Improved Hamiltonians for Quantum Simulations

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The quantum simulation of lattice gauge theories for the foreseeable future will be hampered by limited resources. The historical success of Symanzik-improved lattice actions in classical simulations strongly suggests that improved Hamiltonians will reduce quantum resources for fixed discretization errors. In this work, we consider Symanzik-improved lattice Hamiltonians for pure gauge theories and design quantum circuits for $O(a^2)$-improved Hamiltonians in terms of primitive group gates. An explicit demonstration for $Z_2$ is presented including exploratory tests using the ibmqperth device.

Quantum simulations of lattice field theories avoid the exponentially large resources which plague classical methods for finite-density and dynamics [1–3]. While such resource reduction is dramatic for problems of interest like transport coefficients [4], PDFs [5–7], and the strong-CP problem [8, 9], the number of qubits remains $O((L/a)^d)$ for a $d$ spatial dimensional lattice of physical length $L$ and spacing $a$. An important question for such simulations is which resources are required for practical quantum advantage. Here, we will consider QCD as our fiducial case. Current estimates suggest $10^9$ qubits per gluon link are required [10–16]. This implies that kiloqubyte-sized computers are required for $3+1$D simulations with smaller requirements for $U(1)$ and $SU(2)$ [10–14, 17–34]. Comparable resources are found for qudit devices [14, 35, 36].

To estimate gate costs, one must specify a Hamiltonian for the simulations. Most studies of gauge theories consider the Kogut-Susskind Hamiltonian, $\hat{H}_{KS}$ [37]:

$$\hat{H}_{KS} = \hat{K}_{KS} + \hat{V}_{KS},$$

(1)

$$\hat{K}_{KS} = \sum_{x,i} \frac{g^2 \alpha}{a} \text{Tr} \hat{L}_i(x), \quad \hat{V}_{KS} = - \sum_{x,i<j} \frac{2}{g^2 \alpha} \text{Re} \text{Tr} \hat{P}_{ij}(x).$$

which has discretization errors of $O(a^2)$. The electric field $\hat{L}_i(x)$ is the left generator of gauge transformations on a link $U_i(x)$ [38] while $\hat{P}_{ij}(x)$ is the spatial plaquette term (e.g. $U_1 U_7 U_2^\dagger U_6^\dagger$ in Fig. 1).

When approximating the time evolution operator $\hat{U}(t) = e^{-i\hat{H}_{KS}t}$ via trotterization, the gate count scales $\propto t^{3/2} (L/a)^{d/2} \epsilon^{-1/2}$ [39, 40] for a maximum error $\epsilon$ for any state; although logarithmic corrections may prove important [15]. For one candidate for early practical quantum advantage in $SU(3)$ – the shear viscosity $\eta$, a loose upper bound of $O(10^{49})$ T gates has been estimated [15] where the authors assumed $\epsilon = 10^{-8}$. Given that lattice errors of $O(a^2, e^{-L/a})$ are not accounted for in $\epsilon$ and that current theoretical uncertainties on $\eta$ are $O(1)$ [41], $\epsilon \sim 10^{-2}$ seems a better target for practical quantum advantage. A tighter bound could be obtained by requiring that only low-lying states have errors below $\epsilon$. This greatly reduces the $L$ dependence and prefactors in the gate costs [42, 43]. Even with these reductions the gate cost is expected to be beyond access on near-term devices.

Further exacerbating these problems is the current, noisy status of quantum computers and the open question of how much quantum error correction is required to perform such simulations. General estimates suggest $O(10^{10^{-5}})$ physical qubits per logical qubit [44–46] – so physical qubit requirements could easily rise to the megaqubyte scale.

Gate reductions may be possible using other approximations of $\hat{U}(t)$ [47–52]. At the cost of classical signal-to-noise problems, stochastic state preparation yields shallower circuits [53–56]. Furthermore, performing scale setting classically can reduce quantum resources [57–59]. Lattice field theory specific error correction or mitigation could also potentially decrease quantum costs [60, 61].

