Gauge Equivariant and Invariant Neural Network for Quantum Lattice Model Simulations

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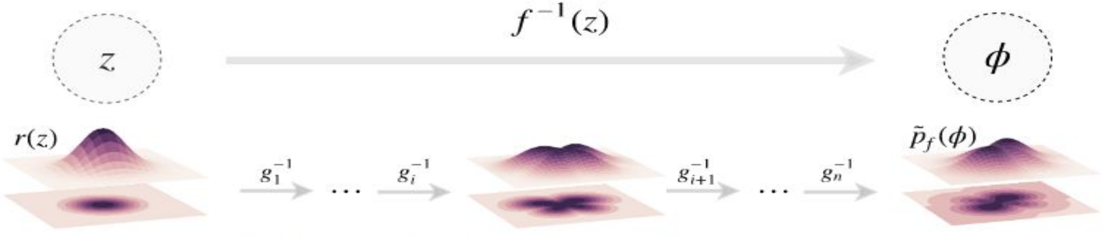
Machine Learning & High Energy Physics

Machine learning accelerated simulation

- Denis Boyda, etc., arxiv.2008.05456
- Gurtej Kanwar, etc., arxiv.2003.06413
- M. S. Albergo, etc., arxiv.1904.12072
- Kim A. Nicoli, etc., arxiv.2007.07115
- Akio Tomiya, etc., arxiv.2103.11965
- Sam Foreman, etc., arxiv.2105.12767
- Yuki Nagai, etc., arxiv.2010.11900
- Matteo Favoni, etc. arxiv.2012.12901
- Gurtej Kanwar, etc. arxiv.2103.02602
- Andrei Alexandru, etc. arxiv.1709.01971
- Boram Yoon, etc, arxiv.1807.05971
- ......



(a) Normalizing flow between prior and output distributions

arxiv.1904.12072

Quantum many-body physics simulation

Spectrum calculation

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

Eg. phase diagram, excited states, correlation function

Real time evolution

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

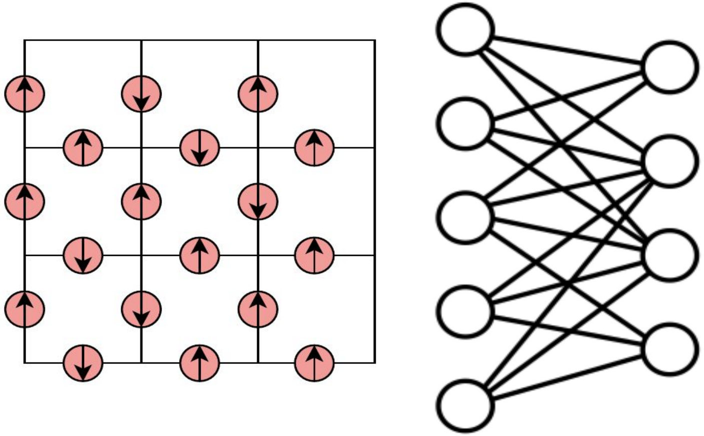
Eg. quantum chaos, quantum circuit simulation, dynamics of gauge theories

Challenges:

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

Challenges: sign problem + high dimensionality

Neural network: low dimensional representation of high dimensional objects

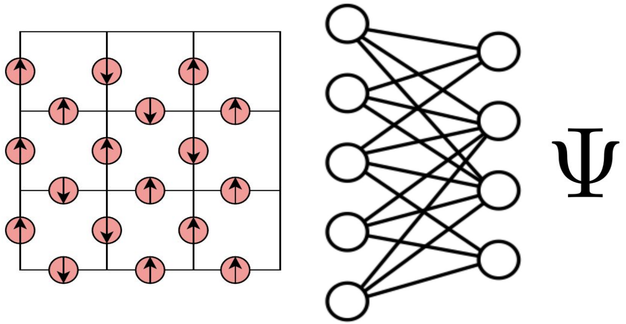


Universal Approximation Theorem [Cybenko]

→ Ψ

Wave function amplitude [Carleo]

Neural network representation



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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

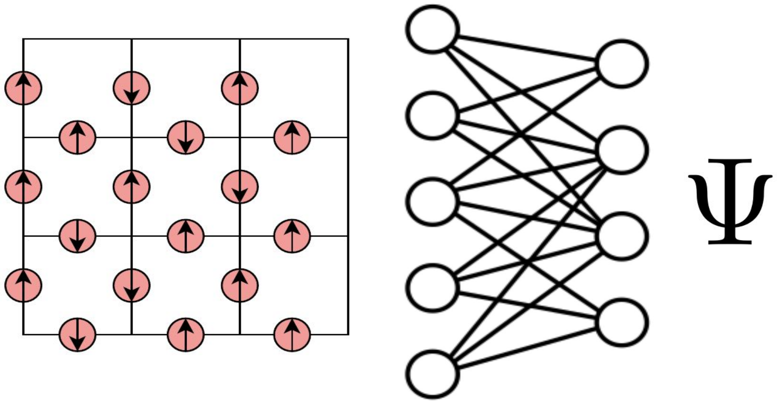
Phys. Rev. X **7**, 021021 – Published 11 May 2017

