



Quantum simulations of lattice field thoeries

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The last several years have seen a massive resurgence of interest in the Hamiltonian simulation of relativistic lattice field theories from the nuclear and high energy physics community. This renewal has largely been driven by rapid advancements in quantum computing hardware and increased access to real quantum computers, not just simulators on classical machines. However, significant breakthroughs in hardware and software must occur to develop fault-tolerant quantum computers, which will most likely be necessary for simulations of physically-relevant nuclear systems. In the meantime, there are many theoretical and algorithmic roadblocks to overcome in order to implement gauge theories onto quantum computers. In this plenary, I present a broad overview of digital quantum simulation, including methods and status of current hardware architectures, followed by a description of the challenges faced when simulating lattice gauge theories on quantum computers.

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1. Introduction and Motivation

The Standard Model of Particle Physics, encapsulating the vast majority of our understanding of the fundamental nature of our Universe, is at its core a gauge theory. Much of the richness of its phenomenology can be traced back to the complicated interplay of its various gauged interactions. Thus, studying the properties of strongly coupled theories from first principles is necessary to fully understand the Standard Model. In particular, Quantum Chromodynamics (QCD), which provides a precise and quantitative description of the strong nuclear force over a broad range of energies, is a strongly coupled gauge theory. Therefore, *ab-initio* calculations are crucial for comparing theoretical predictions of the Standard Model to experimental results. Additionally, due to its strongly coupled nature, this theory gives rise to a complex array of emergent phenomena that cannot be identified from the underlying degrees of freedom. While massive theoretical and algorithmic developments in classical computing have allowed us to probe many of these aspects, there remain a plethora of open questions that do not seem amenable to these methods. For example, the determination of the phase diagram of finite-density QCD and direct, nonperturbative calculations of real-time dynamics of hadrons are exponentially difficult to probe with classical computers due to the notorious sign problem. Even our knowledge of whether the electroweak gauge interactions in the Standard Model can be given a precise, nonperturbatively regularized definition using lattice field theory faces similar difficulties, as sign problems obstruct the verification of candidate regularizations of chiral gauge theories. With an inherently different computational strategy, digital quantum computers hold the promise of simulating quantum field theories from first principles without encountering sign problems. Through this, they would probe these and other fundamental questions of particle and nuclear physics, which currently seem inaccessible through existing classical computing techniques.

The revival of interest in quantum simulations of high-energy physics has been spurred by the rapid evolution of real-world quantum computers, with increasing size and decreasing noise. With large influxes of both intellectual and financial interests, impressive advances in both hardware and software are occurring on yearly timescales, paving the way towards fault-tolerant quantum computation. However, despite this progress, current machines are in the noisy intermediate-scale quantum (NISQ) era [1], characterized by systems of O(100) qubits, susceptible to various types of noise, networked together. Much progress must occur before the promise of fault-tolerant quantum computers can come to fruition; this progress is of key importance to high-energy physicists, as current resource scaling arguments indicate that 3 + 1 dimensional lattice QCD simulations at physical pion masses will require fault-tolerant quantum computers. Additionally, similarly to the early days of classical lattice QCD, there is an enormous amount of theoretical and algorithmic development that needs to occur before this novel computational strategy can be applied to real-word physics problem.

In these proceedings, I will provide a broad overview of the ideas behind quantum simulation, as well as the status, both current and near-term, of several different hardware architectures. I will then briefly discuss the Kogut-Susskind Hamiltonian formulation of an SU(N) lattice gauge theory [2], in order to highlight three key challenges that must be considered for the successful simulation of lattice gauge theories on quantum devices; note that addressing these problems is necessary but not sufficient for real-world simulations. Lastly, I will discuss an alternative formulation of



Figure 1: General schematic for quantum simulation. The precise details of how each of these four steps is carried out will depend heavily on both the experimental platform and the target theory.

an SU(2) lattice gauge theory to demonstrate possible approaches for implementing SU(N) lattice gauge theories onto quantum devices. Note that these proceedings, as well as the plenary on which they are based, are not meant to be an all-encompassing overview of the field. Instead, my goal is to provide a general introduction, suitable for colleagues who are not quantum computing experts, to some of the challenges and hurdles that we face on the path towards implementing the Standard Model onto quantum devices. The main take-away message I hope to instill is that this is a young and vibrant field with many interesting theoretical and algorithmic challenges ahead!