In this letter, we present a new direction for reducing quantum resources by using Symanzik-improved Hamiltonians. The Symanzik program [62–64] has taught us that dramatic reductions in computational resources are possible through the use of lattice theories with reduced discretization errors. To do this, one includes specific additional terms in the Hamiltonian, and uses their relative weight to cancel the leading discretization errors [65, 66]. For example, $\hat{V}_{KS}$ can be series expanded via $\hat{P}_{ij}$,

$$\hat{P}_{ij} = \frac{1}{2} - \frac{g^2 \alpha^4}{2} \left[ F_{ij}^2 + \frac{\alpha^2}{12} (D_i^2 + D_j^2) F_{ij} + O(a^4) \right].$$

(2)

The deviations between lattice and continuous quantum field theories arise not only from discretizing the classical Hamiltonian, but also at the quantum level in the path integral. By adding rectangular and bent six-link loop terms (Fig. 1) to $\hat{H}_{KS}$, the $F_{ij}(D_i^2 + D_j^2)F_{ij}$ term can

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were found to have similar discretization errors to the classical $O(a^4)$ error, leaving the quantum $O(g^2a^2)$ error.

We will define our improved Hamiltonian as $\hat{H}_I = \hat{K}_I + \hat{V}_I$ with improved potential term $\hat{V}_I = \beta_0 V_{KS} + \beta_V V_{\text{rect}} + \beta_{V'} V_{\text{bent}}$. $V_{\text{rect}}$ is defined as
\begin{equation}
\hat{V}_{\text{rect}} = \frac{2}{ag^2} \sum_{x,i<j} \text{Re Tr} \left[ \hat{R}_{ij}(x) + \hat{R}_{ij}(x) \right], \tag{3}
\end{equation}
where $\hat{R}_{ij}(x)$ (e.g. $U_1U_2U_3U_4U_5U_6$ in Fig. 1) is the 6-link rectangular loop term with the $i$-th ($j$-th) direction crossing two units (one unit) of lattice spacing. $V_{\text{bent}}$ has analogous expressions to $V_{\text{rect}}$. The couplings are constrained by $\beta_0 + 8\beta_V + 16\beta_{V'} = 1$ for a consistent definition of $g_0$ [63]. For classical improvement, the couplings are $\beta_0 = \frac{2}{7}$, $\beta_V = -\frac{1}{12}$, $\beta_{V'} = 0$. While classically $\beta_{V'} = 0$, it is generated at $O(g^2a^2)$ [64] but remains suppressed relative to $\beta_V$ [67]. To obtain an improved kinetic term $\hat{K}_I = \beta_{K0}\hat{K}_{KS} + \beta_{K1}\hat{K}_{2L}$, one includes the two-link term:
\begin{equation}
\hat{K}_{2L} = \frac{g_0^2}{a} \sum_{x,i} \text{Tr} \left[ L_i(x) \hat{U}_i(x) L_i(x + a\hat{\sigma}) \hat{U}_i^\dagger(x) \right]. \tag{4}
\end{equation}

$\beta_{K0,1}$ are constrained by $\beta_{K0} + \beta_{K1} = 1$ [66] for a consistent definition of $g_0$. Classical errors of $O(a^2)$ are cancelled when $\beta_{K0} = \frac{2}{5}$ and $\beta_{K1} = \frac{1}{5}$ [66]. Similar to $\hat{H}_{KS}$, the improved Hamiltonian can also be obtained from an improved action via the transfer matrix [65].

For the Lüscher-Weisz action [63], $a = 0.4$ fm lattices were found to have similar discretization errors to $a = 0.17$ fm lattices with the Wilson action [68]. Given that $\hat{H}_I$ is derivable from the Lüscher-Weisz action [65, 66], it is unsurprising that similar scaling is suggested by the limited studies in the Hamiltonian formalism [69]. Therefore, using $\hat{H}_I$ may require $\gtrsim g_0^d$ fewer qubits in realistic quantum simulations for a fixed discretization error compared to $\hat{H}_{KS}$.