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

Neural network representation



- Neural network as a compact approximation to high dimensional function
- Symmetric function plays an important role in physics
- Gauge symmetry is crucial for condensed matter physics and high energy physics

Question:

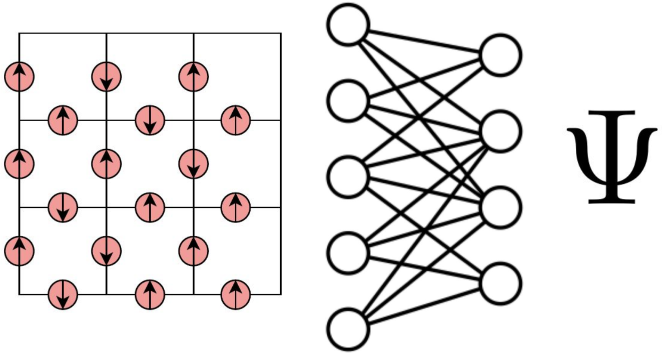
How to incorporate gauge symmetries into neural network constructions?

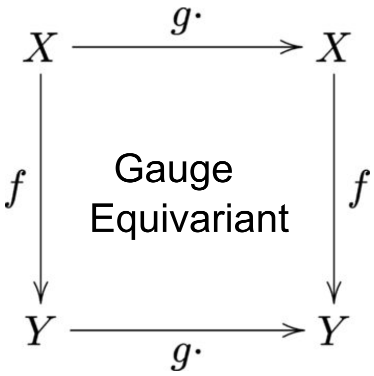
arxiv: 2012.05232

Gauge equivariant neural network for quantum lattice gauge theories

Di Luo[1], Giuseppe Carleo[2], Bryan K. Clark[1], and James Stokes[3]

[1] University of Illinois, Urbana-Champaign
[2] École Polytechnique Fédérale de Lausanne
[3] Center for Computational Quantum Physics and Center Computational Mathematics, Flatiron Institute





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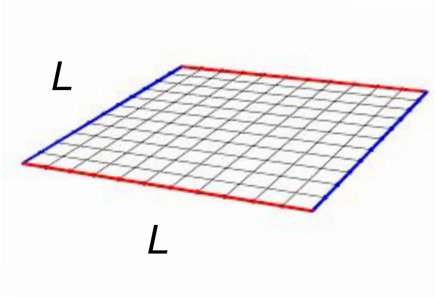
Gauge equivariant neural network

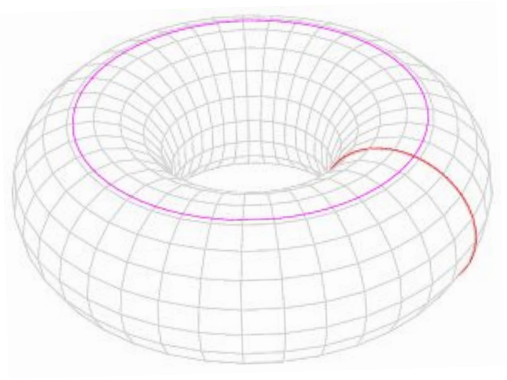
Hilbert Space



- Consider the $L \times L$ lattice with periodic boundary conditions

  $G = (V, E)$ be the associated undirected graph

  with $|V| = L^2$ vertices and $|E| = 2L^2$ edges



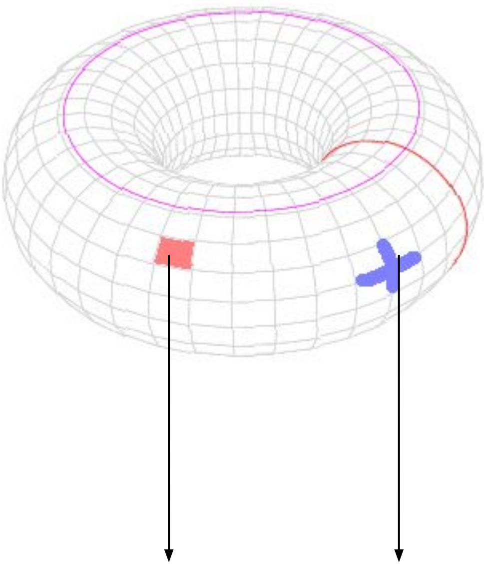
- Consider the Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes |E|}$

  (where $\mathbb{C}^2 = \text{span}\{|0\rangle, |1\rangle\}$) of qubits located the edges

$$\dim \mathcal{H} = 2^{|E|} = 2^{2L^2}$$

arxiv: 2012.05232

Gauge equivariant neural network



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

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

(AY Kitaev, 2003)

