss'law,
U(1) freedom without cutoff,
Exact sampling

Fermionic anti-symmetry



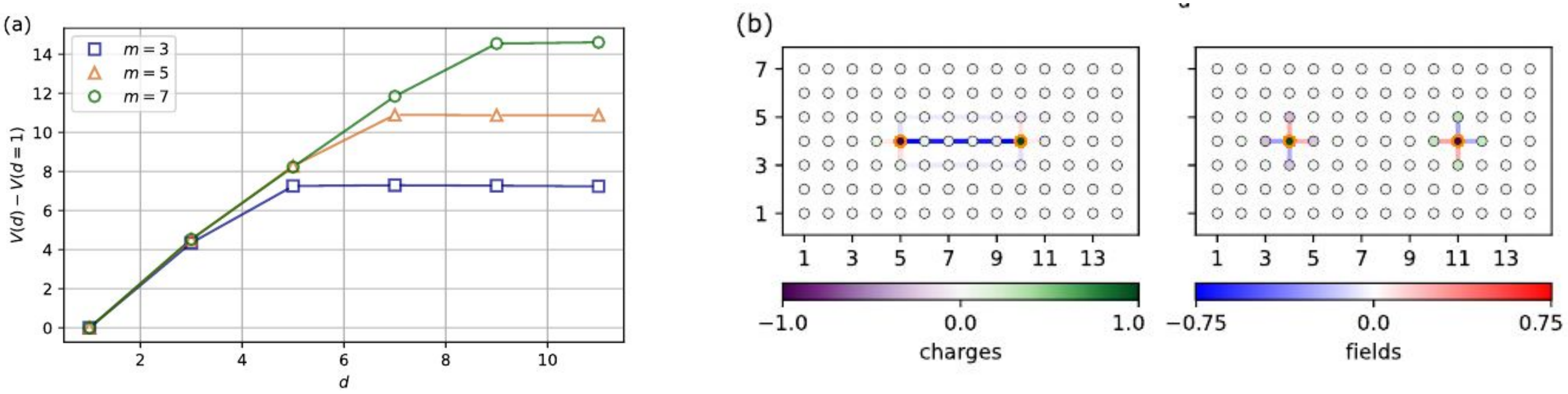
Gauge-Fermion FlowNet

2+1D QED at Finite Density: String Breaking

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Zero density regime: string breaking

