Tailoring non-Abelian lattice gauge theory for quantum simulation

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The prepotential formulation of non-Abelian lattice gauge theories is a promising paradigm for digital quantum simulation due to its gauge invariant basis, its integer-valued towers of states, and the simple action of the Hamiltonian in this basis. In this letter, we introduce matter into a general framework – valid in any dimension – that casts all Gauss law constraints into Abelian form. We explicitly solve one problem of practical importance by constructing Gauss law oracles for SU(2) theories, which can help filter out unphysical errors in a simulation.

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Introduction. Quantum computation is expected to efficiently simulate quantum mechanical many-body problems [1–4], as they can handle the exponential growth of information in entangled quantum systems that overwhelms classical computers. For lattice gauge theories (LGTs), quantum computers offer hope for ab initio studies of non-zero density, topological properties, and real-time phenomena [3][10], which are exponentially hard to solve classically due to sign problems [11–13]. However, with the limitations faced by near-term quantum devices, especially in the NISQ era [14], it is crucial that LGTs be formulated economically and tailored to the capabilities of quantum devices [15–18].

Non-Abelian LGT is conventionally constructed in terms of a local Hamiltonian and a Hilbert space of group representation states, supplemented by a non-Abelian Gauss law for gauge invariance [19, 20]. States in the Hilbert space are predominantly unphysical, and a noisy quantum computer would get lost among them. In order to remove gauge redundancy, one must impose Gauss’s law, which is nontrivial on a quantum computer as its color components are not simultaneously diagonalizable. Apart from that, the different representations to be mapped onto a register of qubits are on different footings under (and mixed by) the action of the Hamiltonian; crafting the action of the Hamiltonian in terms of quantum computer operations – though straightforward in principle – seems rather unnatural to do. In constrast, the prepotential formulation of LGT uses gauge invariant towers of states, characterized by integer quantum numbers. The Hamiltonian acts as a sum of ladder operators on those towers of states, which seems far more natural to digitize using qubits.

Unlike conventional loop formulations of LGTs, where the manifestly gauge invariant Hilbert space suffers from non-locality and a proliferation of loop and string states, prepotentials [21, 22] give an equivalent formulation of Hamiltonian LGT in terms of local gauge invariant operators and states. An exact and orthonormal basis is obtained via a set of local constraints, namely, Abelian Gauss law constraints and Mandelstam constraints. However, Mandelstam constraints are nonlinear, which would have been cumbersome to enforce on a register of qubits. A new variant of the prepotential formulation [20, 27] circumvents that problem.

In this letter, we construct a theoretical framework based on prepotentials that could define a whole new paradigm in digital quantum simulations of non-Abelian gauge theories, making them a reality sooner. We introduce matter into the already existing prepotential formalism in 2D SU(2) gauge theory and then generalize to 3D. The local algebraic structure of this framework is equally simple in any dimension. We particularly show how Gauss law’s and the Hamiltonian dynamics bear a closer resemblance to their U(1) cousins, presenting the novel opportunity for SU(2) simulations to benefit from algorithmic developments made for U(1) theories. As a first exploration of the advantages, we construct oracles for testing physicality of states that are strikingly similar to those in Abelian gauge theories [25]. In 3D, the SU(2) oracles are actually simpler than their U(1) counterparts.

Hamiltonian formulation. A lattice Hamiltonian for SU(2) gauge theory coupled to fundamental matter, using units where the lattice spacing a = 1, may be formulated as [29]

\[
\hat{H} = g^2 \sum_{(x,i)} \hat{E}^2(x,i) + \frac{1}{4a^2} \sum_{x,\square} \text{Tr}(2 - \hat{U}_\square - \hat{U}_\square) \\
+ \sum_{(x,i)} \hat{\psi}^\dagger(x) \hat{U}(x,i) \hat{\psi}(x + e_i) + m \sum_{x} (-)^x \hat{\psi}^\dagger(x) \hat{\psi}(x).
\]

Left and right color electric fields \(\hat{E}_{L/R}^a\) (\(a = 1, 2, 3\)) both form SU(2) Lie algebras. Along with the link operators \(\hat{U}\) (2 × 2 operator matrices) defined on links \((x, i)\), they
The Gauss law operators at any site \( x \) are
\[
\hat{G}^a(x) = \sum_{i=1}^{d} (\hat{E}_{L,i}(x) + \hat{E}_{R,i}(x)) - \frac{1}{2} \hat{\psi}^\dagger \sigma_{\alpha\beta} \hat{\psi}(x),
\]
and physical states are those annihilated by every \( \hat{G}^a(x) \).
In order to have \( [\hat{H}, \hat{G}^a] = 0 \), the gauge invariant Casimirs \( \hat{E}^2 = \hat{E}_L^2 + \hat{E}_R^2 \) and plaquette operators \( \hat{U}_T \) (products of link operators around elementary loops) appear in \( \hat{H}_E \) and \( \hat{H}_B \). The matter Hamiltonian \( \hat{H}_M \) describes staggered fermions coupled to the gauge field \( \hat{U}_{a\beta} \) in a gauge invariant combination, plus a fermion mass term. Solutions to Gauss’s law describe gauge invariant, non-local loop and string states, but these form an overcomplete basis. Mutually dependent loops satisfy Mandelstam constraints \([30,32]\), which are non-local and notoriously hard to solve.