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

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

$$\dim \mathcal{H}_{\text{gauge}} = \frac{2^{|E|}}{2^{|V|-1}} = 2^{L^2+1}$$

- Hilbert space grows exponentially and exhibits curse of dimensionality
- Gauge constraint creates subspace

Gauge equivariant neural network

- Invariant function

$$\psi(T_v x) = \psi(x)$$

For some T_v as Z_2 transition operator

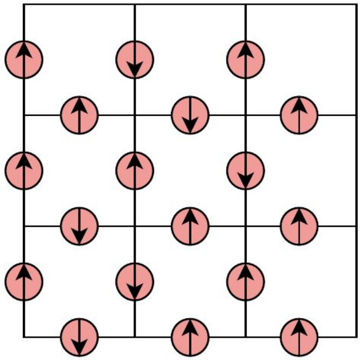
- Equivariant function

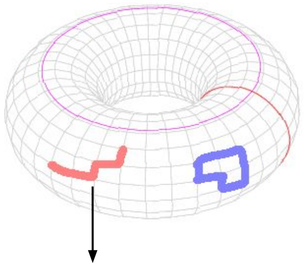
$$f(x) = f_L \circ \cdots \circ f_1(x)$$

$$f_i(T_v x) = T_v f_i(x)$$

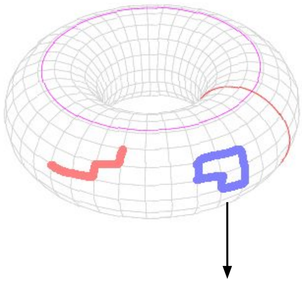
Gauge equivariant neural network

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





curve



loop

arxiv: 2012.05232

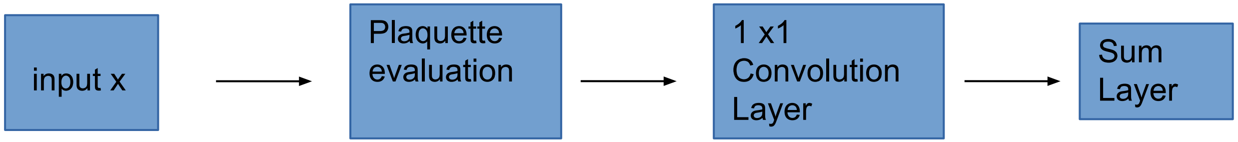
Quantum States with Neural Network Constructions

Theorem The four-fold degenerate ground states of the $\mathbb{Z}_2$ toric code are exactly representable with gauge invariant neural network functions.

- $G_v|\psi\rangle = |\psi\rangle$ automatically satisfied by Z_2 invariant neural network
- $W_f|\psi\rangle = |\psi\rangle$

Analytic construction:

- 1 Z_2 invariant layer

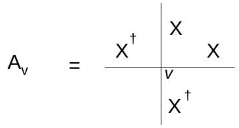


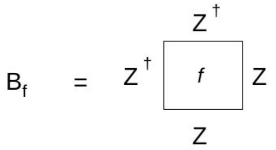
Quantum States with Neural Network Constructions

($\mathbb{Z}_d$ *model*) Consider the usual $L \times L$ square periodic lattice where each edge hosts a d-dimensional qudit. The Hamiltonian defined on $\mathcal{H}(\mathbb{C}^d)^{\otimes E}$ is

$$H = -\sum_{v \in V} \sum_{h \in \mathbb{Z}_d} (A_v)^h - \sum_{f \in F} \sum_{h \in \mathbb{Z}_d} (B_f)^h$$

where A_v and B_f are shown in Figure with





$$X = \sum_{h \in \mathbb{Z}_d} |h+1\rangle\langle h| \ , \qquad Z = \sum_{h \in \mathbb{Z}_d} \omega^h |h\rangle\langle h| \ , \qquad \omega = e^{i2\pi/d}$$

Theorem The ground states of the $\mathbb{Z}_d$ toric code are exactly representable with gauge invariant neural network functions.

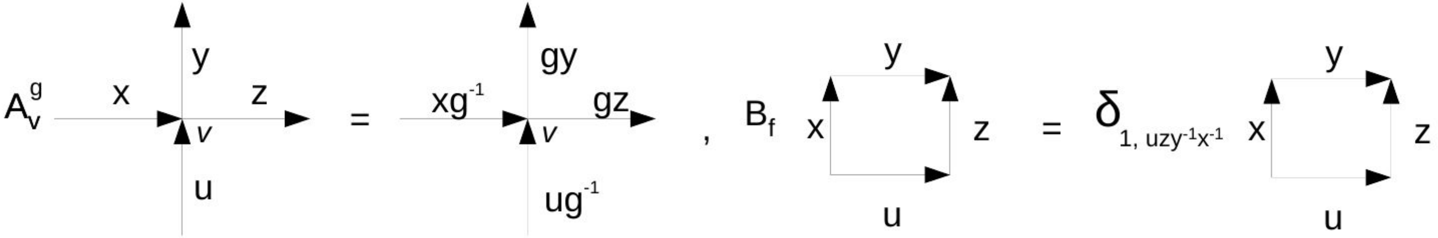
arxiv: 2012.05232

Quantum States with Neural Network Constructions

(*Kitaev $D(G)$ model*) The Hamiltonian defined on $\mathcal{H}(G)^{\otimes E}$ where G is a discrete group