2. Introduction to Quantum Simulation

Quantum simulation is broadly defined as a protocol to manipulate quantum degrees of freedom plus an experimental platform that utilizes the collective quantum properties of the system for calculation. Said more plainly, quantum simulation involves manipulating quantum states in a specific way in order to mirror the properties of a specific target system. In general, this proceeds via three steps, regardless of the experimental platform. First, the quantum system must be initialized into the desired initial state, which is called initial state preparation. Then the system undergoes unitary time evolution. Lastly, measurement takes place. This entire process is repeated a large number of times, due to the probabilistic nature of the computational method. Once a sufficient number of simulations is carried out, post-processing analysis can occur. This general procedure is shown in Figure 1. Note that the use of 'unitary time evolution' carries a double meaning here. The first meaning is the canonical meaning used by physicists *i.e.* the evolution of a quantum system forwards in time. For example, to simulate a heavy ion passing through nuclear matter would require encoding the time-evolution operator for this specific physical process onto the experimental platform. The second meaning is more from the computer science perspective, in that any quantum algorithm is by definition a series of unitary operators acting sequentially. For example, quantum phase estimation [3] is a quantum algorithm that can be used to extract the ground state energies in quantum chemistry¹. While the quantum phase estimation algorithm is not the time-evolution operator of the quantum chemistry system, it is the unitary time evolution of the quantum experimental platform.

Of particular interest to the simulation of lattice gauge theories are two different approaches to quantum simulation: *digital* and *analog* quantum computing. The key difference between the two approaches is whether the unitary time evolution of the system is discrete or continuous. The digital approach is most similar to classical simulation, in that the time evolution of the desired

¹Please see Ref. [4] for an extensive overview of solving quantum chemistry problems on quantum computers.

theory is rewritten into a (quantum) circuit and the system evolves via the sequential application of discrete gates; it is of fundamental importance that this circuit run in reasonable time. In contrast, the analog approach constructs a quantum system that is "close" to the target theory and then the quantum system is simply allowed to evolve in time, given its own internal dynamics. Both of these approaches require approximating the time evolution operator of the target system, though the approximation methods (and the degree to which the error may be quantitatively bounded) do differ. Most of this plenary will focus on digital quantum simulation using circuit formulations, so we will first discuss this approach.

The computational strategy for digital quantum simulation is to construct a quantum circuit by acting on a collection of qubits with unitary operations. A qubit is, by definition, any two-state quantum system. The unitary operations, which generally act on one or two qubits at a time, are called gates, in analogy to classical computation. The benefit of digital simulation is that it offers a path towards a 'universal quantum simulator'. While there is much literature on how one precisely defines a quantum Turing machine, for the purposes of this plenary, I offer my colloquial definition: *a universal quantum computer is one that can simulate any theory, as long as said theory can be rewritten into a quantum circuit*. Therefore, much work is currently being devoted to rewriting lattice gauge Hamiltonians into quantum circuits; the benefit of this approach is that these quantum circuits should run on any digital quantum computer, regardless of the hardware architecture. It is important to note, however, that the resource cost may differ dramatically between different architectures and therefore the choice of architecture is of practical concern.

Many proposals for qubit hardware exist and there are benefits and downsides to each of these technologies. Three examples of qubit systems are shown in Figure 3. The first is superconducting loops, which build on existing semi-conductor technology; as semi-conductor technology is highly advanced, this approach has a great technological advantage. Unfortunately, due to the requirements of superconductivity, these qubits must be kept at O(mK). Additionally, due to the manner in which the qubits are controlled, networking together multiple superconducting qubits results in a system with two-to-two connectivity. This might prove quite limiting for simulations of lattice gauge theories, especially in formulations that are gauge fixed and thus contain non-local interactions. An alternative approach is to use trapped ions, which not only have a higher gate fidelity but can also be networked with all-to-all connectivity. One disadvantage is that the time it takes to carry out a single gate operation is significantly higher than for superconducting qubits. These systems must also be kept cold, but only at O(4K). One last example of qubit systems is diamond vacancies are quite difficult to entangle due to the limited range of their interactions.