In the prepotential formulation \([21,23]\), \( \hat{U} \) and \( \hat{E} \) are replaced by bilinears of harmonic oscillator doublets \( \hat{a}^\dagger_a(L/R) \) (the “prepotentials”) at each end \( L \equiv x \) and \( R = x + e_i \) of every link \( (x,i) \) as
\[
\hat{E}_L^a = \frac{1}{2} \hat{a}^\dagger_a(L) \sigma^a \hat{a}(L) , \quad \hat{E}_R^a = \frac{1}{2} \hat{a}^\dagger_a(R) \sigma^a \hat{a}(R),
\]
\[
\hat{U} = \frac{1}{\sqrt{n_L + 1}} \left( \begin{array}{c}
\hat{a}_1^\dagger(L) \\
\hat{a}_2^\dagger(L) \\
\hat{a}_1(L) \\
\hat{a}_2(L) \\
\end{array} \right) \frac{1}{\sqrt{n_R + 1}} = U_L U_R.
\]
where \( n_L = (n_R) \) is the total occupation number for prepotentials at the left (right) end of link \( (x,i) \). With these definitions, \([\hat{U}] \) follows along with \( \hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = 1 \). Moreover, using \([\hat{U}] \) one can show that \([\hat{U}_{a\beta}, \hat{U}_{\gamma\delta}] = [\hat{U}_{a\beta}, \hat{U}_{\gamma\delta}] = 0 \). Since the SU(2) representations situated at the ends of a link must have the same Casimir \( \hat{E}_L \equiv \hat{E}_R \), there is an Abelian Gauss law constraint on each link:
\[
n_{L}(x,i) = n_{R}(x,i).
\]
In terms of prepotentials, the link operator is broken into a left part \( U_L \) and a right part \( U_R \), denoting the SU(2) group to be localized at each end. In \([\hat{U}] \), the staggered fermions, which are SU(2) doublets, also live on lattice sites. Thus, the prepotential operators and the matter fields can all be uniquely associated with sites and they transform in the same way. (The essential difference between matter and prepotentials is their statistics.) This feature enables one to construct local SU(2) invariants combining both prepotentials and matter, resulting in a local loop (SU(2) invariant) basis. The local loop states, together with flux flowing along the links following the Abelian Gauss law \([\hat{U}] \) yield non-local Wilson loops.

In the next section we discuss the local loop and string states in the simplest case of 1D with fundamental matter.
The last two actions give rise to dynamical pair production and string breaking phenomena, which can be simulated locally. Any other state is annihilated by the matter field in the string operators.

**2D lattice** Prepotential formulation of pure SU(2) gauge theory on a 2D lattice has been studied in great detail in [21][25]. This particular formulation yields local loop basis, however, that is again overcomplete and are associated with Mandelstam constraints in a local form. Solving these constraints is nontrivial and becomes increasingly difficult in higher dimensions.

In a recent development [26][27], a virtual “point splitting” of lattice sites in 2D was found to be particularly useful, as it bypasses the Mandelstam constraints and casts all constraints of the theory into the Abelian form of $[3]$. Below, we show that coupling to matter and generalizing to higher dimensions introduces minimal extra complication in this framework. This seems a vital step toward building digital quantum simulators for 3D non-Abelian LGTs, which has never been attempted so far.

**Virtual hexagonal lattice with matter.** A virtual splitting of a lattice site is shown in Fig. 2. In 2D, point splitting results in a hexagonal lattice. One can now formulate prepotentials on this virtual hexagonal lattice as in [4] and [5]. On this hexagonal lattice, physical lattice directions are along 1 and 2, and only the electric fields along these two directions contribute to $\hat{H}_E$. However, in $\hat{H}_B$, the elementary loops are indeed hexagonal plaquettes. The matter field, originally at sites $x$ of the square lattice, now lives on sites $x_m$, as shown in Fig. 2. This is the middle of the virtual link along 3. We treat the sites $x', x''$ on the same footing as in pure gauge theory [20] (to be explained below), whereas $x_m$, being connected to only two virtual links, is effectively handled as a site on a 1D lattice as in Fig. [4].