$$H = -\sum_{v \in V} A_v - \sum_{f \in F} B_f$$

where $A_v = \frac{1}{|G|} \sum_{g \in G} A_v^g$ is the Gauss' law and the gauge constraint.



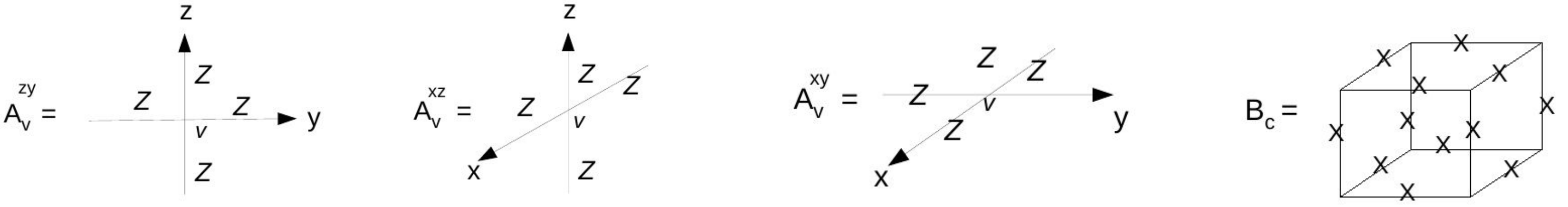
Theorem The ground states of the Kitaev $D(G)$ model are exactly representable with gauge invariant neural network functions.

arxiv: 2012.05232

Quantum States with Neural Network Constructions

(*X-cube fracton model*) The Hamiltonian is defined on a cubic lattice by

$$H = -\sum_{v \in V, i} A_v^i - \sum_{c \in C} B_c$$



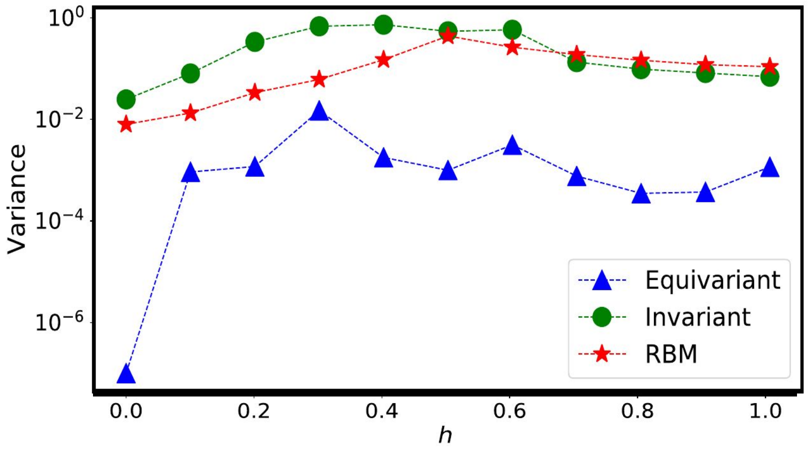
Theorem The ground states of the X-cube fracton model are exactly representable with gauge invariant neural network functions.

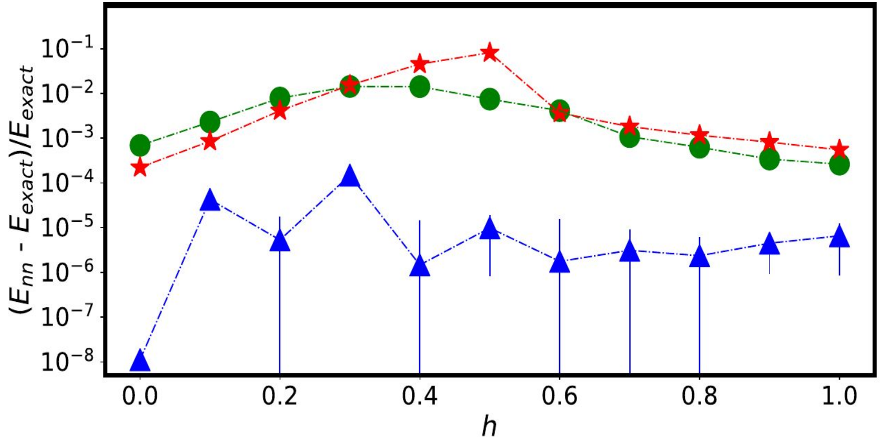
arxiv: 2012.05232

Gauge equivariant neural network

Toric code hamiltonian with transverse field (L=3)