For many of these proposals of qubit hardware, there now exist examples of 'real-world' quantum computers *i.e.* quantum systems of entangled qubits that can carry out various calculations. However, despite recent advancements, we are in NISQ-era, which is defined by having machines of O(100) qubits that are sensitive to various sources of noise, including bit flips, phase flips, decoherence and dephasing. In particular, current machines have gate error rates of $O(10^{-3})$, which implies that circuit depths cannot exceed O(100) gates before the measurement is pure noise. The path out of the NISQ-era and towards simulations of 3 + 1-dimensional QCD rests on two intertwined ideas: *quantum-error correction* and *fault-tolerant quantum computing*. The end goal of this is 'the protection of quantum information as it *dynamically* undergoes *computation*' [8]. To



(a) Roadmap for IBM's quantum computing efforts, which utilize superconducting qubits [5], released in September 2020. An updated roadmap was released in Dec. 2023 [6].



(**b**) Roadmap for IonQ's quantum computing efforts, which utilize trapped ions, released in December 2020. This roadmap includes the projected use of error-correction encoding to allow for logical qubits [7]

Figure 2: Near-term roadmaps for two different commercially-developed quantum hardware architectures.

give a sense of how much work remains to be done, the quantum simulation of 3 + 1-dimensional QCD at physical pion masses will likely require tens of millions of qubits and orders of magnitude many more gates.² Note that these qubits will need to be *logical* qubits and the gates *fault-tolerant*; logical qubits are abstract qubits that are acted upon as specified by a quantum circuit, built out of many physical qubits that are the actual quantum hardware; a similar idea holds for fault-tolerant gates. To give a sense of the current hardware capabilities, Figure 2 presents roadmaps for two different qubit technologies, as implemented in a commercial setting. The two technologies are superconducting loops, which are used by IBM, and trapped ions, used by IonQ.

As mentioned previously, there exists an alternative approach to digital quantum computers, namely analog quantum computers. In analog quantum computing, the computational strategy is to 'tweak' the natural degrees of freedom of a quantum system to mimic the behavior of a target model. I like to think of analog quantum computers as 'effective field theories made physical'. Analog simulators are incredibly useful, as not only do they allow for continuous time evolution with zero error in the time-evolution operator, but they can also simulate toy models not yet achievable on digital computers. The downside is that they are non-universal and so each target theory requires a somewhat different experimental set-up. Additionally it is not always clear how to quantify the errors that arise due to the experimental quantum system not being the same as the target theory; in particular, the time-evolution operator being simulated without error is not the exact time-evolution operator of the target theory. The name of the game for analog quantum simulation is finding a target

²One way of understanding this resource scaling is to assume that each spatial lattice site (for fermions) and each spatial lattice link (for gauge fields) will have at least one qubit associated with it; additionally assuming that quantum simulations for 140 MeV pions will require similar lattice volumes and spacings, a quantum simulation will require at least $O(10^7)$ qubits. Note that this number underestimates the number of qubits dramatically as non-abelian gauge theories will certainly require more than a single qubit per link. Circuit depth, which can be thought of as the number of gates that need to be run in series, is a bit more difficult to estimate, as it strongly depends on the specific Hamiltonian formulation. However, we can arrive at a rough scaling by noting that the magnetic component of the Hamiltonian will typically entail a sum over plaquettes. Since each plaquette includes four link variables and the same link variable will appear in multiple plaquettes, plaquette terms will generally need to be run in series and not in parallel. Therefore, the number of quantum gates will roughly scale with the number of plaquettes. Requiring at least six gates per plaquette (by assuming one two-qubit gate for each pair of links in the plaquette) will result in $O(10^7)$ gates. Both of these estimates are very rough and should be considered more as a motivating guideline than a rule.



Figure 3: Three examples of two-state systems that can be used for constructing qubits. Images are reproduced from Ref. [15], which offers a historical overview of recent advances in various qubit technologies.

theory that is both interesting and that can be successfully modeled in an experimental set-up. A good example of this is the 1+1 Ising Model. This model displays confinement, which is of obvious great interest. Additionally, this theory can be implemented on a variety of experimental set ups, including trapped ions and Rydberg atoms [9, 10]. In terms of implementing gauge theories onto analog devices, the key observation is that gauge theories emerge from simple condensed matter systems once local constraints are imposed; a high-energy physicists might say the inverse statement, that local constraints (Gauss' Law) naturally emerge from gauge theories. These two statements are, of course, complementary. For more in-depth overviews of analog quantum simulation of lattice gauge theories, see Refs. [11–14]

