Simulating (2+1)d Lattice Gauge Theories with Fermionic Tensor Networks

Institute for Nuclear Theory, Seattle

Universiteit Leiden The Netherlands

April 04, 2023 | Patrick Emonts | Lorentz Institute, Leiden University

Why do we need Lattice Gauge Theories?



Image adapted from Alexandre Deur, Stanley J. Brodsky, and Guy F. de Téramond (2016) Progress in Particle and Nuclear Physics 90 pp. 1–74



Modeling Nature



Mari Carmen Bañuls and Krzysztof Cichy (2020) Rep. Prog. Phys. **83** p. 024401; John Kogut and Leonard Susskind (1975) Phys. Rev. D **11** pp. 395–408; Kenneth G. Wilson (1974) Phys. Rev. D **10** pp. 2445–2459



Path integral formalism in QFT

pure QED

$$S_{QED}[A_{\mu}] = -\frac{1}{4} \int dx^{\alpha} F_{\mu\nu}(x_{\alpha}) F^{\mu\nu}(x^{\alpha}) = \int dx^{\alpha} \partial_{\mu} A_{\nu}(x^{\alpha}) \partial^{\nu} A^{\mu}(x^{\alpha})$$

vacuum expectation value

$$\langle \Omega | O[A_{\mu}] | \Omega \rangle = \frac{\int \mathcal{D}AO[A_{\mu}] e^{iS_{QED}[A_{\mu}]}}{\int \mathcal{D}A e^{iS_{QED}[A_{\mu}]}}$$

Problems

- × Numerator oscillating
- ✗ Integration measure ill-defined



Wick rotation

Shift to imaginary time

$$t \rightarrow -i\tau$$

Change of metric from Minkowski to Euclidean

$$e^{iS_M} = e^{i\int dx_M^{\alpha}\mathcal{L}(x_M^{\alpha})} \longrightarrow e^{-\int dx_E^{\alpha}\mathcal{L}(x_E^{\alpha})} = e^{-S_E}$$

Problems

- Numerator converging
- ✗ Integration measure ill-defined





Discretization: Lattice Gauge Theory



$$A_{\mu}
ightarrow U_{\mu} = e^{i a A_{\mu}}$$

Find the lattice action \tilde{S}_E that agrees with S_E in the continuum limit of vanishing a

$$\tilde{S}_E[U] \to S_E[A](a \to 0)$$

Vacuum expectation value

Vacuum expectation value

$$\langle O[U] \rangle = \frac{\int \mathcal{D} U O[U] e^{-S_E[U]}}{\int \mathcal{D} U e^{-S_E[U]}}$$
 with $\mathcal{D} U = \prod_{x^{\alpha}} dU_{\mu}(x^{\alpha})$

Problems

Numerator converging

Integration with the Haar measure



Monte Carlo

Vacuum expectation value

$$\langle O[U] \rangle = \frac{\int \mathcal{D} U O[U] e^{-S_E[U]}}{\int \mathcal{D} U e^{-S_E[U]}}$$
 with $\mathcal{D} U = \prod_{x^{\alpha}} dU_{\mu}(x^{\alpha})$

Monte Carlo

Sampling from the distribution $p(U) = \frac{e^{-S_E[U]}}{\int \mathcal{D}U e^{-S_E[U]}}$ and calculate the expactation value as

$$\langle O[U] \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O[U(i)]$$

Fermions in lattice gauge theories

Action of the fermions

$$S_{f}[\Psi, \bar{\Psi}, U]$$

$$= \sum_{x,\mu} \bar{\Psi}(x)\gamma^{\mu}U_{\mu}(x)\Psi(x + e_{\mu}) - h.c. + m\bar{\Psi}(x)\Psi(x)$$

$$= \bar{\Psi}_{x}M_{xy}[U]\Psi_{y}$$



Integrating out the fermions

$$\int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi e^{-\bar{\Psi}M[U]\Psi} = \det(M[U])$$