$$H = -J \sum W_f - h \sum_{e \in E} X_e$$





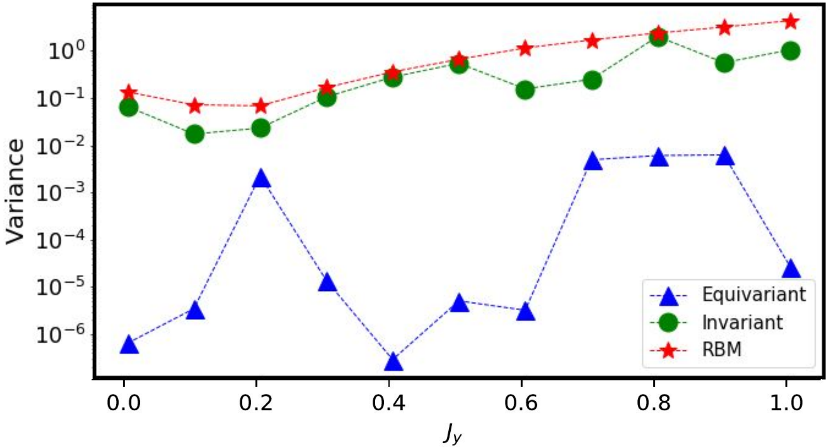
- Gauge equivariant neural network requires fewer parameters and has better performance.

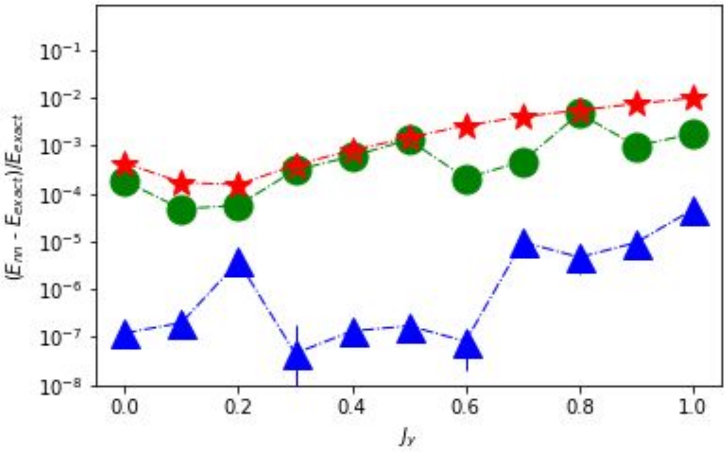
arxiv: 2012.05232

Gauge equivariant neural network

Hamiltonian with sign problem (L=3)

$$H = -J\sum W_f - h\sum_{e\in E} X_e - J_y \sum \prod_{\square} Y_e$$





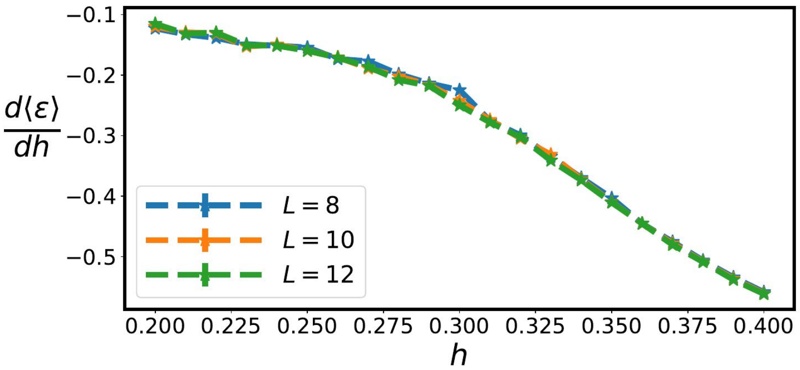
- Gauge equivariant neural network requires fewer parameters and has better performance.