3. Hamiltonian Formulations of Lattice Gauge Theories

Due to an inherently different computational strategy, it is significantly more natural to use the Hamiltonian formulation when simulating physical systems on quantum computers. In contrast to classical simulations of path integrals, time is kept as a continuous variable and only the spatial dimensions are made discrete³. In order to ensure that Schrödinger's equation is gauge-invariant, the Hamiltonian for lattice gauge theories is derived in Weyl gauge, $A_0 = 0$. There is a long history of constructing Hamiltonians for lattice gauge theories, with the Hamiltonian for QCD first proposed in the 1970s in Ref. [2]. An explicit derivation from the partition function of lattice gauge theories, as defined by Wilson, is given in Ref. [18]; the derivation proceeds via the transfer matrix and requires that all temporal links are set to the identity.

Before delving into the non-Abelian Hamiltonian, let us first look at the Abelian version. In this case, the Hamiltonian is given by

$$\hat{H} = \frac{1}{2a} \left[g^2 \sum_{\ell \in links} \hat{E}_{\ell} \hat{E}_{\ell} + \frac{1}{g^2} \sum_{p \in plaquettes} \operatorname{Tr} \left(2I - \hat{P}_p - \hat{P}_p^{\dagger} \right) \right]$$
(1)

³Time is, additionally, made discrete when working with digital quantum computers and using Suzuki-Trotter methods for approximating the time-evolution operator [16, 17]. There are other approaches in which time is kept continuous and the time-evolution operator is approximated via different methods. However, all of these approaches require constructing a quantum circuit that uses discrete gates.





(a) The operators that appear in the Kogut-Susskind Hamiltonian are the electric link operators \hat{E}_{ℓ} and plaquette operators \hat{P}_p ; the plaquette operators are constructed out of gauge link operators \hat{U}_{ℓ} , which act as raising operators for the electric link operators.

(b) Example of a state that obeys Gauss's law, written in the electric basis. Assuming a positive orientation for each link (each link points in the positive \hat{x} or \hat{y} direction),the sum of the electric fields going into each lattice site is the same as the sum going out.

Figure 4: Abelian version of the Kogut-Susskind formulation of a gauge theory on a 3×3 lattice with periodic boundary conditions.

where \hat{E}_{ℓ} are electric link operators and \hat{P}_p are purely-spatial plaquette variables constructed out of gauge link variables, \hat{U}_{ℓ} ; see Figure 4a for an explicit mapping onto a two-dimensional spatial lattice. The variables E_{ℓ} and U_{ℓ} obey the commutation relations

$$\left[\hat{E}_{\ell}, \hat{U}_{\ell'}\right] = \hat{U}_{\ell} \delta_{\ell, \ell'} , \qquad (2)$$

which inform how these operators can be mapped onto qubits. More specifically, in order to simulate the time evolution of this system, it is necessary to decide on a specific basis in which to work. This choice is not unique and different bases will have different strengths and weaknesses; we shall come back to this point later. One possible basis choice is the electric basis, in which the electric link operators are all diagonal. In this basis, the operators are given by

$$\hat{E} = \sum_{\epsilon} \epsilon |\epsilon\rangle \langle \epsilon| \qquad \hat{U} = \sum_{\epsilon} |\epsilon + 1\rangle \langle \epsilon| \tag{3}$$

where we have suppressed the link index. In particular, this implies that the electric link operator has integer eigenvalues and the gauge link operator acts as a raising operator. In Figure 4b, we show one possible state of the system, using electric field eigenvalues; this state obeys Gauss' law as the sum of the electric fields going into any one lattice site is the same as the sum of electric fields going out.