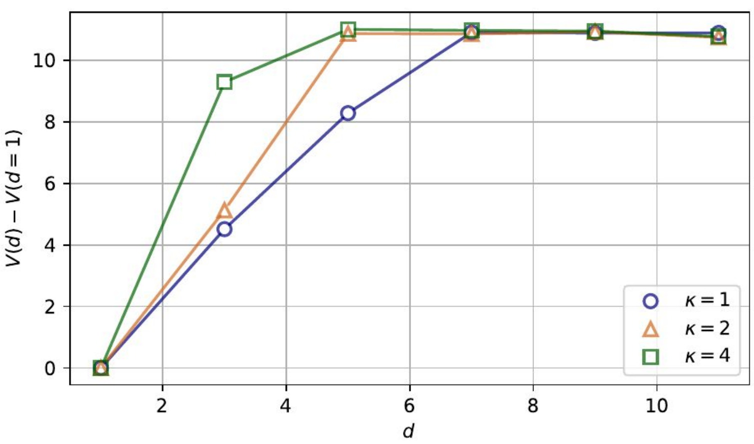
$$g_E^2 + 4m < g_E^2/2 \times L + 2m$$



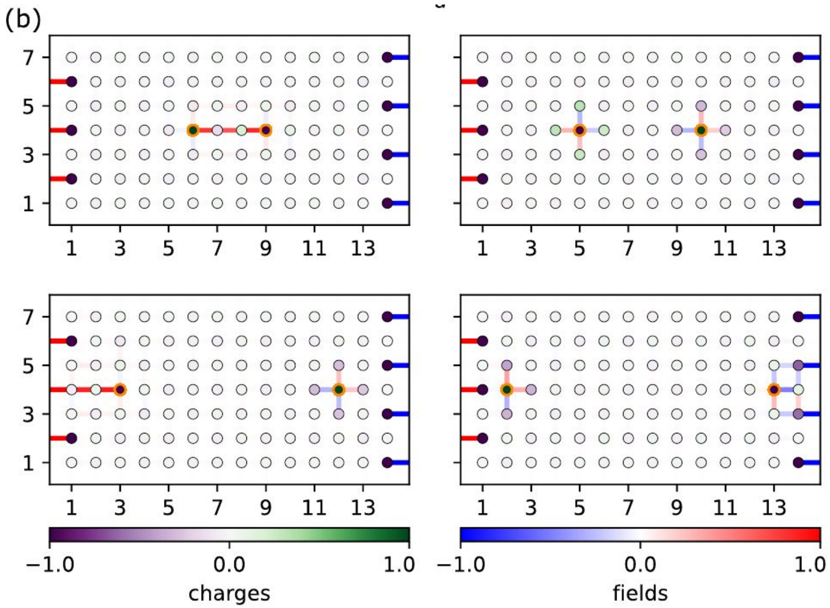
2+1D QED at Finite Density: String Breaking

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Zero density: hopping effect on string breaking



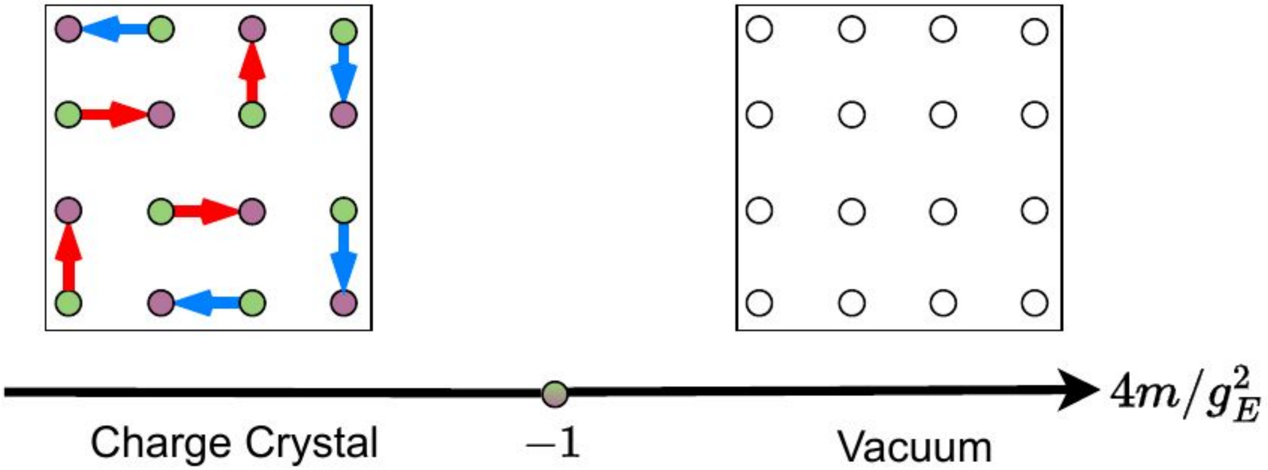
Finite density fixed doping: string breaking



2+1D QED at Finite Density: Charge Crystal to Vacuum Transition

$$H=\sum_k \frac{g_E^2}{2}E_k^2+\frac{2}{g_B^2}B_k^2-\kappa\psi_k^\dagger U_k\psi_{k+1}+m(-1)^k\psi_k^\dagger\psi_k$$

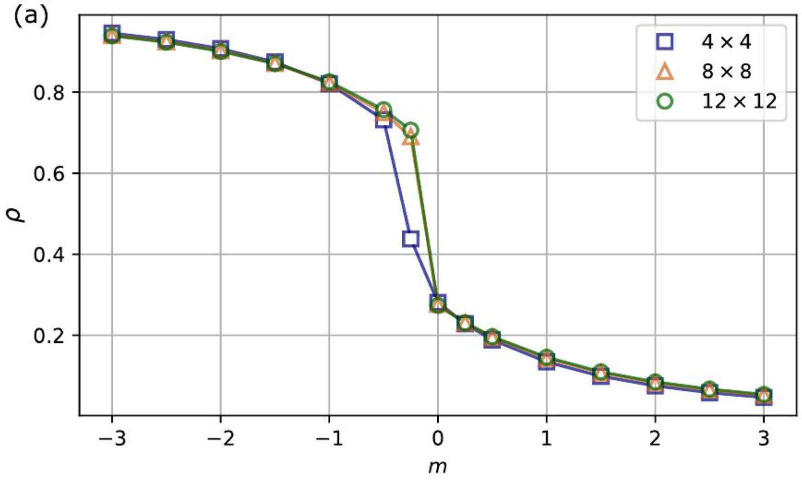
Classical picture: 1st order transition between charge crystal phase to vacuum phase