So far, we have only discussed the classically-improved couplings. For determining the quantum-corrected couplings, a number of methods exist. Perturbative calculations of the couplings in the Hamiltonian formalism analogous to those in [63] could be obtained. To remove these $O(g^2a^2)$ errors, one should nonperturbatively tune the couplings via lattice computations. Part of the tuning can be done by resumming tadpole contributions [67, 70, 71]. As non-perturbatively determining the couplings on quantum computers will cost considerable resources, one may opt to extract them via the analytic continuation of classical computations [59].

While we occupy ourselves with the improvements to the gauge Hamiltonian, the $O(a)$ fermionic Hamiltonian should be improved as well. Many methods exist in the action formulations. Some preliminary work in formulating $1+1d$ improved fermions has been considered [72] but more work is required – particularly for the interesting case of chiral fermions.

We construct quantum circuits to implement the improvement terms in Eq. (3) and Eq. (4) for a generic gauge theory, using the primitive gates acting on group element registers [73]: the inverse gate $U^{-1}$, the left/right product gates $U^L/R$, the trace gate $V_T$, the Fourier transform gate $V_F$ and a phase gate $U_{\text{phase}}$. The improved potential term includes the square Wilson loops $\hat{P}_{ij}(x)$ for every individual plaquette and the rectangle ones $\hat{R}_{ij}(x)$ for every neighboring two plaquettes in the spatial lattice. The group element basis $|U\rangle$ diagonalizes both $\hat{P}_{ij}$ and $\hat{R}_{ij}$. Optimal quantum circuits depend on the underlying architecture – in particular connectivity. We present the quantum circuits that only require register connectivity between every pair of links sharing one common site (linear register connectivity). The circuit for the rectangle one $U_{\text{rect}} = e^{-i\theta \text{Re Tr} \hat{R}_{ij}(x)}$ is shown in Fig. 2, with the coupling and trotter step information encoded in the parameter $\theta$. The same circuit as Fig. 2 with registers $U_2, U_3, U_4$ replaced by $U_2', U_3', U_4'$ in Fig. 1 implements $U_{\text{phase}}$. The circuit for the unimproved potential term can be constructed similarly to that in Ref. [73] but with linear register connectivity.

The unimproved kinetic term can be implemented by $U_{\text{phase}}$ in the Fourier basis which diagonalizes $\hat{L}_i^2(x)$ [73]. To construct a circuit for the two-link term $\hat{K}_{2L}$ in Eq. (4) and avoid dealing with $L$ and $U$ operators simultaneously,
we will rewrite it using the right electric field operator [38]:
\[
\hat{R}_t(x) \equiv \hat{U}_i(x) \hat{L}_i(x) \hat{U}_i(x) = \hat{R}_{t_0}^b(x) T_b,
\]
\[
\hat{R}_t^b(x) = 2 \text{Tr}[\hat{U}_i(x) \hat{L}_i(x) \hat{U}_i(x) T_b].
\] (5)

With \(\hat{R}_t(x)\), we can then construct \(\hat{K}_{2L}\) term by term as
\[
\hat{K}_{2L} = \frac{g_2^2}{a} \sum_{x,i} \text{Tr}[\hat{R}_t(x) \hat{L}_i(x + a\vec{i})],
\] (6)

where summands commute.

For simplicity, we denote the two succeeding links in one direction as \(U_1\) and \(U_2\) following Fig. 1. For Abelian gauge theories, \(\hat{R}_t(x) = \hat{L}_i(x)\), \(\hat{R}_t \hat{L}_2\) can be straightforwardly implemented in the Fourier basis. There are at least two obstacles in non-Abelian gauge theories. Firstly, \(\hat{R}_t \hat{L}_2\) with different \(c\) do not commute, and Hamiltonians as sums of non-commuting terms are in general difficult to implement. Secondly, for a generic discrete non-Abelian group, although \(\hat{L}_2\) is easy to define through the group Fourier transformation, for \(\hat{L}_c\) it is less clear. We can bypass both obstacles by decomposing \(\hat{R}_t \hat{L}_2\) as
\[
\text{Tr}(\hat{R}_t \hat{L}_2) = \frac{1}{2} \text{Tr}[\hat{L}_2^2 + \hat{R}_t^2 - (\hat{L}_2 - \hat{R}_t)^2].
\] (7)