The structure of the SU(N) Hamiltonian is quite similar, though now both the electric links and

the gauge links carry SU(N) color indices. The Hamiltonian is given by

$$\hat{H} = \frac{1}{2a} \left[g^2 \sum_{\ell \in links} \hat{E}^a_\ell \hat{E}^a_\ell + \frac{1}{g^2} \sum_{p \in plaquettes} \operatorname{Tr} \left(2I - \hat{P}_p - \hat{P}^\dagger_p \right) \right]$$
(4)

where the trace of the plaquette operator, in terms of gauge links, is

$$\mathrm{Tr}\hat{P}_{p} = \hat{U}_{ab}(n, e_{i})\hat{U}_{bc}(n + e_{i}, e_{j})\hat{U}_{cd}^{\dagger}(n + e_{j}, e_{i})\hat{U}_{da}^{\dagger}(n, e_{j})$$
(5)

where the plaquette p is specified by site index n and two directions, \hat{e}_i, \hat{e}_j . Note that due to the non-Abelian nature of this theory, the gauge links transform under gauge transformations as

$$\hat{U}(n,e_i) \longmapsto \Omega(n) \,\hat{U}(n,e_i) \,\Omega(n+e_i)^{\dagger} \tag{6}$$

i.e. gauge transformations at sites n and $n+e_i$ will affect the link via left and right group composition. This implies that there are two different translation operators that need to be defined, and therefore two different electric link operators. For simplicity, we define these electric link operators to be E_L^a and E_R^a , with each set of operators satisfying their own independent Lie algebra,

$$\left[\hat{E}_{L}^{a}, \hat{E}_{L}^{b}\right] = -if^{abc}\hat{E}_{L}^{c} \qquad \left[\hat{E}_{R}^{a}, \hat{E}_{R}^{b}\right] = if^{abc}\hat{E}_{R}^{c} \qquad \left[\hat{E}_{L}^{a}, \hat{E}_{R}^{b}\right] = 0.$$
(7)

As before, the commutation relations will inform how this Hamiltonian can be mapped onto a quantum device. For the SU(N) theory, we now have two different commutation relations correspond to left and right group composition

$$\left[\hat{E}_{L}^{a},\hat{U}_{mn}^{j}\right] = T_{mm'}^{ja}\hat{U}_{m'n}^{j} \qquad \left[\hat{E}_{R}^{a},\hat{U}_{mn}^{j}\right] = \hat{U}_{mn'}^{j}T_{n'n}^{ja},\tag{8}$$

where T^{ja} are the generators of the Lie group in the *j* representation, with j *not* summed. One possible basis choice is the *irrep* basis, sometimes called the *electric* basis due to electric component of the Hamiltonian being diagonal. As an illustrative example, if we take the gauge group to be SU(2), the states are defined by three quantum numbers: *J*, M_L and M_R , reminiscent of angular momentum quantum numbers. The action of the electric operators on these states is given by

$$\hat{E}^{z}|J, M_{L}, M_{R}\rangle = J(J+1)|J, M_{L}, M_{R}\rangle$$

$$\hat{E}_{L}^{z}|J, M_{L}, M_{R}\rangle = M_{L}|J, M_{L}, M_{R}\rangle$$

$$\hat{E}_{R}^{z}|J, M_{L}, M_{R}\rangle = M_{R}|J, M_{L}, M_{R}\rangle$$
(9)

where $\hat{E}^2 \equiv \hat{E}_L^2 = \hat{E}_R^2$. while the gauge link operator can be written as

$$\langle J'M'_LM'_R|\hat{U}^j_{m_Lm_R}|JM_LM_R\rangle = \sqrt{\frac{\dim(J)}{\dim(J')}}\langle JM_Ljm_L|J'M'_L\rangle\langle J'M'_R|JM_Rjm_R\rangle \tag{10}$$

where the matrix elements on the right-hand side are SU(2) Clebsch-Gordan coefficients.

An astute observer will notice that the Kogut-Susskind Hamiltonian was derived almost fifty years ago and yet there has recently been a massive resurgence of interest in Hamiltonian formulations of lattice gauge theories. Why is that? Many recent works have focused on three fundamental

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considerations that must be addressed in order to simulate lattice gauge Hamiltonians on real-world devices. While similar hurdles exist for digital and analog devices, we will mostly speak in terms of digital devices. The first two issues to confront arise because the Hamiltonians that we would like to simulate - namely QCD and other Standard Model gauge groups - are all infinite-dimensional; however, by construction, quantum computers contain a finite number of degrees of freedom. Therefore, the Hamiltonian must be truncated while still faithfully capturing the desired physics. For lattice gauge theory, this truncation is two-fold. Firstly, the Hamiltonian must be reduced such that its energy eigenstates have good overlap with the phenomena of interest; this can usually be thought of as a UV cut-off, analogous to regularization methods in path integral methods. Secondly, the gauge degrees of freedom have to be appropriately discretized or sampled. This must be done carefully, as there is a risk of either inducing (uncontrollable) gauge violation into the theory or simulating a theory that is so unlike the target theory that any numerical results are functionally unusable. Note that while these two obstacles are related, addressing one does not automatically address the other. The last obstacle is that Gauss' Law is not automatically satisfied. This is due to the fact that Gauss' Law is the constraint associated with the A_0 Lagrange multiplier, which is set to zero in Weyl gauge. Unless additional constraints are imposed, the Hilbert space is a tensor product of all the different charge sectors, as shown in Figure 5a.