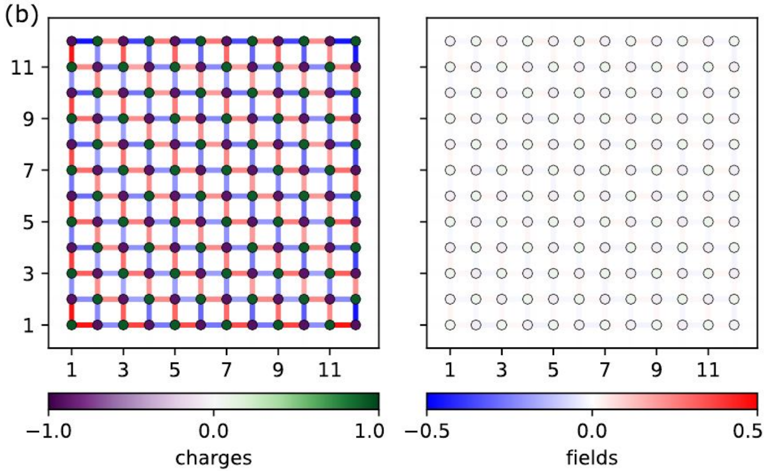


2+1D QED at Finite Density: Charge Crystal to Vacuum Transition

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Zero density: charge crystal to vacuum transition



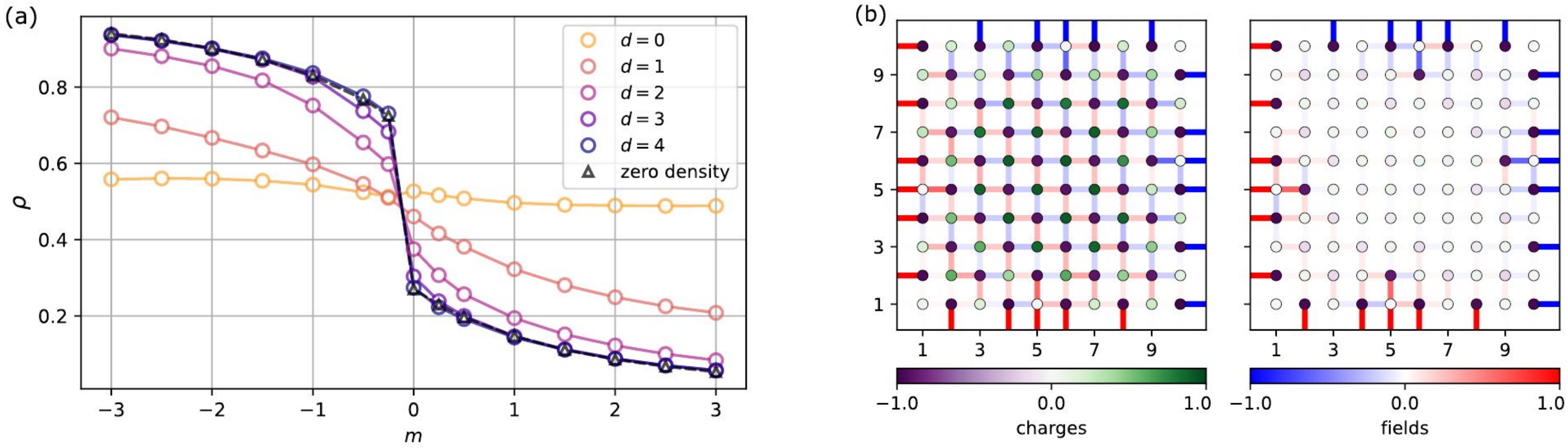


$$\rho \equiv 1/N \sum_n \left\{ \frac{1}{2}[(-1)^n + 1] \left\langle \hat{\psi}_n^\dagger \hat{\psi}_n \right\rangle - \frac{1}{2}[(-1)^n - 1] \left\langle \hat{\psi}_n \hat{\psi}_n^\dagger \right\rangle \right.$$