Sign Problem

$$\langle O[U] \rangle = \frac{\int \mathcal{D}U \mathcal{D}\Psi \mathcal{D}\bar{\Psi} O[U] e^{-S_{E}[U] - \bar{\Psi}M[U]\Psi}}{\int \mathcal{D}U \mathcal{D}\Psi \mathcal{D}\bar{\Psi} e^{-S_{E}[U] - \bar{\Psi}M[U]\Psi}}$$

$$= \frac{\int \mathcal{D}U O[U] \det(M[U]) e^{-S_{E}[U]}}{\int \mathcal{D}U \det(M[U]) e^{-S_{E}[U]}}$$

$$Probability distribution$$

$$p(U) = \frac{\det(M[U]) e^{-S_{E}[U]}}{\int \mathcal{D}U \det(M[U]) e^{-S_{E}[U]}}$$

But for finite potential $\mu > 0$: det(M[U]) ≥ 0



(Incomplete) Overview of fTN Approaches

TRG



Nouman Butt et al. (2020) Phys. Rev. D **101** p. 094509 Shinichiro Akiyama and Daisuke Kadoh (2021) J. High Energ. Phys. **2021** p. 188

Tree TN



Timo Felser et al. (2020) Phys. Rev. X **10** p. 041040

fPEPS/fMERA



Philippe Corboz et al. (2010) **81** p. 165104; Manuel Schneider et al. (2021) **104** p. 155118

Mari Carmen Bañuls and Krzysztof Cichy (2020) Rep. Prog. Phys. 83 p. 024401

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Modeling Nature



Mari Carmen Bañuls and Krzysztof Cichy (2020) Rep. Prog. Phys. **83** p. 024401; John Kogut and Leonard Susskind (1975) Phys. Rev. D **11** pp. 395–408; Kenneth G. Wilson (1974) Phys. Rev. D **10** pp. 2445–2459

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Many-body physics - How hard can it be?

We take a system that can take two states \uparrow and \checkmark



Number of possibilities

$$Z = 2^{N}$$

Storage of minimal configuration (classical)

 $|\psi_0\rangle = 0101101010$



Many-body physics – How hard can it be?

We take a system that can take two states \clubsuit and \checkmark



Number of possibilities

$$Z = 2^{N}$$

Storage of minimal configuration (quantum)

$$|\psi_0\rangle = \sum_{\{i\}} c_{i_0,\ldots,i_N} |i_1,i_2,\ldots,i_N\rangle$$



Finding an Ansatz

Idea

Use an Ansatz with polynomially many parameters although the Hilbert space has exponentially many states



We explore only a small part of the Hilbert space

M. Fannes, B. Nachtergaele, and R. F. Werner (1992) Commun.Math. Phys. 144 pp. 443-490



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Tensor Networks: A motivation

General superposition state

$$|\psi\rangle = \sum_{i_1,\dots,i_N} c^{i_1,\dots,i_N} |i_1,\dots,i_N\rangle$$

An example system: Ising spins



How to get to polynomial scaling?

Can we just skip the small coefficients?

 $\begin{array}{l} c^{0,0,1,0,1} = 0.3623 \\ c^{0,1,1,0,1} = 0.0003 \\ c^{1,0,0,0,0} = -0.0004 \\ c^{0,1,0,0,1} = 0.5203 \end{array}$



Tensor Networks: A motivation

General superposition state

$$|\psi\rangle = \sum_{i_1,\dots,i_N} c^{i_1,\dots,i_N} |i_1,\dots,i_N\rangle$$

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Tensor Network Notation



- The number of legs determines the number of indices of the object
- A connection ⇔ Contraction of indices



Calculations with pictures





SVD – Splitting a state

Singular value decomposition

 $M = USV^{\dagger}$

Tensor Network Notation

Properties

U, *V* unitaries *S* diagonal, real, non-negative



Construction of a state



Jacob C. Bridgeman and Christopher T. Chubb (2017) 50 p. 223001

General state

$$|\psi\rangle = \sum_{\{i\}} c^{i_1, \cdots, i_N} |i_1, \cdots, i_N\rangle$$

Matrix Product State

$$|\psi\rangle = \sum_{\{i\}} \sum_{\{\alpha\}} A_{1,\alpha_1}^{i_1} A_{\alpha_1,\alpha_2}^{i_2} \cdots A_{\alpha_{N-1},1}^{i_N} |i_1, \cdots, i_N\rangle$$



SVD – Selecting the important bits

Best approximation

The best approximation with rank r in the Frobenius norm for a given matrix M is to truncate to r singular values.





