#### Gauge invariant Trotterization via shears

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#### Jesse Stryker

Maryland Center for Fundamental Physics University of Maryland, College Park

Iowa State University Seminar 2021/02/17

## Big picture

Physics targets:

- Simulation of quantum chromodynamics
  - Hadronization
  - Microscopic understanding of nuclear interactions
- Complete phase diagram of QCD
- Equation of state for nuclear matter

How to make these predictions?

- Nonperturbative problems
  - Numerically simulate QCD degrees of freedom





Conjectured phase diagram credit: G. Endrödi J.Phys.Conf.Ser. 503 (2014) 012009

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#### Traditional lattice field theory



- Defines a field theory nonperturbatively
- Spacetime discretized with a lattice (e.g. square, cubic, hypercubic)
- Matter particles such as quarks are described "live" on the sites
- Gauge bosons live on oriented links joining sites
- Gauge fields belonging to some Lie group–the "gauge group" *G*



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#### Traditional lattice field theory



 Real-time dynamics and nonzero baryon density both suffer from 'sign problems' in classical simulations



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#### Classical problems.. quantum solutions?

Digital quantum computers:



- Unitary gates:  $e^{-it\hat{H}}$  with Hamiltonian of interest
- Want to simulate nonperturbative gauge theory
  - ➤ Gauge theory on the lattice
  - Hamiltonian lattice gauge theory
- Has no apparent sign problems

General problem:

How to map a Hilbert space  $\,\,{\cal H}$  , and  $\,\,\hat{H}$  , on to qubits & quantum gates?



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#### Gate-based quantum computing model

Two state, qubit system – computational basis

Two qubit basis: |00>, |01>, |10>, |11>





Nielsen & Chuang (2001)

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Lattice gauge theory Hilbert space structure

• An Abelian group, U(1)



*Gauge transformations:* 

$$\hat{U}_{n,i} \to e^{i(\theta_n - \theta_{n+e_i})} \hat{U}_{n,i}$$

Kogut & Susskind (1975); Creutz (1983), Smit (2002)

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Quantized with canonical, same-link. commutation relations.

$$U\left|q
ight
angle=\left|q+1
ight
angle$$

"U raises E"

[E, U] = U







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Lattice gauge theory Hilbert space structure

• Non-Abelian group, e.g. SU(2)



$$\langle g|j,m,n
angle = \sqrt{rac{d_j}{|G|}} D_{m,n}^{(j)}(g)$$
  
representation  
basis

$$E^{a}_{L/R}, E^{b}_{L/R}] = if^{abc}E^{c}_{L/R}$$
$$[E^{a}_{R}, U] = UT^{a}$$
$$[E^{a}_{L}, U] = -T^{a}U$$

Left and right electric fields each have 'colored' components in addition to





"Left" and "right" electric fields to generate

the independent left/right rotations.

 $\hat{U}_{n,i} \rightarrow \overline{\Omega_n \hat{U}_{n,i} \Omega_{n+e_i}^{\dagger}}$ 

Gauge transformations:

Lattice gauge theory Hilbert space structure

• Non-Abelian group, e.g. SU(2)

"ILadde representations"

$$U_{m,m'} | j, M, M' \rangle = C_{+}(j, m, m', M, M') \times \times | j + 1/2, M + m, M' + m') \times + C_{-}(j, m, m', M, M') \times \times | j - 1/2, M + m, M' + m')$$

#### Non-Abelian Hamiltonian

$$\hat{H}_E = \frac{g^2}{2} \sum_{n,i} \hat{E}^{\alpha}_{n,i} \hat{E}^{\alpha}_{n,i}$$

$$\hat{H}_B = -\sum_n \frac{1}{2g^2} \operatorname{tr}(\hat{U}_{n,\Box} + \hat{U}_{n,\Box}^{\dagger})$$

SU(2) example for the 2x2 link operator

Zohar & Burrello (2015)

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#### Potential issues simulating KS formulation

• Qubits wasted on physical states



- Non-Abelian constraints mean individual basis states are virtually never allowed by themselves
- Quantum noise will create components along unphysical directions
- Gauge invariance not necessarily respected by algorithms, even for noiseless simulation



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Off-diagonal gauge invariant operators

$$\psi^{\dagger}(x)\psi(x+1)U(x) \rightarrow \psi^{\dagger}\chi U \rightarrow \sigma_{\psi}^{-}\sigma_{\chi}^{+}U$$

- Gauge invariant terms, e.g. hopping term, change multiple quantum numbers simultaneously
- Increments on a binary register (*E* register) involve *every* qubit
- Naive Pauli decompositions quickly blow up in number of terms
  - U(1) plaquette w/ two-qubit cutoff: 922 Pauli term
- Approximation via "sub-Trotter steps" liable to have unphysical transitions