With \(\hat{R}_t^2 = \hat{L}_2\), the first two terms can be absorbed into \(\hat{K}_{KS}\) by taking \(\beta_{K0}\) to \(\beta_{KK} + \beta_{KL} = 1\). Thus, for \(\hat{K}_t\) the only new term is \(\text{Tr}(\hat{L}_2 - \hat{R}_t)^2\), which commutes with \(\hat{U}_1 \hat{U}_2\). Defining the evolution operator \(U_{K_{2L}} \equiv e^{i\theta \text{Tr}(\hat{L}_2 - \hat{R}_t)}\), the matrix elements \(\langle U_1, U_2 \rangle U_{K_{2L}} [U_1, U_2]\) are only non-zero for \(U_1^* U_2 = U_1 U_2\). We can write down the following expression:
\[
\langle U_1, U_2 \rangle U_{K_{2L}} [U_1, U_2] = \delta(U_1^* U_2 - U_1 U_2) \mathcal{A}(U_1, U_2, U_1^*).
\] (8)

By integrating over \(U_2^*\) and changing the variable \(U_2^*\) to \(V \equiv U_2^{-1} U_1^{-1} U_1 U_2\), we can determine \(\mathcal{A}(U_1, U_2, U_1^*).\)

Using the invariance of the Haar measure and the property \(\langle U_1, U_2 \rangle = \langle U_1^* U_2 \rangle e^{i\alpha L_2^z}\), we have:
\[
\mathcal{A}(U_1, U_2, U_1^*) = \langle U_1^*, U_2 \rangle \int dV e^{i\alpha L_2^z} U_{K_{2L}} [U_1, U_2].
\] (9)

The integral over all group transformations \(\int dV e^{i\alpha L_2^z}\) is equivalent to projecting the \(U_2\) register to the ground state of \(\hat{L}_2^z\) \((J_2 = 0)\) up to a normalization factor fixed to be consistent with \(\int dV = |G|^2\) [74]:
\[
\int dV e^{i\alpha L_2^z} = |G| |J_2 = 0 \rangle \langle J_2 = 0 | = |G| \hat{P}_{J_2=0}.
\] (10)

Substitute Eq. (10) into Eq. (9) and notice that, as \(U_{K_{2L}}\) commutes with \(\hat{R}_t^2\), it conserves the quantum number \(J_2\), and therefore, \(\hat{P}_{J_2=0} U_{K_{2L}} = \hat{P}_{J_2=0} U_{K_{2L}} \hat{P}_{J_2=0}\). Insert another \(\hat{P}_{J_2=0}\) after \(U_{K_{2L}}\) in Eq. (9) and we find \(\mathcal{A}\) is:
\[
\mathcal{A}(U_1, U_2, U_1^*) = \langle U_1^*, U_2 \rangle \int dV e^{i\theta \text{Tr} \hat{R}_t^2} |U_1\rangle.
\] (11)

Using Eq. (11), the circuit in Fig. 3 implements Eq. (8) by first storing the conserved quantity \(U_1 U_2\) in the \(U_2\) register via \(U^L_2\), and then performing \(e^{i\theta \hat{R}_t^2}\) on \(|U_1\rangle\) with the sequence \(U_2^U_2 U_{\text{phase}} U_F\) gates. Finally, we multiply back to ensure the conserved product using the information stored in \(|U_2\rangle\) via \(U_{-1} U_s U_{-1}\).