Carl Eckart and Gale Young (1936) Psychometrika 1 pp. 211–218



SVD – An example

Original Image









SVD – An example

Original Image



Truncated Image (20 SV)





Putting it all together – Approximating the state

Reducing to polynomially many parameters \Im

Truncate to a virtual bond dimension *D* to reduce to polynomially many parameters.

$$\begin{split} |\psi\rangle &= \bigcirc & \bigcirc & \bigcirc & & \bigcirc \\ &= \sum_{\{i\}} \sum_{\{\alpha\}} A_{1,\alpha_1}^{i_1} A_{\alpha_1,\alpha_2}^{i_2} \cdots A_{\alpha_{N-1},1}^{i_N} | i_1, \cdots, i_N \rangle \end{split}$$

Notation

 $A^{i}_{\alpha,\beta}: d \times D \times D$ tensors Physical index: i_{j} Virtual index: α_{j}



What did we gain? - Counting Parameters

$$|\psi\rangle = \sum_{\{i\}} c_{i_0,\ldots,i_N} |i_1, i_2, \ldots i_N\rangle$$

 d^N

MPS

$$|\psi\rangle = \sum_{\{i\}} \sum_{\{\alpha\}} A_{1,\alpha_1}^{i_1} A_{\alpha_1,\alpha_2}^{i_2} \cdots A_{\alpha_{N-1},1}^{i_N} | i_1, \cdots, i_N \rangle$$

Number of parameters

Number of parameters

 $N(D \times D \times d)$

Full state



MPS as 1D PEPS





Lattice Systems



Hilbert space

$$\mathcal{H} \subset \mathcal{H}_{\mathsf{gauge fields}} \otimes \mathcal{H}_{\mathsf{fermions}}$$

A general state

$$\begin{aligned} |\Psi\rangle &= \int \mathcal{D}\mathcal{G} |\mathcal{G}\rangle \left|\Psi_{F}(\mathcal{G})\right\rangle \\ \text{with } \mathcal{D}\mathcal{G} &= \prod_{\mathbf{x},k} dg(\mathbf{x},k) \end{aligned}$$

Erez Zohar and J. Ignacio Cirac (2018) Phys. Rev. D **97** p. 034510 Patrick Emonts and Erez Zohar (2020) SciPost Phys. Lect. Notes p. 12



Gauss law

Gauss law

$$\sum_{k} \left(E_{k}(\mathbf{x}) - E_{k}(\mathbf{x} - \mathbf{e}_{i}) \right) |\text{phys}\rangle = 0 \quad \forall \mathbf{x}$$

Classical analogue in (cont.) electrodynamics

 $\nabla\cdot {\bf E}=0$

$$E_1(\mathbf{x} - \mathbf{e}_1) \xrightarrow{E_2(\mathbf{x})} E_1(\mathbf{x})$$



Expectation value of an Observable

Assume that *O* acts only on the gauge field and is diagonal in the group element basis:

$$\begin{split} \langle O \rangle &= \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle} \\ &= \frac{\int \mathcal{D}\mathcal{G} \langle \mathcal{G} | O | \mathcal{G} \rangle \langle \Psi_F(\mathcal{G}) | \Psi_F(\mathcal{G})}{\int \mathcal{D}\mathcal{G}' \langle \Psi_F(\mathcal{G}') | \Psi_F(\mathcal{G}') \rangle} \\ &= \int \mathcal{D}\mathcal{G}\mathcal{F}_O(\mathcal{G}) p(\mathcal{G}) \end{split}$$
with $p(\mathcal{G}) &= \frac{\langle \Psi_F(\mathcal{G}) | \Psi_F(\mathcal{G}) \rangle}{\int \mathcal{D}\mathcal{G}' \langle \Psi_F(\mathcal{G}') | \Psi_F(\mathcal{G}') \rangle} = \frac{\langle \Psi_F(\mathcal{G}) | \Psi_F(\mathcal{G}) \rangle}{Z}$