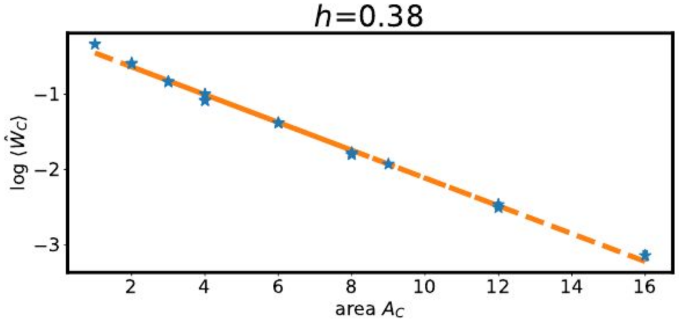
arxiv: 2012.05232

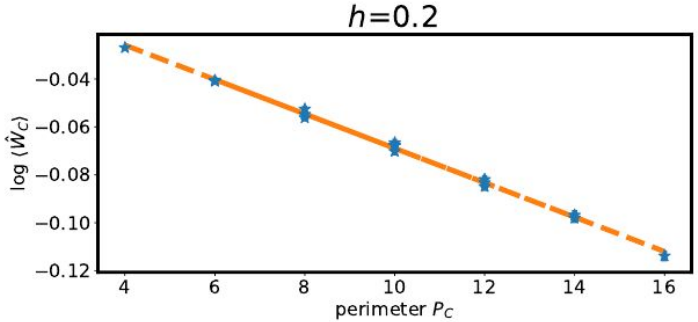
Gauge equivariant neural network

$$H = -J \sum W_f - h \sum_{e \in E} X_e$$

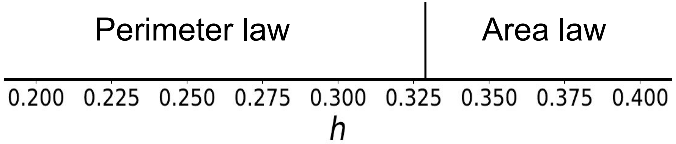
Study Area-law to Perimeter-law transition on







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



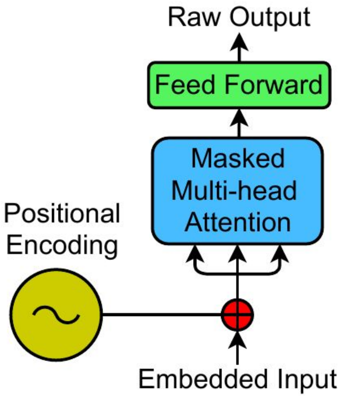
(J Vidal, et al. 2009)

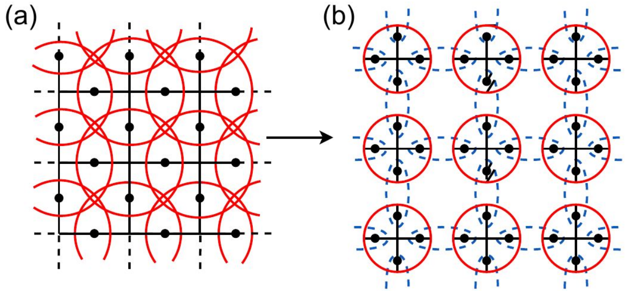
arxiv: 2012.05232

Autoregressive gauge invariant neural network for quantum lattice models

Di Luo†, Zhuo Chen†, Kaiwen Hu, Zhizhen Zhao, Vera Mikyoung Hur, and Bryan K. Clark

University of Illinois, Urbana-Champaign





Gauge invariant neural network

arxiv: 2101.07243

Autoregressive gauge invariant neural network

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

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

Gauge invariant neural network

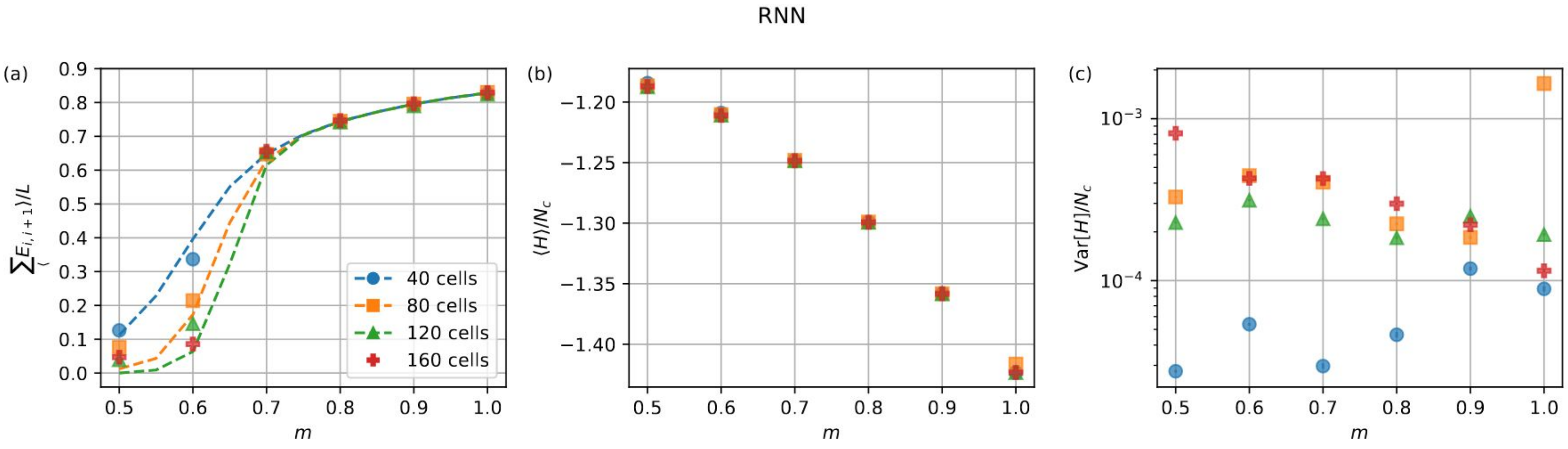
arxiv: 2101.07243

Quantum Link Model

(1+1-d QED)