### Schwinger model hopping term (2020)

• Schwinger model

Martinez et al (2016); Klco et al (2018) Shaw, Lougovski, JRS, Wiebe (2020)







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# Schwinger model hopping term: Shears



$$\xi_1 = \delta_{n_{\psi},0} + \delta_{n_{\psi},1}\lambda^- ,$$
  
$$\xi_1 T_{\text{hop}} \xi_1^{\dagger} = \sigma_{\psi}^- \sigma_{\chi}^+ (1 - \delta_{E,E_{\text{max}}})$$



$$\xi_2 = \delta_{n_{\psi},0} + \delta_{n_{\psi},1} X_{\chi} ,$$
  
$$\xi_2(\xi_1 T_{\text{hop}} \xi_1^{\dagger}) \xi_2^{\dagger} = \delta_{n_{\chi},1} \sigma_{\psi}^- (1 - \delta_{E,E_{\text{max}}}) .$$



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#### Schwinger model hopping term: Circuit





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### $U(1) \text{ or } Z(\mathcal{N}) \text{ Plaquette}$

• Four link plaquette

$$U_{\Box} = U_0 U_1 U_2^{\dagger} U_3^{\dagger}$$
  
=  $\lambda_0^+ \lambda_1^+ \lambda_2^- \lambda_3^- \times$   
 $[1 - \delta_{N_0, -1}] [1 - \delta_{N_1, -1}] [1 - \delta_{N_2, 0}] [1 - \delta_{N_3, 0}]$ 

• Off-diagonal on four registers



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### Toy plaquette

• Consider a two-link "plaquette"

$$U_{\Box} = U_1 U_2^{\dagger} = \lambda_1^+ \lambda_2^- [1 - \delta_{N_1, -1}] [1 - \delta_{N_2, 0}] .$$





 $\Xi_{12}U_{\Box}\Xi_{12}^{\dagger} = \lambda_1^+ [1 - \delta_{N_1, -1}] [1 - \delta_{N_2, N_1}].$ 

### Toy plaquette

• The couplings can be expressed as a sum of two terms



$$U_{\Box} + U_{\Box}^{\dagger} \xrightarrow{\Xi_{12}} h_e + h_o ,$$

$$h_e \equiv \sigma_{1,\text{lsb}}^- [1 - \delta_{N_1,-1}] [1 - \delta_{N_2,N_1}] + [1 - \delta_{N_1,-1}] [1 - \delta_{N_2,N_1}] \sigma_{1,\text{lsb}}^+ ,$$

$$h_o \equiv \lambda_1^+ \sigma_{1,\text{lsb}}^- \lambda_1^- [1 - \delta_{N_1,-1}] [1 - \delta_{N_2,N_1}] + [1 - \delta_{N_1,-1}] [1 - \delta_{N_2,N_1}] + [1 - \delta_{N_1,-1}] [1 - \delta_{N_2,N_1}] \lambda_1^+ \sigma_{1,\text{lsb}}^+ \lambda_1^- .$$

 $X_{1,\mathrm{lsb}} P_e$ 

 $\lambda_1^+ [X_{1, \text{lsb}} P_o] \lambda_1^-$ 



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#### Toy plaquette: Circuit





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#### Outlook

- The true, four-link plaquette is solved using shears in a 4D space
- Shearing appears to work when gauge constraints are *simultaneously diagonalizable* 
  - Can characterize each matrix element of H as an allowed or unallowed transition
  - Off-diagonal, product of ladder operators + shearing → Controlled ladder operator on one quantum number
  - Can use sub-Trotter steps safely as long as we reproduce all the allowed transitions
- Non-Abelian? SU(2)?
  - Kogut-Susskind unlikely to help
  - Loop-String-Hadron has Abelian (commuting) constraints



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### Loop-String-Hadron

- Loop-String-Hadron has formal lattice consisting of 'quark sites' and 'gluonic sites'
  - Quark sites have a local basis  $|n_i,n_o,n_l
    angle$
  - Gluonic sites have a local basis  $|\ell_{qr},\ell_{rp},\ell_{pq}
    angle$







Constraints known as "Abelian Gauss Law": Abelian flux must be conserved along each link



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### Summary

- Off-diagonal terms such as hopping terms in Schwinger model or plaquette operators in d>1 U(1) gauge theories require correlated changes of quantum numbers
- Shears can help change basis such that off-diagonal operators change one quantum number only
  - Other registers may still be involved as controls
- Commuting constraints and Cartesian 'space of quantum numbers' seem key
- Non-Abelian will no doubt be harder, but there is reason to be optimistic