Let us first address the question of Gauss's Law in lattice gauge theories. In this discussion, it is important to remember that the three ideas of *Gauss' law*, *gauge invariance* and *charge conservation* are intricately related and none of them can be discussed without the other two. To begin, recall that Weyl gauge, which is necessary for ensuring that Schrödinger's equation is gauge invariant, is an incomplete gauge-fixing procedure. In particular, gauge transformations that only depend on spatial coordinates are still allowed. However, the physical Hilbert space must only contain states that obey the Gauss law constraint *i.e.* states that are all invariant under spatial gauge transformations. In particular, for an SU(N) theory without fermions, Gauss's law is given by

$$\underbrace{\sum_{i=1}^{d} D_i E_i^a = 0}_{\text{continuum}} \qquad \underbrace{\hat{G}^a(n) = \sum_{i=1}^{d} \left[\hat{E}_R^a(n - e_i, e_i) - \hat{E}_L^a(n, e_i) \right]}_{\text{lattice}}$$
(11)

where *a* is a color index. Despite the incomplete gauge fixing procedure, notice that the Hamiltonian given in Eq. (4) commutes with the generators of Gauss' law. This implies that if a simulation is initiated on a state with a given charge distribution, assuming zero noise, the charge distribution will *not* change. Another way to see this is by looking at Figure 4b and noticing that the application of the plaquette operator will change the electric field value on all four links but will not change the electric flux through any of the sites. Therefore, there are generally two approaches to dealing with the problem of Gauss' law for quantum simulation. The first approach is to not impose any additional gauge fixing and instead rely on initial state preparation to initialize the system in a given charge sector and then utilize fault-tolerant time evolution to keep the system within that sector; an energy penalty can be added to the Hamiltonian to discourage non-physical transitions in noisy simulations [19]. The downside of this approach is that, due to the inclusion of many unphysical states in the Hilbert space, the simulation must utilize many more qubits than is strictly necessary. Additionally, initial state preparation is proving to be quite challenging in practice for lattice



(a) Symbolic representation of the disconnected charge sectors that make up the full Hilbert space that is spanned by the Kogut-Susskind Hamiltonian



(**b**) The interplay between Gauss law, gauge invariance and charge conservation underlies many of the difficulties of implementing phenomenologically-relevant lattice gauge Hamiltonians onto quantum devices.



gauge theories and fault-tolerant quantum computing is still (probably) decades away. The second approach is to carry out additional gauge-fixing procedures in order to try to reduce the Hamiltonian such that it only spans the physical Hilbert space. While this greatly reduces the dimensionality of the Hilbert space and therefore the necessary number of qubits, there are two major downsides to this approach. The first is that it is not always obvious how to systematically impose additional gauge fixing so that the resultant Hamiltonian only spans the physical Hilbert space. The second downside is that imposing constraints *a priori* typically leads to an increase in non-locality and therefore to more complicated and deeper quantum circuits; the choice between superconducting qubits versus trapped ions will further affect the circuit depth for these formulations. At this point in time, it is not obvious which approach will be most beneficial in the long run.