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Gate & \(K_{KS} + V_{KS}\) & \(K_{2L} + V_{\text{rect}}\) \\
\hline
\(U^F\) & 2 & 2 \\
\(U_{\text{phase}}\) & 1 & 1 \\
\(U^V\) & \(\frac{d-1}{2}\) & \(d-1\) \\
\(U_{-1}\) & 3(d-1) & 2 + 8(d-1) \\
\(U_s\) & 6(d-1) & 4 + 20(d-1) \\
\hline
\end{tabular}
\caption{Number of primitive gates per link register in \(d\) spatial dimensions, for a single trotter step neglecting boundary effects.}
\end{table}

While using \(\hat{H}_t\) should require \(\gg 2^d\) times fewer qubits, it requires more gates per link register. Since the dominant quantum errors today are the \(O(10^{-2})\) two-qubit gate error rates and decoherence [75–77], this increased cost may lead to consternation. We list the gate costs for a general gauge group in terms of primitive gates in Tab. I for one trotter step using both \(\hat{H}_{KS}\) and \(\hat{H}_t\). Studies of \(Z_N\) and \(D_N\) [78] suggest that different primitive gates take approximately the same order of entangling native gates. Depending on which primitive gates dominate the circuits, the gate cost for \(\hat{H}_t\) is 2 to 4 times that of \(\hat{H}_{KS}\) for the same number of qubits. Since \(\hat{H}_t\) should require \(\gg 2^d\) fewer qubits, for the interesting cases of \(d = 2, 3\) we anticipate the same or fewer total gates to be required.

For \(Z_2\) gauge theory, \(\hat{H}_t\) can be mapped to Pauli matrices. Choosing the computational basis to be the group element basis, \(\hat{U} = \hat{\sigma}^+\) and \(\hat{L} = 1 - \hat{\sigma}^+\). Thus \(U_s\) is the CNOT gate. \(U_{-1}\) is \(\hat{I}\), and \(U_F\) is the Hadamard gate. With these primitive gates, the circuit implementation for the \(U_{\text{rect}}\) and \(U_{K_{2L}}\) are found in Fig. 4a and Fig. 4b respectively.

One should ask what existing quantum errors are and what are required to benefit despite the additional circuit depth. As a test case, we implement the most expensive
$Z_2$ gate, $U_{V_{rect}}$, on the 7-qubit ibm.perth device (Fig. 4c) and study its fidelity. The connectivity of ibm.perth prevents implementing $U_{V_{rect}}$ exactly as shown in Fig. 4a and a transpiled version of the circuit with 12 CNOTs and 20 additional one-qubit gates is used.

We consider the quantum fidelity metric $F_q = \frac{1}{N} \sum_n^N \text{Tr} |\Psi_n U_{V_{rect}} \Psi_n|^2$ where the summands are defined as $F_q^{(n)}$. For a noiseless simulation, each $F_q^{(n)} = 1$ because the state preparation and $U_{V_{rect}}$ are exactly cancelled by their complex conjugations, and thus the entire circuit is simply $I$. Alas, accurately determining $F_q$ is prohibitively expensive since it requires summing over all possible $|\Psi_n\rangle$ – including entangled ones which introduce additional CNOT errors [79]. Therefore we consider a restricted set of unentangled initial states $|\Psi_n\rangle = \prod_i H_{m_i} |0000000\rangle$ where $n$ indicates the number of qubits to which a Hadamard gate is applied. The strongly coupled vacuum state of $Z_2$ corresponds to $|\Psi_0\rangle$. Taking the reported CNOT error rate of 2% [75–77] and assuming the CNOT errors are incoherent and state-independent, for $U_{V_{rect}}$ one bounds the fidelity $F_q \lesssim (0.98)^{12} = 0.78$. Evolving a two-plaquette lattice by $\hat{H}_I$ for a single trotter step, $U_δ$, requires at least 28 CNOTs and thus an upper bound of $F_q^δ \lesssim (0.98)^{28} = 0.56$.

