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Smearing lattice gauge fields on a quantum computer

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Smearing of gauge-field configurations in lattice field theory improves the results of lattice simulations by suppressing high energy modes from correlation functions. In quantum simulations, high kinetic energy eigenstates are introduced when the time evolution operator is approximated such as Trotterization. While improved Trotter product formulae exist to reduce the errors, they have diminishing accuracy returns with respect to resource costs. Therefore having an algorithm that has fewer resources than an improved Trotter formula is desirable. In this work I develop a representation agnostic method for quantum smearing and show that it reduces the coupling to high energy modes in the discrete nonabelian gauge theory $\mathbb{D}_4$.

1 Introduction. Classical lattice gauge theory (LGT) offers the ability for high precision determinations of observables such as decay constants, hadron masses, scattering amplitudes below multiparticle thresholds, finite temperature QCD, and equations of state [1–9]. However, these simulations struggle to extract multiparticle threshold final states and dynamical quantities such as viscosities which encounter sign problems using stochastic methods [10, 11]. Quantum computers offer a method to circumvent this sign problem entirely by using a Hamiltonian formulation for the deterministic evolution of a quantum system [12–14].

There has been a significant effort to develop methods for simulating LGTs on quantum computers [15–73]. The benefits for high energy physics from quantum simulators stems from the ability to do real-time simulations and study finite density physics. However it is known that many time evolution methods introduce couplings to other energy modes which is undesirable [40, 74, 75].

Implementations of the time evolution operator for quantum simulations involve approximating this operator [76–86]. One method, Trotterization, break the Hamiltonian, H, is broken into commuting terms, e.g. potential (V) and kinetic (K), such that $e^{itH} \approx (e^{i\delta t/2K} e^{-i\delta t V} e^{i\delta t/2K})^{t/\delta t}$, which are easily implemented on a quantum computer [76, 77, 87]. All approximations distort the Hamiltonian spectrum. Trotterization affects the spectrum by introducing terms proportional to $(t/n)^3$ multiplied by commutators such as $[K,[V,[V,K]]$; this significantly affects observables such as time dependent correlation functions [74]. The spectrum distortion induces couplings to higher and lower energy states [75, 88]. Therefore one wants a band-pass filter that cuts out the energy modes unconnected to the states of interest; higher order Trotter product formulae do this [77]. However, higher order Trotter products become increasingly more expensive in terms of gates and have diminishing accuracy returns [89]. The calculation of gate costs for quantum electrodynamics (QED) and quantum chromodynamics (QCD) simulations in Ref. [90] is cost prohibitive in terms of T gates for a fault tolerant quantum computer; therefore, finding methods to bring these costs down is crucial. One method would be finding an alternative way to bring down the systematic errors from Trotterization other than higher order product formulae.

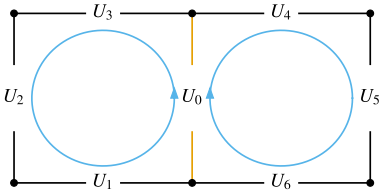

FIG. 1. Depiction of the plaquettes connected to a link in 2d. The orange line indicates the link to be smeared and the blue circles indicate the plaquettes that are taken as inputs to the smearing algorithm.

Classical LGT theory developed tools such as smearing [91–100] and gradient flow [101–104] as a method for dealing with high energy states in lattice configurations. This allows for classical simulations with $100\times - 1000\times$ fewer statistics and coarser lattices [100, 105–107]. Smearing averages neighboring fluctuations on a lattice configuration to remove ultraviolet (UV) contamination; gradient flow moves the configuration along the renormalization group and dampens high-momentum field modes which can be used as a continuous method of smearing [102, 103, 108, 109]. In addition smearing comes in two forms: operator smearing and link smearing. Operator smearing mitigates the excited state contamination from a lattice operator choices, link smearing suppresses the noise from UV fluctuations from the background field configurations themselves. Since one does not know the UV state explicitly one approximates them by the using the kinetic energy operator as a proxy. Smearing smooths away the UV fluctuations on the underlying signal.

Therefore one would like to have a quantum equivalent of classical lattice link smearing that is both cost effective and removes some couplings to high energy modes induced by Trotterization or state preparation. The quantum case of smearing can be understood as introducing a small imaginary component to the kinetic energy operator that will suppress their contribution to time dependent observables. In many cases these non-unitary algorithms can yield shorter local circuits than their unitary counter

parts at the expense of some probability of failure [40, 110–114].