The rest of this talk

Expectation value

$$\langle O \rangle = \int \mathcal{D}\mathcal{G}\mathcal{F}_O(\mathcal{G})p(\mathcal{G})$$

with $p(\mathcal{G}) = \frac{\langle \Psi_F(\mathcal{G}) | \Psi_F(\mathcal{G}) \rangle}{Z}$

TODO List

- **1** How do we construct $|\Psi_F(\mathcal{G})\rangle$?
- **2** How do we efficiently calculate $p(\mathcal{G})$?
- 3 Are those states useful?



Let's use a tensor network



with

 $a \in \{r, u, l, d, \Psi\}$



Building a state



Formula





Building a state



Formula

$$|\psi_0\rangle = \langle \Omega_{\nu}| \prod_{\ell} \omega_{\ell} \prod_{\mathbf{x}} \mathcal{A}(\mathbf{x}) |\Omega\rangle$$



Global Invariance

Global Gauge Transformation

$$e^{i \wedge \sum_{\mathbf{x}} Q(\mathbf{x})} |\psi_0\rangle$$

Gauge Invariance of the tensors

Acting on a physical degree of freedom with a gauge transformation is equivalent to acting on all auxiliary degrees of freedom.



Gauge Invariance of the projectors

The projectors are invariant under auxiliary gauge transformations.





Virtual vs Physical Gauge Invariance

Virtual Gauge Invariance



- Physical charge, virtual electric fields
- X Physical symmetry is global

Physical Gauge Invariance

- **?** Physical charge, physical electric fields
- Physical symmetry is local

Global Gauge Transformation

 $e^{i\wedge\sum_{\mathbf{x}}Q(\mathbf{x})}|\psi_{0}\rangle = |\psi_{0}\rangle$

Local Gauge transformation

$$e^{i\wedge \mathcal{G}(\mathbf{x})} \ket{\psi} = \ket{\psi}$$



Minimal coupling of a state

Goal

Couple the gauge field to the state such that it is locally invariant under gauge transformations.

Substitution procedure

$$|\psi_0
angle = \left< \Omega_{\nu} \right| \prod_{\ell} \omega_{\ell} \prod_{\mathbf{x}} \mathcal{A}(\mathbf{x}) |\Omega
angle$$

Erez Zohar and Michele Burrello (2016) New J. Phys. 18 p. 043008; Erez Zohar and J. Ignacio Cirac (2018) Phys. Rev. D 97 p. 034510



Minimal coupling of a state

Goal

Couple the gauge field to the state such that it is locally invariant under gauge transformations.

Substitution procedure

$$\begin{split} |\psi_{0}\rangle &= \left\langle \Omega_{v} \right| \prod_{\ell} \omega_{\ell} \prod_{\mathbf{x}} \mathcal{A}(\mathbf{x}) |\Omega\rangle \\ &\rightarrow \left\langle \Omega_{v} \right| \prod_{\ell} \omega_{\ell} \prod_{\mathbf{x}} \mathcal{A}(\mathbf{x}) |0\rangle_{\mathbf{x},1} |0\rangle_{\mathbf{x},2} |\Omega\rangle \end{split}$$



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Erez Zohar and Michele Burrello (2016) New J. Phys. 18 p. 043008; Erez Zohar and J. Ignacio Cirac (2018) Phys. Rev. D 97 p. 034510



Where are we now?

TODO List

- **1** How do we construct $|\Psi_F(\mathcal{G})\rangle$? \checkmark
- **2** How do we efficiently calculate $p(\mathcal{G})$?
- 3 Are those states useful?