2+1D QED at Finite Density: Charge Crystal to Vacuum Transition

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Finite density fixed doping: phase separation and charge penetration blocking caused by magnetic interaction



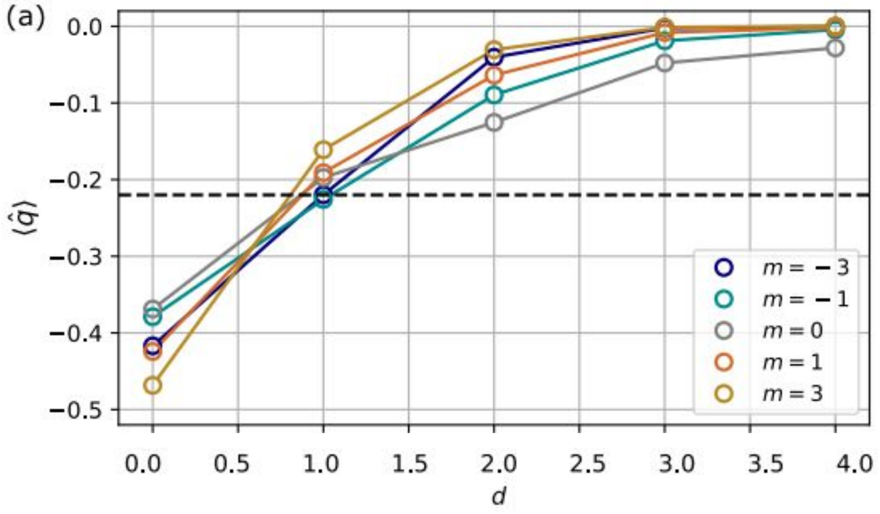
Bulk approaches zero density phase

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

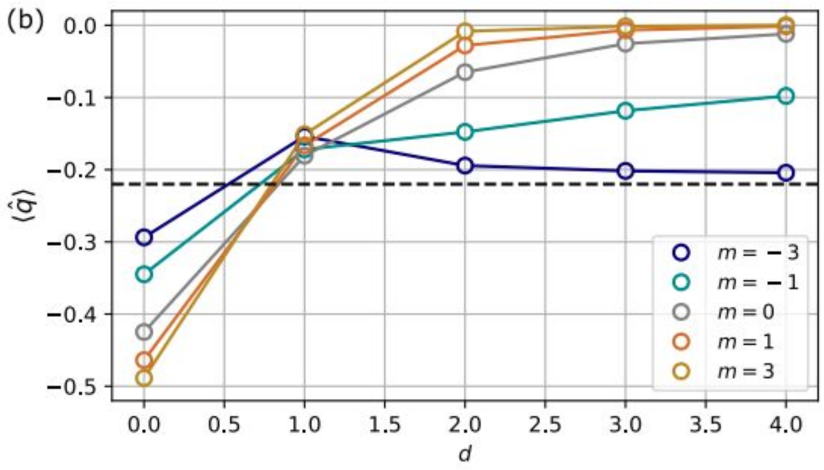
2+1D QED at Finite Density: Charge Crystal to Vacuum Transition

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Finite density fixed doping: phase separation and charge penetration blocking caused by magnetic interaction



Existence of magnetic interaction

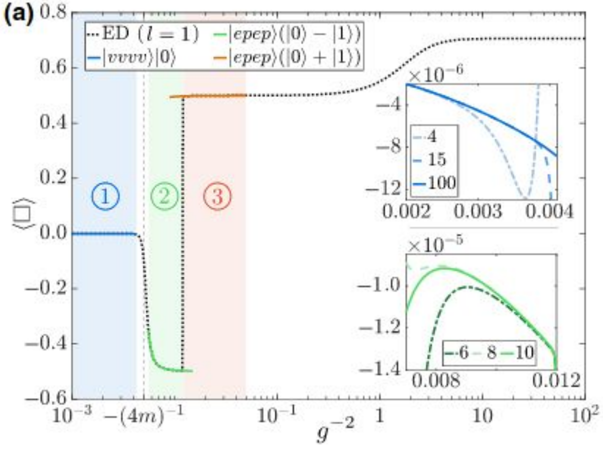


Absence of magnetic interaction
(also in tensor network simulation PhysRevX.10.041040)