$$H_{\rm QLM} = -\sum_i \left[\psi_i^\dagger U_{i,i+1}\psi_{i+1} + \psi_{i+1}^\dagger U_{i,i+1}^\dagger \psi_i\right] + m\sum_i (-1)^i \psi_i^\dagger\psi_i + \frac{g^2}{2}\sum_i E_{i,i+1}^2$$

$$\widetilde{G}_x = \psi_x^\dagger\psi_x - E_{x,x+1} + E_{x-1,x} + \tfrac{1}{2}\left[(-1)^x - 1\right]$$



Ground state calculation in gauge sector

Gauge invariant neural network

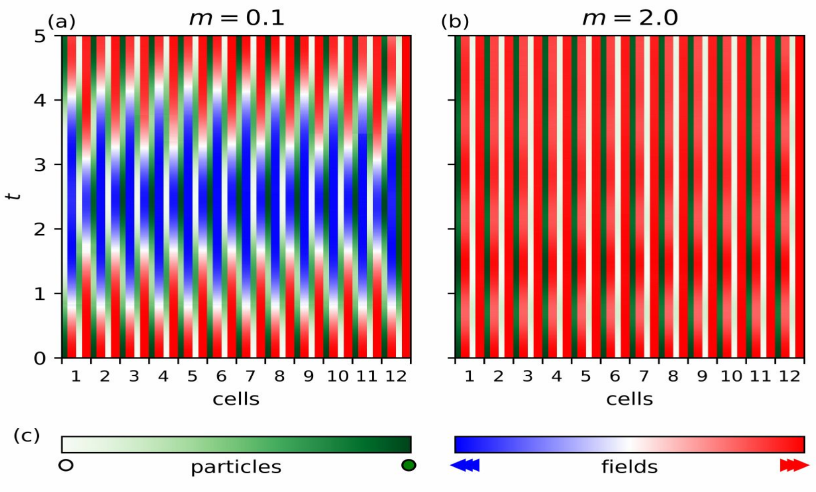
arxiv: 2101.07243

Quantum Link Model

(1+1-d QED)

$$H_{\mathrm{QLM}} = -\sum_i \left[\psi_i^\dagger U_{i,i+1}\psi_{i+1} + \psi_{i+1}^\dagger U_{i,i+1}^\dagger \psi_i\right] + m\sum_i (-1)^i \psi_i^\dagger \psi_i + \frac{g^2}{2}\sum_i E_{i,i+1}^2$$

$$\widetilde{G}_x = \psi_x^\dagger \psi_x - E_{x,x+1} + E_{x-1,x} + \frac{1}{2}\left[(-1)^x - 1\right]$$



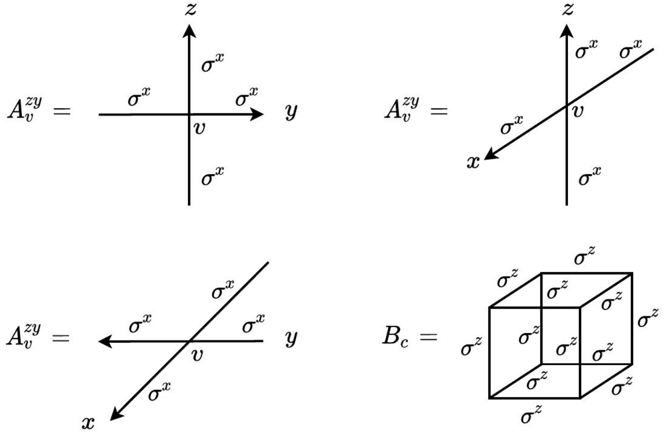
String inversion of real-time dynamics

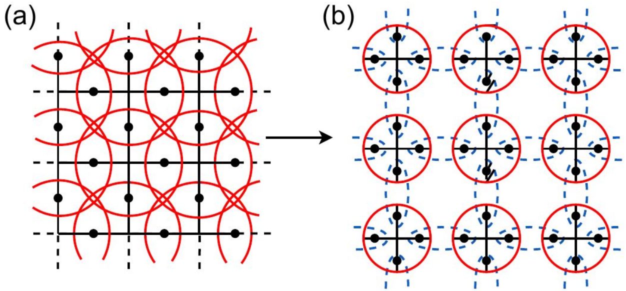
Gauge invariant neural network

arxiv: 2101.07243

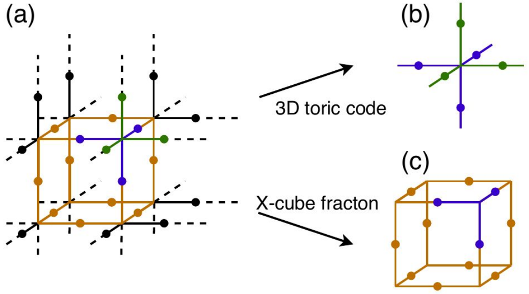
Applications to 2D, 3D Toric code and X-cube Fracton model