The probability

$$p(\mathcal{G}) = \frac{\left\langle \Psi_{F}(\mathcal{G}) | \Psi_{F}(\mathcal{G}) \right\rangle}{\int \mathcal{D}\mathcal{G}' \left\langle \Psi_{F}(\mathcal{G}') | \Psi_{F}(\mathcal{G}') \right\rangle}$$



Who is scared of norms?

Matrix Product State

Efficient computation of

- Norm
- Expectation values
- Correlation functions

(canonical form)

PEPS

No efficient way to compute exactly

- Norm
- Expectation values
- Correlation functions

Norbert Schuch et al. (2007) Phys. Rev. Lett. 98 p. 140506



Is $|\Psi_{\mathsf{F}}(\mathcal{G})\rangle$ special?

The fermionic state $|\Psi_{F}(\mathcal{G})\rangle$

$$\Psi_{\mathsf{F}}(\mathcal{G})\rangle = \langle \Omega_{\mathsf{V}} | \prod_{\mathsf{x}} \omega(\mathsf{x}) \prod_{\mathsf{x}} \mathcal{U}_{\Phi(\mathsf{x})} \prod_{\mathsf{x}} \mathcal{A}(\mathsf{x}) | \Omega \rangle$$

$$\mathcal{A}(\mathbf{x}) = \exp\left(\sum_{ij} T_{ij} a_i^{\dagger}(\mathbf{x}) a_j^{\dagger}(\mathbf{x})\right)$$
$$\omega(x) = \omega_0(\mathbf{x}) \omega_1(\mathbf{x}) \Omega(\mathbf{x}) \omega_1^{\dagger}(\mathbf{x}) \omega_0^{\dagger}(\mathbf{x})$$
$$\omega_0(\mathbf{x}) = \exp(l^{\dagger}(\mathbf{x} + \mathbf{e}_1) r^{\dagger}(\mathbf{x}))$$
$$\omega_1(\mathbf{x}) = \exp(d^{\dagger}(\mathbf{x} + \mathbf{e}_2) u^{\dagger}(\mathbf{x}))$$



Gaussian States

Definition

Fermionic Gaussian states are represented by density operators that are exponentials of a quadratic form in Majorana operators.

 $\rho = K \exp\left(-\frac{i}{4}\gamma^T G\gamma\right)$

Covariance matrix

Covariance matrix for a state Φ :

$$\Gamma_{ab} = \frac{i}{2} \left\langle [\gamma_a, \gamma_b] \right\rangle = \frac{i}{2} \frac{\left\langle \Phi | [\gamma_a, \gamma_b] | \Phi \right\rangle}{\left\langle \Phi | \Phi \right\rangle}$$

Sergey Bravyi (2005) Quantum Inf. and Comp. 5 pp. 216–238

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What is actually on the computer?

Covariance matrices all the way

$$|\psi(\mathcal{G})\rangle = \langle \Omega_{v} | \underbrace{\prod_{\mathbf{x}} \omega(x) \prod_{\mathbf{x}} \mathcal{U}_{\phi(\mathbf{x})}}_{\sim \sim \Gamma_{in}(\mathcal{G})} \underbrace{\prod_{\mathbf{x}} A(\mathbf{x})}_{\sim \sim \Gamma_{M}} | \Omega \rangle$$

Norm of the state

$$\langle \Psi_F(\mathcal{G}) | \Psi_F(\mathcal{G}) \rangle = \sqrt{\det\left(\frac{1 - \Gamma_{in}(\mathcal{G})D}{2}\right)}$$







The whole framework for a given set of parameters





Variational Monte Carlo





Where are we now?