**2D pure gauge theory.** At each site $x$ (standing for either $x'$ or $x''$) of the hexagonal lattice, links emerge in three directions, labeled as 1, 2, 3. Each link is associated with prepotential creation and annihilation operators $\{\hat{a}_\alpha^\dagger(x, i), \hat{a}_\alpha (x, i)\}$ for $i = 1, 2, 3$ and $\alpha = 1, 2$. Using $[3]$ in $\hat{H}_B$, one obtains the following gauge invariant operators and their conjugates at each site,

$$\hat{L}^+_{ij} = \hat{a}_\alpha^\dagger(i)\hat{a}_\alpha(j) \quad \hat{L}^-_{ij} = \hat{a}_\alpha(i)\hat{a}_\alpha^\dagger(j) \quad (11)$$

Above, $\hat{a}_\alpha^\dagger \equiv \epsilon^{\alpha\beta\gamma}\hat{a}_\beta^\dagger$, $\hat{a}_\alpha \equiv \epsilon_{\alpha\beta\gamma}\hat{a}_\beta$, and $i, j$ are direction indices with $i \neq j$. It is clear from the definitions that when acting on $|0\rangle$ only $\hat{L}^+_{ij}$ is non-zero and will build up the local loop Hilbert space. For the 2D hexagonal lattice, the local loop space is characterized by three independent linking numbers $l_{ij}$ (cf. Fig. 2) denoting the flux flowing along three $(ij)$ directions $(12, 23, 31)$. The action of these operators on a general orthonormal loop state,

$$|l_{12}, l_{23}, l_{31}\rangle \equiv \frac{(\hat{L}^+_{12})^{l_{12}}(\hat{L}^+_{23})^{l_{23}}(\hat{L}^+_{31})^{l_{31}}}{(l_{12} + l_{23} + l_{31})!} |0\rangle , \quad (12)$$

is given by

$$\hat{L}^+_{ij}|l_{ij}\rangle = \sqrt{(l_{ij} + 1)(l_{12} + l_{23} + l_{31} + 2)}|l_{ij} + 1\rangle , \quad (13)$$

$$\hat{L}^-_{ij}|l_{ij}\rangle = \sqrt{l_{ij}(l_{12} + l_{23} + l_{31} + 1)}|l_{ij} - 1\rangle , \quad (14)$$

$$\hat{L}^-_{ij}|l_{ij}\rangle = -\sqrt{l_{ik}(l_{jk} + 1)}|l_{ij} - l_{jk} - 1, l_{ik} + 1\rangle . \quad (15)$$

These simple local loop actions, glued together along the links following [4], reproduce the non-local loops and strings of the original theory. Moreover, these loop operators now act more like their U(1) counterparts: loop operators in U(1) theories shift $E$ by unit increments along infinite tower of states, although there the normalization factor is always trivial.

**2D lattice with matter.** Putting matter at site $x$ corresponds to putting matter at the middle of the virtual 3–3 link in the point-split picture. As indicated by Fig. 2 the gauge invariant Hilbert space associated with the virtual sites is as follows: (i) The two sites $x', x''$ have only loop states $|l_{12}, l_{23}, l_{31}, x', x''\rangle$, being treated identically as in pure gauge theory. (ii) The third virtual site $x_m$ along the 3–3 direction contains both local loop and string states $|l_{33}, s_3, s_3\rangle$, being structurally identical to a site with matter in 1D. (iii) The Abelian Gauss laws along the three directions of the hexagonal lattice are

$$n_1(x) = n_1(x + e_1) , \quad n_2(x) = n_2(x + e_2) , \quad (16)$$

$$n_3(x) + s_3 = n_3(x + e_3) + s_3 , \quad (17)$$

where $n_1 = l_{12} + l_{33}$, $n_2 = l_{12} + l_{33}$, and $n_3 = l_{23} + l_{33}$ count prepotential occupation numbers at each site.

The structure of the 2D theory with matter is therefore equivalent to pure gauge theory in 2D, plus gauge fields coupled to matter in 1D.
3D lattice with matter. The same scheme would continue as one generalizes to any arbitrary dimension. For example, in 3D, each site splits into four three-point vertices and matter is added at another intermediate two-point vertex, as shown in Fig. 3. As shown for 2D, the local loop Hilbert space remains identical (three linking numbers) to the pure gauge theory on all virtual sites in Fig. 3. Matter is added at the middle of one virtual link, i.e., along 5 – 5 in Fig. 3 such that the gauge invariant Hilbert space at the additional site has two string numbers and one loop number, just like the 3 – 3 links in the 2D or 1 – 1 links in 1D. The modified Abelian Gauss laws on the 3D lattice are

\[ n_i(x) = n_i(x + e_i), \quad (i = 1, 2, 3, 4, 6) \] (18)
\[ n_5(x) + s_5 = n_5(x + e_5) + s_5. \] (19)

This scheme generalizes straightforwardly to any arbitrary dimension. All of these can be checked straightforwardly on a quantum computer using oracles described below.