In this context we can estimate the cost of smearing for a larger group that could approximate QCD, $S(1080)$. Using the chosen smearing strength is $\rho = 0.2$ from Ref [115] as an approximate value for the smearing parameter used for a quantum simulation of $S(1080)$, we find that the quantum smearing operator has an approximate nonunitarity of $\eta = 0.0005$ for a single link using the definition of η in Ref. [116]. If we estimate that a stochastic implementation such as in [113] of the non-unitary operator succeeds with probability $1-\eta$, we find that every time we want to smear all the links it will succeed with probability $(1-\eta)^{d*L^d}$ where d is the number of dimensions and L is the number of sites on the lattice in one direction. Using the volume and lattice size as an estimate for gluon viscosity from Ref. [90], this would imply that for a 10^3 lattice using smearing 50 times would succeed stochastically with probability 10^{-33}. This is clearly impossible and the unitary method provided in this work would win out even with a subexponential increase in the number of required qubits.

In this letter, I develop a unitary quantum smearing algorithm in a representation agnostic way. This quantum smearing algorithm scales linearly with the number of qubits and circuit depth. Using a discrete nonabelian gauge theory on a 2×1 lattice I demonstrate that the high energy modes are suppressed and the underlying physics is not distorted.

2 Stout smearing as a classical algorithm. Smearing lattice configurations reduces the UV artifacts by replacing link variables U by U' such that the underlying configuration is smoother [95–100]. The special case of stout smearing takes a linear combination of plaquettes connected to a link, see Fig. 1, and then uses an exponential mapping of the linear combinations to transform the target link to a smeared link. Following the notation in Ref. [97], I cover the basics of stout smearing.

The staples connected to our target link $U_\mu(n)$ in the direction ν are defined as

$$\begin{aligned} C_{\mu,\nu}(n) =& U_\nu(n)U_\mu(n+\hat{\nu})U_\nu^\dagger(n+\hat{\mu}) \\ &+ U_\nu(n-\hat{\nu})^\dagger U_\mu(n-\hat{\nu})U_\nu(n-\hat{\nu}+\hat{\mu}). \end{aligned} \tag{1}$$

Next, one defines the linear combination of plaquettes as

$$\Omega_\mu(U_\mu(n)) = \Omega_\mu(n) = \sum_{\nu\neq\mu} C_{\mu,\nu}(n)U_\mu^\dagger(n). \tag{2}$$

A new variable, $\mathcal{Q}_\mu(n)$, defined as

$$\mathcal{Q}_\mu(n) = \frac{i}{2}\Big(\Omega_\mu(n) - \Omega_\mu^\dagger(n) - \frac{1}{N}Tr(\Omega_\mu(n) - \Omega_\mu^\dagger(n))\Big), \tag{3}$$

creates a traceless Hermitian matrix which is a generator for a group element. The target link is then transformed to

$$U'_\mu(n) = \mathcal{P}\{e^{-i\rho\mathcal{Q}_\mu(n)}\}U_\mu(n), \tag{4}$$

where ρ is a tunable parameter to determine how strong the smearing is and $\mathcal{P}$ indicates that some projection back onto the group may be required. Hereinafter the element $\mathcal{P}\{e^{-i\rho\mathcal{Q}(n)}\}$ will be referred to as the shift element, $\mathcal{S}(\rho,\mathcal{Q})$. A graphical depiction of these terms is shown in Fig. 1. The benefits of this algorithm are that it smears out fluctuations at the lattice scale and is gauge invariant.

3 Stout smearing as a quantum algorithm. Smearing does not work straightforwardly as a quantum algorithm because it irreversibly (nonunitarily) writes over information which is difficult to implement deterministically on a quantum computer. Smearing also requires making a copy of the lattice; this is not allowed in quantum computation [117–121]. The copying procedure is required to avoid stroboscopic approximations. Therefore we need to alter the smearing algorithm to allow for reversibility which increases the required physical quantum resources compared to the classical algorithm.

Before introducing the algorithm, I will cover the necessary quantum operations needed for this algorithm. One requires three primitive group operations: $\mathfrak{U}_\times$ which multiplies two group elements together, $\mathfrak{U}_{-1}$ which inverts a group element, and $\mathcal{S}(\rho,\mathcal{Q})$ which generates the shift elements. The algorithm is summarized in Fig. 2.