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- **1** How do we construct $|\Psi_F(\mathcal{G})\rangle$?
- 2 How do we efficiently calculate $p(\mathcal{G})$?
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Application to pure \mathbb{Z}_2

Properties

- 1 No physical fermions
- 2 Abelian gauge theory

Kogut Susskind Hamiltonian

$$\begin{split} H &= H_E + H_B \\ &= \frac{g^2}{2} \sum_{\ell} \left[2 - (P_{\ell} + P_{\ell}^{\dagger}) \right] + \frac{1}{2g^2} \sum_{p} \left[2 - (Q_{p_1}^{\dagger} Q_{p_2}^{\dagger} Q_{p_3} Q_{p_4} + \text{H.c.}) \right] \end{split}$$

John Kogut and Leonard Susskind (1975) Phys. Rev. D **11** pp. 395–408 D. Horn, M. Weinstein, and S. Yankielowicz (1979) Phys. Rev. D **19** pp. 3715–3731



Application to pure \mathbb{Z}_2

Kogut Susskind Hamiltonian

$$\begin{split} H &= H_E + H_B \\ &= \lambda \sum_{\ell} \left[1 - \sigma_{\ell}^z \right] + \frac{1}{\lambda} \sum_{\rho} \left[1 - \sigma_{\rho_1}^x \sigma_{\rho_2}^x \sigma_{\rho_3}^x \sigma_{\rho_4}^x \right], \end{split}$$



$$egin{aligned} & P_\ell^2 = Q_\ell^2 = 1 & P_\ell^\dagger P_\ell = Q_\ell^\dagger Q_\ell = 1 \ & P_\ell^\dagger Q_\ell P_\ell = e^{i\pi} Q_\ell. \end{aligned}$$



What changes in the Ansatz

The full state

$$\left|\Psi\right\rangle = \int \mathcal{D}\mathcal{G} \left|\Psi_{F}(\mathcal{G})\right\rangle \left|\mathcal{G}\right\rangle \longrightarrow \left|\Psi\right\rangle = \sum_{\mathcal{G}} \left|\Psi_{F}(\mathcal{G})\right| \left|\mathcal{G}\right\rangle$$

Ansatz with physical fermions

$$|\psi_{\mathsf{F}}(\mathcal{G})\rangle = \langle \Omega_{\mathsf{v}} | \prod_{\mathsf{x}} \omega(\mathsf{x}) \prod_{\mathsf{x}} \mathcal{U}_{\Phi(\mathsf{x})} \prod_{\mathsf{x}} A(\mathsf{x}) | \Omega \rangle$$

Ansatz without physical fermions

$$\psi_{\mathsf{F}}(\mathcal{G}) = \left\langle \Omega_{\mathsf{V}} \right| \prod_{\mathsf{x}} \omega(\mathsf{x}) \prod_{\mathsf{x}} \mathcal{U}_{\Phi(\mathsf{x})} \prod_{\mathsf{x}} \tilde{A}(\mathsf{x}) \left| \Omega_{\mathsf{V}} \right\rangle$$



Talking about bond dimension



MPS

$$|\psi\rangle = \sum_{\{i\}} \sum_{\{\alpha\}} A_{1,\alpha_1}^{i_1} A_{\alpha_1,\alpha_2}^{i_2} \cdots A_{\alpha_{N-1},1}^{i_N} |i_1,\cdots,i_N\rangle$$

Minimal Ansatz

1 virtual fermion per link

Optimized Ansatz

2 virtual fermions per link



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Results for an exact contraction calculation (L=2)



Patrick Emonts et al. (2023) Phys. Rev. D 107 p. 014505



Magnetic and electric energy





Energy minimization with Monte Carlo calculations



Patrick Emonts et al. (2023) Phys. Rev. D 107 p. 014505

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Energy minimization with Monte Carlo calculations



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Science is a team effort



Ariel Kelman



Snir Gazit



Umberto Borla



Sergej Moroz



Erez Zohar





Summary and Outlook

Summary

- A Hamiltonian approach shows promising possibilities (time evolution, finite chemical potential)
- Carefully designing the Ansatz is important (analytical guarantee on gauge-symmetry)
- Good results for the energy minimization across the whole spectrum for \mathbb{Z}_2

Open Questions

- What happens in three space dimensions?
- What happens if we add physical fermions?
- And if we do not use tensor networks?



Advertisement

A variational Monte Carlo algorithm for lattice gauge theories with continuous gauge groups: a study of (2+1)-dimensional compact QED with dynamical fermions at finite density

> Julian Bender, PE, Ignacio Cirac arxiv:2304.*



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