2+1D QED at Finite Density: Magnetic Phase Transition

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Competition between kinetic energy and magnetic energy



One plaquette study
PRXQuantum.2.030334

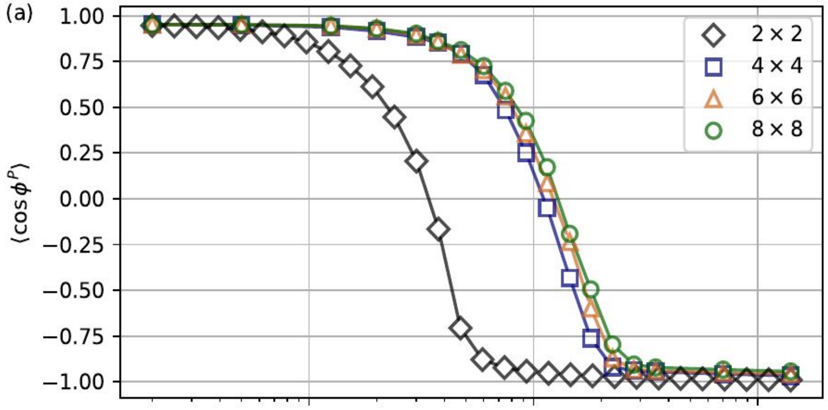
Questions:

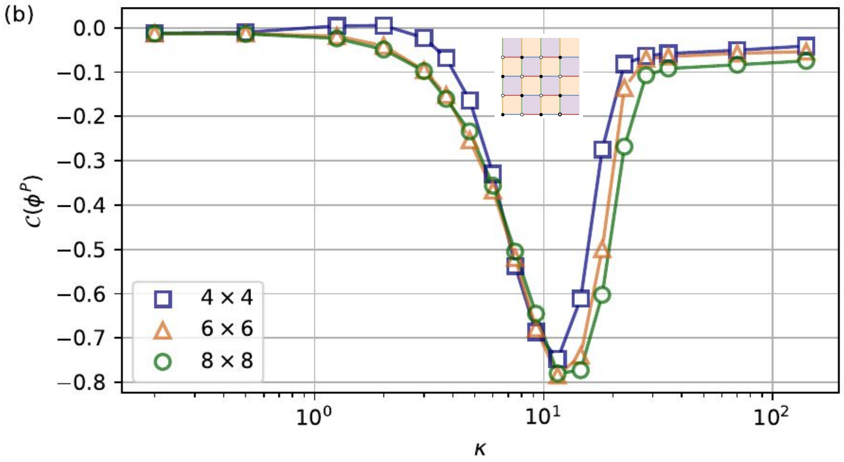
1. What is the large system size phenomena?
2. What are the nature of the phase transitions?

2+1D QED at Finite Density: Magnetic Phase Transition

$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Competition between kinetic energy and magnetic energy





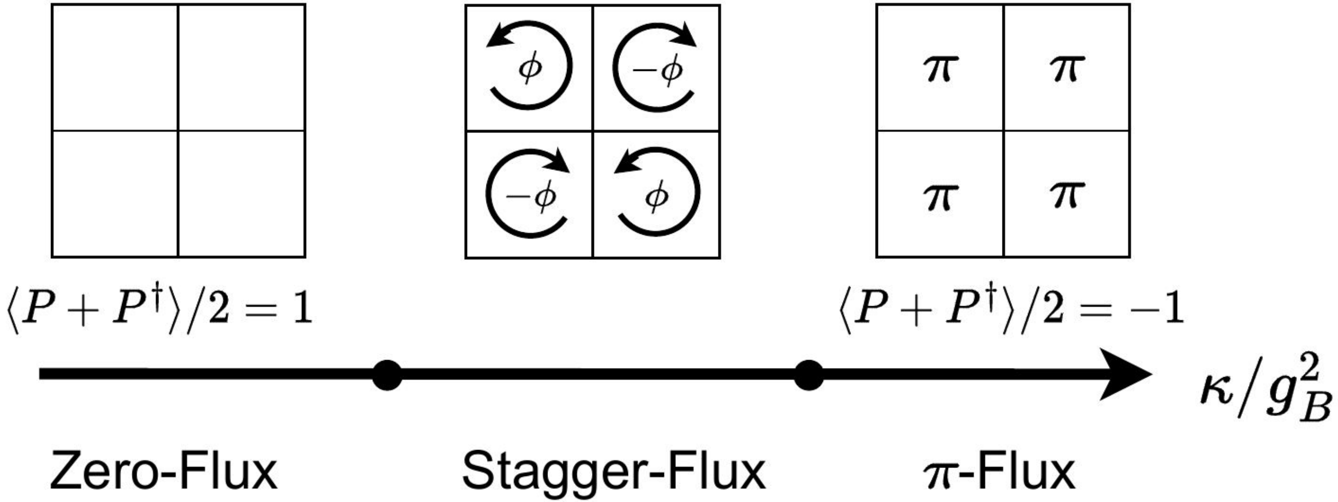
$$\langle \cos\phi^P \rangle \equiv \frac{1}{L^2} \sum_{i,j} \langle \cos\phi^P_{i,j} \rangle = \frac{1}{2L^2} \sum_{i,j} \langle \hat{P}_{i,j} + \hat{P}^\dagger_{i,j} \rangle$$