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for Link, $U_\mu(n)$, on the lattice **do**
  Store each plaquette in Eq. (2) onto scratch registers.
  Generate the link variable corresponding to $\mathcal{S}(\rho,\mathcal{Q})$.
  uncompute the plaquettes on the scratch register
end for
for Link, $U_\mu(n)$, on the lattice **do**
  Multiply the register with $\mathcal{S}(\rho,\mathcal{Q})$ to respective $U_\mu(n)$.
end for

FIG. 2. Pseudocode describing the quantum stout smearing algorithm.

This algorithm is representation agnostic; any Hamiltonian formulation requires a method to represent group element basis states. However, the process of implementing $\mathfrak{U}_\times$, $\mathfrak{U}_{-1}$, and $\mathcal{S}(\rho,\mathcal{Q})$ is representation dependent. Nevertheless, given group element basis exists this the function $\mathcal{S}(\rho,\mathcal{Q})$ is equivalent to a function that takes as inputs numbers and outputs a new number onto a clean scratch register which is a valid unitary operation on a quantum computer [117]. A side effect of this algorithm is that a new lattice's worth of qubits is required every time the smearing operation is applied in order to ensure reversibility. Therefore there is a linear cost in the number of qubits to use this algorithm.

We show in Fig. 3 how to construct the state $|\mathcal{S}(\rho,\mathcal{Q})\rangle$ on an ancilla register for any group and formulation. It is straight forward once all shift elements have been constructed to multiply these elements with their corresponding physical lattice link using the $\mathfrak{U}_\times$ operator.

4 $\mathbb{D}_4$ gauge theory example. It is illustrative to demonstrate smearing by a using discrete group as these are

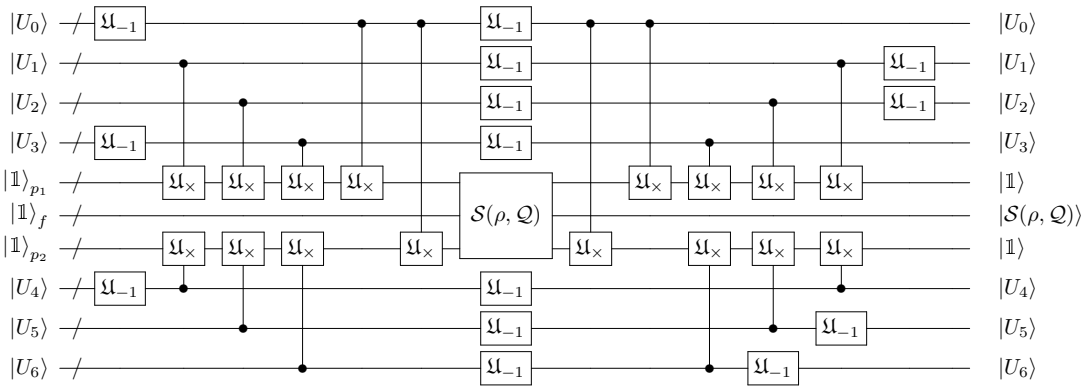

FIG. 3. Quantum circuit for constructing the projected element $\mathcal{S}(\rho, \mathcal{Q})$ on a 2d lattice. The forward slash indicates that the register maybe composed of multiple qubits. The registers $|U_m^\dagger\rangle$ correspond to the links in Fig. **??**. The three register gate $\mathcal{S}(\rho, \mathcal{Q})$ takes the $|\rangle_{p_1}$ and $|\rangle_{p_2}$ scratch plaquette registers as inputs and outputs the closest group element to $e^{i\rho\mathcal{Q}}$ onto the scratch register $|\mathbb{1}\rangle_f$.

realizable in the near future [122] and have the benefit of being defined explicitly in the group element basis. A dihedral group, $\mathbb{D}_4$, whose primitive gates have been derived in Refs. [122, 123], is useful as a proof of principle example. The elements of the group are $g = (\sigma^x)^a(e^{i\pi/2\sigma^z})^{2b+c}$ with $0 \leq a, b, c \leq 1$ and σ^x and σ^z are two of the Pauli matrices. This example uses a two plaquette theory with periodic boundary conditions as shown in Fig. 4 The Hamiltonian for this theory is

$$H = -\beta(ReTr(U_0U_1U_2^\dagger U_1^\dagger + U_2U_3U_0^\dagger U_3^\dagger)) + \log(T_K), \quad (5)$$

where $\log(T_K)$ is the kinetic term of the Hamiltonian, K, and is defined in [123] and $-\beta(ReTr(U_0U_1U_2^\dagger U_1^\dagger + U_2U_3U_0^\dagger U_3^\dagger))$ is the potential term of the Hamiltonian, V. In this example $\beta = 0.75$.