In fact, the CNOT errors are expected to be dominated by coherent noise. To mitigate this, we implemented Pauli twirling [80–84] which allows us to convert coherent errors from various noise channels into random errors in Pauli channels and has found success in low-dimensional lattice field theories [85]. To do this, we modified the circuit by wrapping each CNOT with a set of Pauli gates $\{I, X, Y, Z\}$ randomly sampled from sets which satisfy

$$\left( \prod_i (\sigma_i^b)^{\delta_i} \right) \text{CNOT} \otimes 1_4 \left( \prod_i (\sigma_i^a)^{\delta_i} \right) = \text{CNOT} \otimes 1_4,$$

(12)

where the $i$-th qubit (including spectators) was rotated by $\delta_i^{a,b}$ before the CNOT and by $\delta_i^{a,b}$ after. For our 24-CNOT $U_{V_{rect}}$ circuit there are 16 ways to twirl the target and control qubits, and 4 ways to twirl the 4 spectators, so $(16 \times 4^4)^2 = 10^8$ possible circuits. Prior work found that sampling $O(10)$ circuits was sufficient [80], thus we ran 15 unique circuits each with $N_{shots} = 2^{13}$. We also computed $F_q^{(6)}$ without Pauli twirling to gauge its effect.

In the zero-noise limit, the expected measurement for all $|\Psi_n\rangle$ should be all shots in the $|0000000\rangle$ state. Thus, we can infer information about the noise by comparing the probability of measuring this state to all others. One way to group the data is by the number of 1-bits observed – the Hamming weight $w_H$. We present results for these probabilities $P(w_H)$ for selected $|\Psi_n\rangle$ in Fig. 5. In the noise-dominated limit, one expects all states are equally populated with $P(w_H) \propto 6^{-w_H}$. For the $n = 6$ state without Pauli twirling ($|\Psi_6\rangle_{noPT}$), we observed that $P(w_H)$ is indistinguishable from the noise-dominated limit while all the Pauli-twirled results are skewed toward the noise-less result, with states of lower $w_H$ (and consequently less average entanglement) being closer to the desired value.

Our measured $F_q^{(n)} = \sqrt{P(w_H = 0)}$ from ibm.perth are presented in Table II. Comparing the results for $|\Psi_0\rangle$ with and without Pauli twirling we observe a fourfold improvement in fidelity – clearly demonstrating the advantage gained from this error mitigation. Together these results yield $F_q = 0.550$ for $U_{V_{rect}}$.

Using this refined upper bound on $F_q$, we can estimate $F_q^δ \lesssim 0.25$ based on it containing $\frac{16}{15}$ more CNOTs. This low $F_q^δ$ suggests that while current devices are inadequate for dynamics, a two-plaquette $Z_2$ lattice appears possible in the next two years given the expected hardware improvements [44–46], allowing for direct comparisons.
TABLE II: Measured state-dependent quantum fidelities with and without Pauli twirling.

| \( |\Psi_0\rangle \) | \( |\Psi_1\rangle \) | \( |\Psi_2\rangle \) | \( |\Psi_3\rangle \) | \( |\Psi_4\rangle \) | \( |\Psi_5\rangle \) | \( |\Psi_6\rangle \) _no PT |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0.650          | 0.575          | 0.605          | 0.599          | 0.579          | 0.442          | 0.425          | 0.1194         |

between Hamiltonians. Alternatively, classical simulators could explore larger lattices up to \( 7^2 \) [86].

In this letter, we designed the quantum circuits for simulating the Symanzik-improved Hamiltonian. In comparison to \( \hat{H}_{KS} \), \( \hat{H}_1 \) should allow quantum simulations with \( \gtrsim 2^d \) fewer qubits. With this reduction, we expect the gate count is comparable or less than that for \( \hat{H}_{KS} \) for theories with \( d \geq 2 \) despite increases of gate costs per link. For near-term numerical demonstrations, we constructed the circuits for \( \hat{H}_1 \) of the \( \mathbb{Z}_2 \) gauge group and found that for \textit{ibm} _pert the fidelity of the 12 CNOT with and without Pauli twirling.

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<th>( \hat{H}_{KS} )</th>
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<td>0.650</td>
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<td>0.605</td>
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<td>0.579</td>
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<td>0.425</td>
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Our results suggest that alongside hardware improvements, improved Hamiltonians can accelerate quantum simulations by years, with optimistic prospects for \( 2 + 1d \) \( \mathbb{Z}_2 \) simulations in the near future.

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[34] H. Liu and S. Chandrasekharan, Qubit Regularization and Qubit Embedding Algebras (2021), arXiv:2112.02090 [hep-lat].