$$\mathcal{C}(\phi^P) \equiv \frac{1}{2L(L-1)} \sum_{\langle i_1,j_1;i_2,j_2 \rangle} \langle \sin\phi^P_{i_1,j_1} \sin\phi^P_{i_2,j_2} \rangle$$

2+1D QED at Finite Density: Magnetic Phase Transition

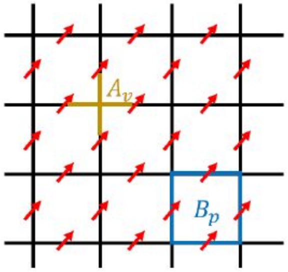
$$H = \sum_k \frac{g_E^2}{2} E_k^2 + \frac{2}{g_B^2} B_k^2 - \kappa \psi_k^\dagger U_k \psi_{k+1} + m(-1)^k \psi_k^\dagger \psi_k$$

Competition between kinetic energy and magnetic energy: spontaneous symmetry breaking of time-reversal symmetry



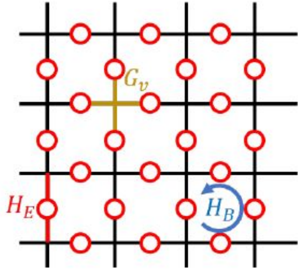
Towards General Quantum Field Theories

$\mathbb{Z}_2$ toric code model



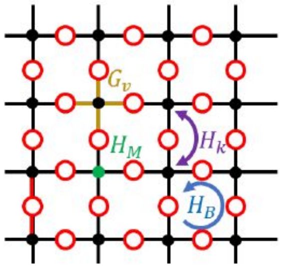
$\mathbb{Z}_2$ gauge theory
A_v: Gauss's law