The only additional gate necessary for quantum stout smearing is a quantum circuit implementation of $\mathcal{S}(\rho, \mathcal{Q})$. The realization of the circuit depends on the chosen value of ρ. In order to ensure that smearing occurs but is not too significant that it distorts the underlying physics, let $\rho = 0.26$. For ρ less than this value no smearing will take place. Since $\mathbb{D}_4$ is discrete, ρ within given ranges will yield the same $\mathcal{S}(\rho, \mathcal{Q})$. Fig. 5 shows the implementation of this quantum circuit for $\rho = 0.26$. The time evolution operator $\mathbf{U}_n(t) = e^{-itH}$, where n is the Trotterization order, is at second order

$$\mathbf{U}_2(t; \delta t) = (e^{-i\delta t/2K}e^{-i\delta tV}e^{-i\delta t/2K})^{t/\delta t}, \quad (6)$$

and third order

$$\mathbf{U}_3(t; \delta t) = (e^{-i7\delta tV/24}e^{-i2\delta tK/3}e^{-i3\delta tV/4}e^{i2\delta tK/3} e^{-i\delta tV/24}e^{-i\delta tK})^{t/\delta t} \quad (7)$$

where K and V are the kinetic and potential parts of the Hamiltonian. For these simulations $\delta t = 0.85$. This is an example which shows contributions from other eigenstates.

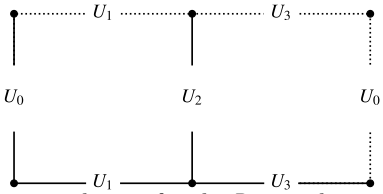

FIG. 4. 2 Plaquette lattice for the $\mathbb{D}_4$ simulation. The dashed lines indicate repeated links from periodic boundary conditions.

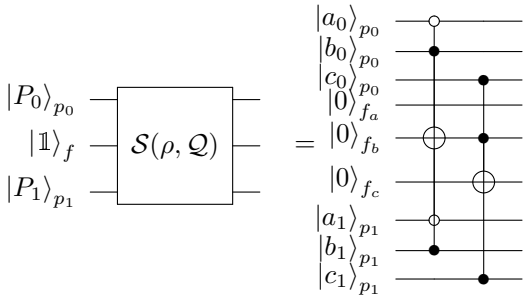

FIG. 5. Quantum Circuit that implements the operator $\mathcal{S}(\rho = 0.26, \mathcal{Q})$ for $\mathbb{D}_4$. 1

Fig. 6 shows the time evolution with $\delta t = 0.85$, of the plaquette correlator,

$$\langle P(t)\rangle = \langle\Omega|U^\dagger(t; \delta t)PU(t; \delta t)|F\rangle, \quad (8)$$

where $\langle\Omega|$ is the gauge invariant ground state, $|F\rangle$ is the gauge invariant projection of the first excited state, and P is the plaquette $ReTr(U_0U_1U_2^\dagger U_1^\dagger)$. A third order Trotterization at $\delta t = 1.0$ which has roughly the same errors as the smeared evolution is also shown. While the third order Trotterization is superior to the second order Trotterization with and with out smearing before