$$H_{\text{fracton}} = -\sum_{v \in V, i} A_v^i - \sum_{c \in C} B_c$$





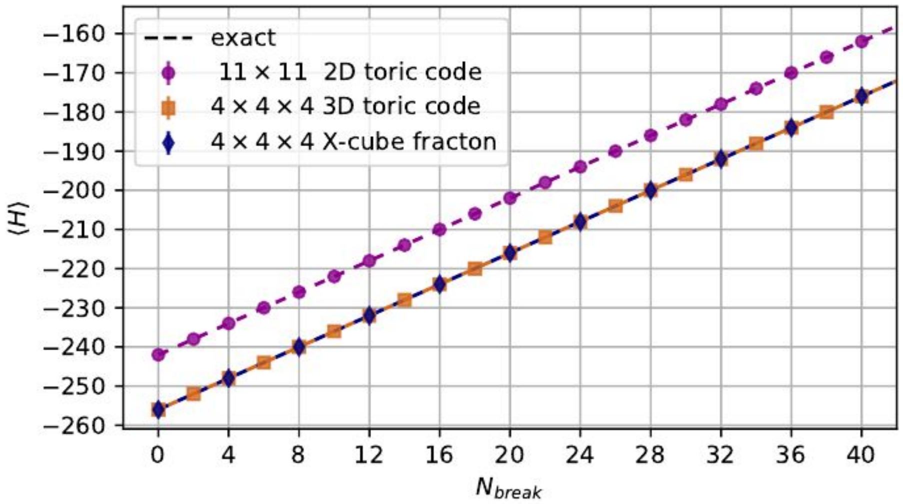
2D toric code



Gauge invariant neural network

arxiv: 2101.07243

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



Exact representation of grounds states and excited states for:

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

Gauge invariant neural network

arxiv: 2101.07243

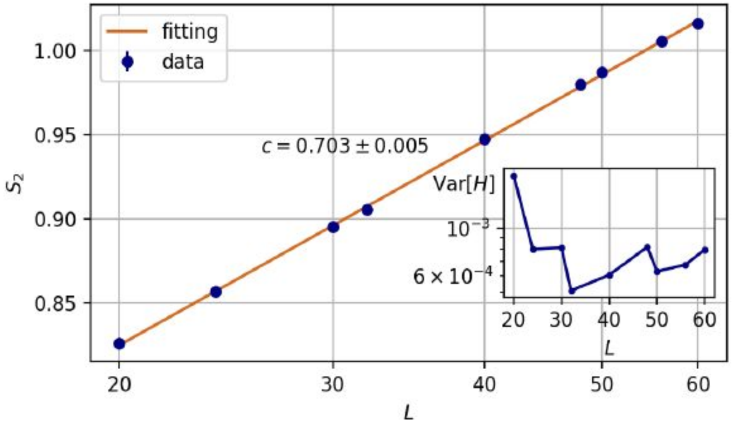
SU(2)₃ Fibonacci anyons

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

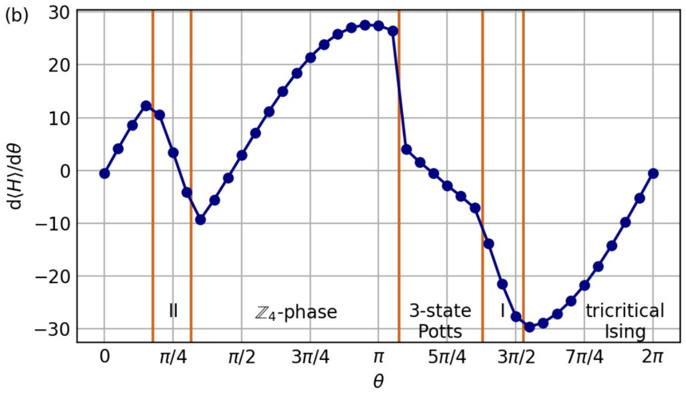
$$H(\theta) = -\cos\theta \sum_i H_i^{(2)} - \sin\theta \sum_i H_i^{(3)}$$

2-body

3-body



Extract central charge $S_2 \sim \frac{c}{4}\log(L)$



Phase Diagram

Summary & Outlook

- Gauge equivariant and gauge invariant neural networks are proposed to study gauge theories
- Applications for studying phase diagrams and excited states of different models with symmetries constraint
- Applications for real time dynamics of gauge theories