Physicality oracles for SU(2) gauge theory. In Fig. 4(a) we construct an oracle for checking the Abelian Gauss law constraints along a link. We define \( F = 1 \) if the link satisfies Gauss’s law and \( F = 0 \) otherwise. The circuit specifically considers \( |l_{ij}\rangle \), i.e., a 3 – 3 link in 2D with matter. Here, \( |l_{ij}\rangle \) means an \( N \)-qubit binary number in the computational basis. \( s_3 \) acts as an incoming “carry qubit” \( s_3 \) to the addition subroutines \( A \), which can have the effect of adding one unit to the overall sum \( l_{31} + l_{23} (l_{31} + l_{33}) \) [cf. Fig. 4(b)]. The sums on each side of (17) are then compared bit-wise by a string of \( N \) CNOTs, as displayed in Fig. 4(c). A conditional phase -1 is applied if and only if they are identical (\( F = 1 \)). An auxiliary query qubit \( |q\rangle \) is flipped if \( F = 1 \), and the remaining gates restore the qubit registers to their original configurations. Matterless links would have \( |s_{3/3}\rangle \rightarrow |0\rangle \) and the appropriate \( l_{ij}'s \) as inputs in order to check (16). For 3D, again the only difference is the input \( l_{ij}'s \) and \( s_i's \), implying that the same simple routine can indeed check all the constraints that define a physical loop configuration in SU(2) lattice gauge theory, in any dimension. For \( N \)-qubit link registers, the oracle can be constructed using no more than \( 17N + 5 \) CNOTs, 8N Toffolis, and the \( C^N(Z) \) gate \( 34 \). This is likely to involve far less \( T \) gates than any Trotter step unless \( N = 1 \).

These routines are likely to be useful in digital simulations because non-gauge invariant errors can easily arise from the Trotter approximation to \( e^{-it_H} \) or from quantum noise \( 28 \). Previously these were only constructed for Abelian theories. Because our framework has cast all constraints into an Abelian form, we can benefit from the same techniques. An analogous construction using the conventional group representation states is much less straightforward because different components of the non-Abelian Gauss law operator are not simultaneously diagonalizable. Constructing physicality oracles for SU(3) is a goal for future work.

Discussion. We see several virtues of using the prepotential framework for simulating lattice gauge theories. The immediate benefit is that non-Abelian gauge redundancy is absent in the constructed Hilbert space, enabling one to attain a higher cutoff on the physical Hilbert space than when working with all the redundant gauge degrees of freedom. Abelian Gauss law constraints are still required on the links, but these can be validated straightforwardly by constructing Gauss oracles for SU(2), in any dimension. Another virtue is working with infinite towers of states rather than multiplets of varying dimensions, so it is far more obvious how to truncate to some dimensionality that is a power of two and map them onto qubits. Operating on towers of states more closely resembles U(1) gauge theory, so it is conceivable that other algorithms developed for Abelian theories can also be ported over to SU(2).

We have noted that the point splitting technique increases the number of links to be simulated and that plaquette operators must deal with more links; it is our hope and expectation that this drawback is outweighed by the simpler action of individual link operators in a plaquette. Our construction nonetheless stands to more directly benefit from any progress made in algorithms for implementing U(1) plaquette operators.

The framework presented in this letter can be generalized to SU(3) using \( 24 \), as we have not explicitly relied on knowing any Clebsch-Gordon coefficients specific to SU(2). Generalizing this work to SU(3) will no doubt be a milestone towards quantum simulation of lattice QCD. Our immediate goal is to characterize the simulation of time evolution using prepotentials, which we expect to do by Trotterization. The work in this direction is in progress.

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FIG. 3. One site \( x \) on a 3D square lattice is virtually split into four sites \( x', x'', x''' \equiv x''' \) connected by three intermediate links in virtual directions 4 – 4, 5 – 5, and 6 – 6. Matter is added on direction 5 – 5 at site \( x_m \).
FIG. 4. (a) A routine for measuring physicality, i.e., the Abelian Gauss law, in our framework. The qubit registers correspond to a $3 \times \overline{3}$ link in 2D with matter. The net effect is that the “query” qubit $|q\rangle$ is flipped if and only if the configuration physical.

(b) A generic adder circuit $A$ for $(y, z) \rightarrow (y, z + y)$. Adder circuits taking an incoming carry bit $c_0 = 0, 1$ can compute $z + y + c_0$ using exactly the same gates that compute $z + y$.

(c) $N$ CNOTs are used to compare two $N$-bit numbers $y$ and $z$.