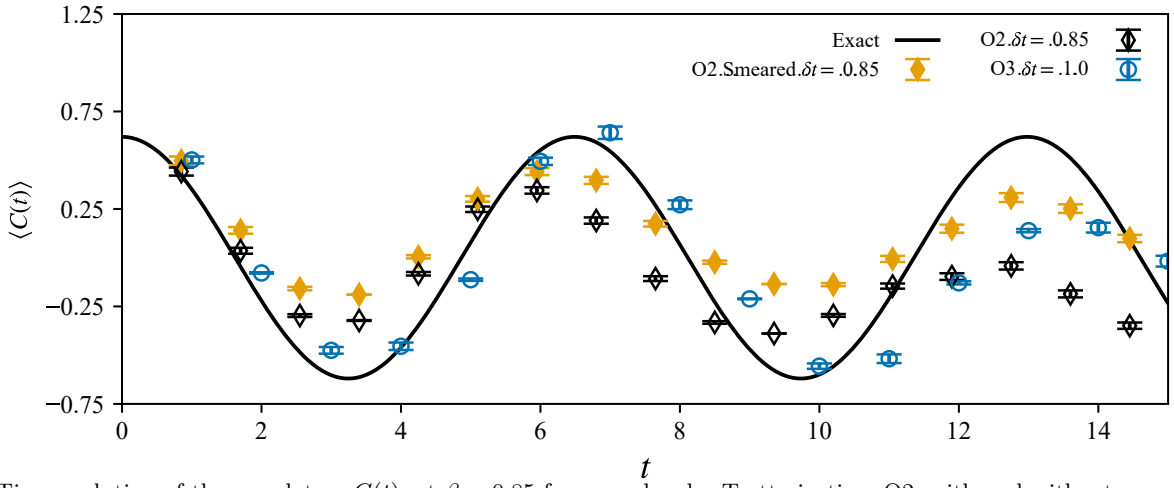

FIG. 6. Time evolution of the correlators $C(t)$, at $\beta = 0.85$ for second order Trotterization, O2, with and without smearing and third order Trotterization, O3, at $\delta t = 1.2$ for equivalent accuracy.

$t = 10$, afterwards the higher energy states begin to distort the time evolution which is expected for a coarse Trotterization and aligns with the second order smeared Trotterization. The ancilla registers are reset in order to minimize the memory resource requirements on the classical simulations.

It is worth examining the resource costs of smearing in a fault tolerant perspective. Many error correcting codes for fault tolerant quantum computing have costly single qubit rotation operations such as the T-gate [124–129]. For this reason T-gates are an important metric for algorithm costs on fault tolerant quantum computers.

TABLE I. T gate costs for various operations on a 2×1 plaquette for $\mathbb{D}_4$.

operator	T gates
2^{nd} order Trotter	$696 + 46\log_2(1/\epsilon)$
3^{rd} order Trotter	$1008 + 131.1\log_2(1/\epsilon)$
smearing	560

The T-gate costs of a single second order Trotter step for $\mathbb{D}_4$, third order Trotter, and the smearing operator on the whole lattice in Tab. I. These costs are derived from the gates provided in Refs. [122, 123] and the single qubit gates are approximated using the repeat until success method with T gate cost $1.15\log_2(1/\epsilon)$ where ϵ is the desired gate infidelity [130]. The total cost for third order Trotterization for infidelity, $\epsilon = 10^{-8}$ and $\delta t = 1$ requires 1.75 times more T gates than a second order Trotterization at $\delta t = 0.85$ with smearing and 2.5 times as many T-gates if the third order Trotterization is used with $\delta t = 0.85$. This T gate saving should increase for larger groups as the projection operation will not require approximations using T-gate synthesis. The second order smeared evolution has fewer high energy oscillations than the unsmeared evolution. Examining the Fourier spectrum for the smeared and unsmeared evolution using second order Trotterization (see Fig. 7) shows that many high kinetic energy modes are mitigated. It is found that smearing does not uniformly suppress higher order energies.

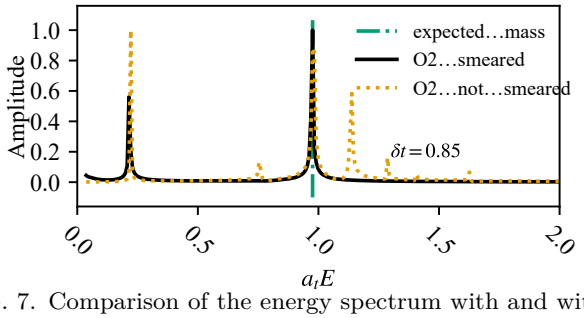

FIG. 7. Comparison of the energy spectrum with and without smearing at $\delta t = 0.85$ using second order Trotterization denoted O2.

5. Conclusions This work has developed a unitary algorithm for smearing real-time quantum simulations of LGTS. Somewhat analogously to classical LGT, this algorithm acts as expected by reducing higher energy modes. For the small lattice size investigated the benefits of smearing are noticable. The representation agnostic method in which this algorithm is presented allows it to be applied to a wide range of Hamiltonian formulations [43, 50, 71, 115, 122, 131–149]for quantum simulation of LGTs and will likely bring down the cost of many fault tolerant applications.

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