U(1) pure gauge theory

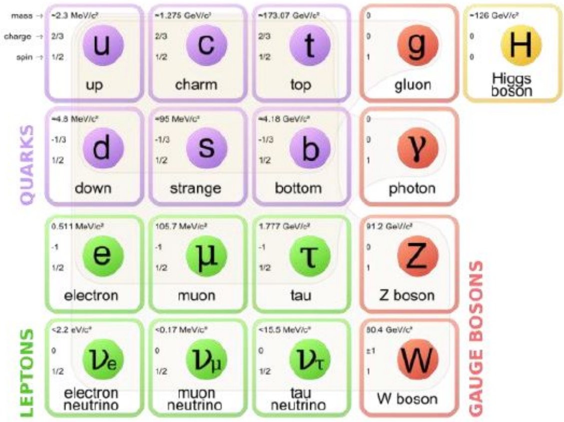


Continuous gauge theory
Infinite degree of freedom

U(1) gauge theory with fermions



Gauge field fermion interaction
Fermionic sign problem



Neural Quantum Field States for Continuum QFT

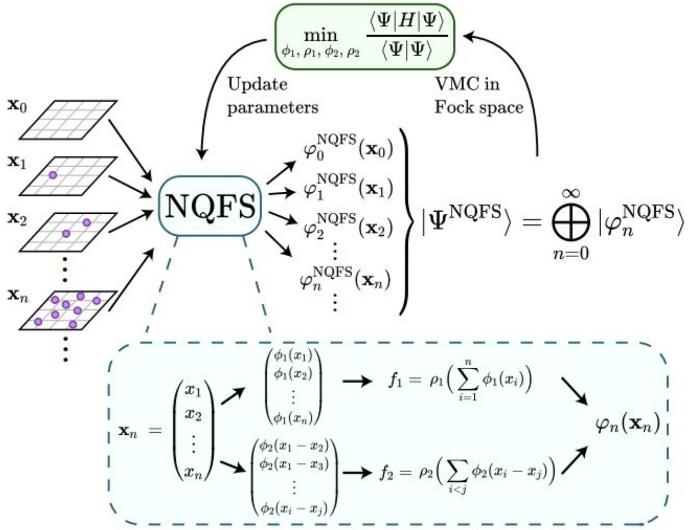
Q: How to simulate continuum quantum field theories?

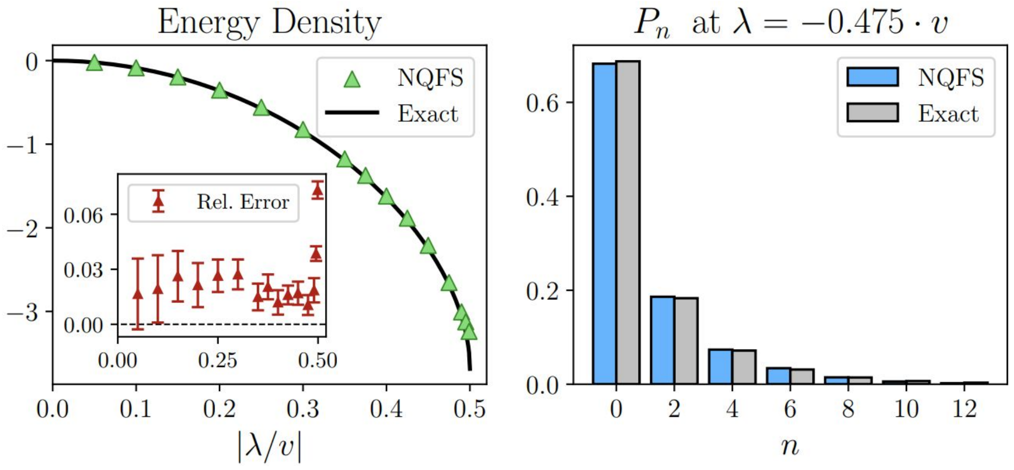
A: Neural quantum field states

John M. Martyn, Khadijeh Najafi, Di Luo. Phys. Rev. Lett. 131, 081601

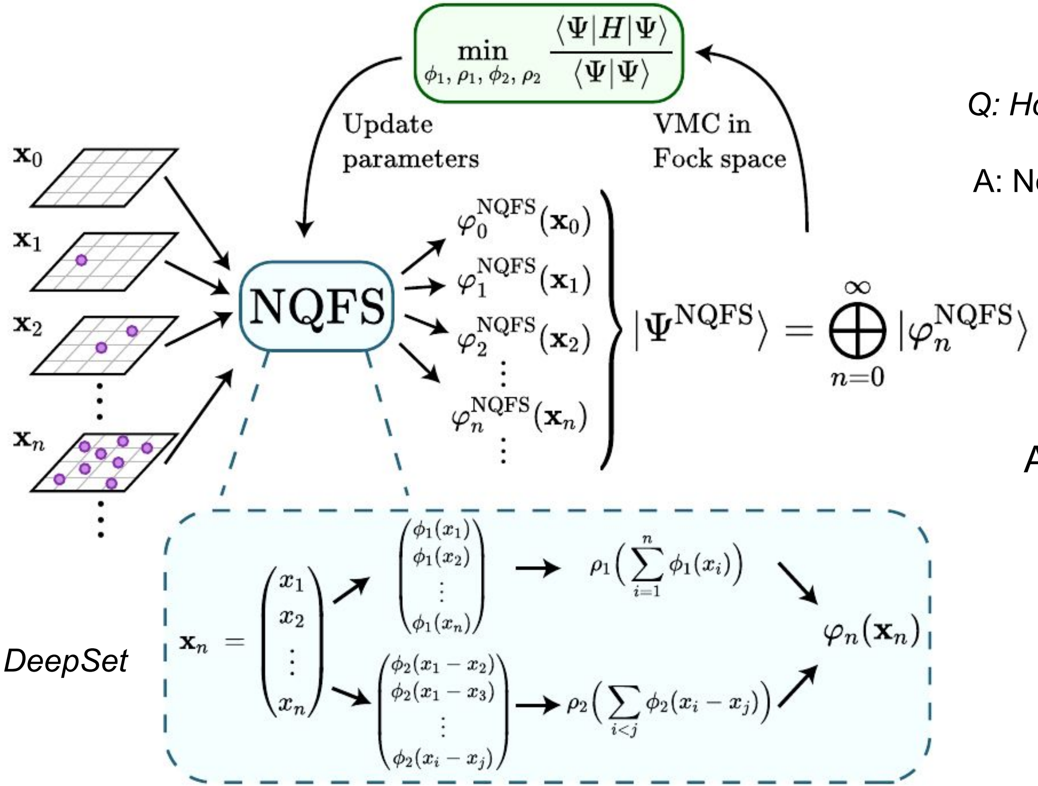
Variational Neural-Network Ansatz for Continuum Quantum Field Theory

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





Neural Quantum Field States for Continuum QFT



DeepSet

Q: How to simulate continuum quantum field theories?

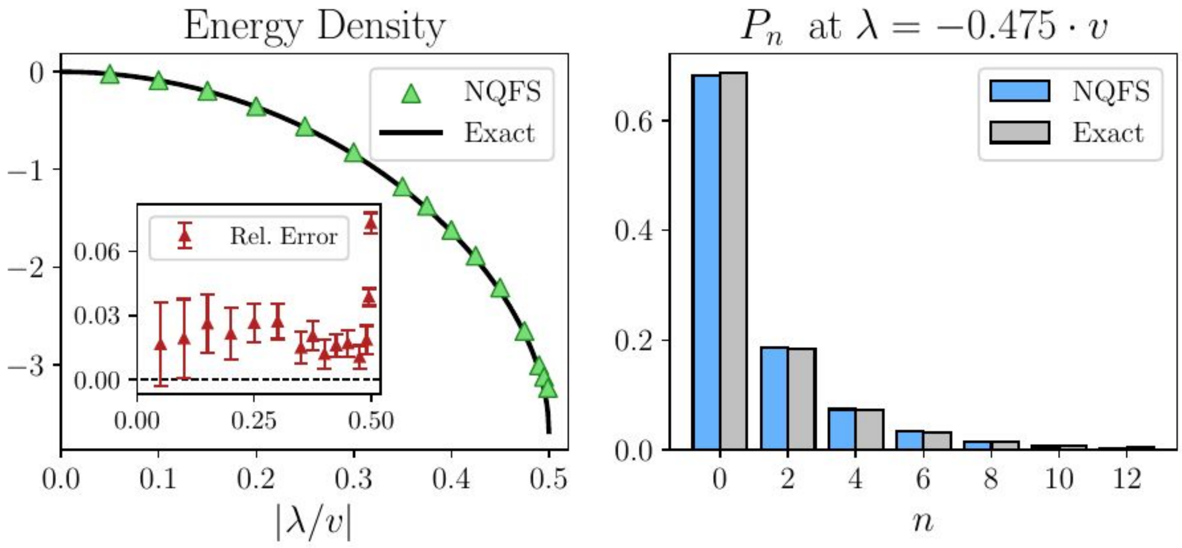
A: Neural quantum field states

Applications:

- Lieb-Liniger Model
- Calogero-Sutherland Model
- Regularized Klein-Gordon Model

Neural Quantum Field States for Continuum QFT

Regularized Klein-Gordon Model



$$H_{\mathrm{KG}} = \frac{1}{2}\int dx\ |\hat{\pi}(x)|^2 + |\nabla\hat{\phi}(x)|^2 + m^2|\hat{\phi}(x)|^2$$

Conclusions and Outlook

- New opportunities from neural quantum states for simulating quantum field theories
- New attempts to handle gauge symmetries, sign problems, continuous fields
- Study ground state phase diagram, finite temperature physics, and real-time dynamics of quantum field theories