The first two considerations mentioned above - the need to truncate a formally infinitedimensional Hamiltonian of a continuous gauge group - cannot be as succinctly explained and, at least in theory, addressed. However, by discussing a practical consideration, namely the choice of basis for the Hamiltonian, some clarity might be gained. The question of basis is also a deeply important one, as different bases are expected to perform better or worse depending on the value of the bare coupling. In particular, recall that the Hamiltonian is given by

$$\hat{H} = \underbrace{\frac{g^2}{2a} \sum_{\ell} \hat{E}_{\ell}^a \hat{E}_{\ell}^a}_{Electric} + \underbrace{\frac{1}{2ag^2} \sum_{p} \operatorname{Tr} \left(2I - \hat{P}_p - \hat{P}_p^{\dagger} \right)}_{Magnetic}$$
(12)

where we have explicitly labeled the electric and the magnetic contribution. Notice that the theory has fundamentally different properties at large and small (bare) coupling. At strong coupling, the electric component of the Hamiltonian dominates and the irrep basis is a good choice. In this case, assuming an SU(2) gauge group, the basis states are defined by three quantum numbers, $|J, M_L, M_R\rangle$, which are the eigenstates of the electric operator. There are several advantanges to this basis, namely that the states are naturally discretized and there is also a intuitive UV truncation scheme, namely eliminating all states with $J > J_{max}$. Additionally, since Gauss' Law is a function of electric fields, it is easier to impose additional gauge-fixing constraints in this basis. The downside of this basis is that the continuum limit corresponds to the weak (bare) coupling limit and so the irrep basis is generally not efficient as it will have large truncation errors unless the cut-off is increased as the bare coupling is sent to zero. An alternative to the irrep basis is the so-called group element basis, where the basis states are defined by the group elements $|g\rangle$. In this basis, the gauge links are diagonal and so this basis is well-suited for 'close-to-continuum' physics, as this corresponds to the weak-coupling limit in which the magnetic component of the Hamiltonian dominates. The downside of this basis is that the electric link operators are significantly more complicated and the digitization and truncation of the gauge links must be done more carefully. We shall expand on this point in the next section of these proceedings.

Due to the complicated and interconnected nature of these three hurdles, there have been many proposals for Abelian and non-Abelian formulations and bases. This includes the Kogut-Susskind formulation in the irrep/'angular momentum' basis [20, 21] and the group element basis [22–24], gauge magnets/quantum link models [25], tensor lattice field theory [26], dual/rotor formulations [27–31], casimir variables / "local-multiplet basis" [32, 33], purely fermionic formulations in 1+1D and with open boundary conditions [34–36], prepotential/Schwinger boson formulations [37–40], loop-string-hadron formulation [41–45], light-front formulation [46], qubit models [47] and q-deformed Kogut-Susskind models [48]; note that this is not an exhaustive list of formulations and bases, nor references.⁴

4. Mixed-Basis Approach to Digitizing Group Element Basis

In order to demonstrate how the three challenges mentioned in the previous section might be addressed, let me discuss one example in detail. My choice of example is purely based on this being the formulation with which I am most familiar and comfortable; it is not an indication that this is the right or best approach. Much of the excitement I have for the coming years is discovering the benefits and drawbacks of different approaches and learning how to best optimize for far-future simulations. Additionally, having multiple formulations of the same physical systems allows for important cross-checks. This method, developed in Ref. [49] utilizes additional gauge fixing in order to reduce the Hilbert space, ideally all the way down to only the physical subspace. An additional benefit of working with a fully gauge-fixed theory is that all states of the Hamiltonian are gauge-invariant and so the Hilbert space can be sampled efficiently without concern for the gauge structure of the theory. Once the theory has been gauge-fixed, it is possible to introduce an efficient sampling scheme by making use of a mixed basis, where some variables are labeled by magnetic quantum numbers and some are labeled by electric quantum numbers. For this reason, we call this approach the *mixed basis approach*.

The first step in deriving this formulation is to take the Kogut-Susskind formulation of Eq. (4) and gauge fix using the maximal-tree gauge fixing procedure developed in Ref. [50]. The benefit of this gauge choice is that it can be easily implemented for general lattices and that it fixes all local gauge transformations; note that it does not fix global gauge transformations, though this can be addressed. In order to implement this gauge, the lattice must be partitioned into two disjointed sets:

⁴I gratefully acknowledge Jesse Stryker's talk 'Formal and algorithmic developments for quantum-simulating non-Abelian and higher-dimensional gauge theories" at the topical workshop 'Toward Quantum Advantage in High Energy Physics' in May 2023. His talk provides a fantastic overview of this topic.



(a) Method for constructing loops in maximum tree gauge. Physical links are shown in dashed green links and tree links are shown in dotted red. The convention used here is that tree links are links in the \hat{x} directions for y = 0 and all links in the \hat{y} direction.



(**b**) Results for one plaquette system of Eq. (19). The asymptotic solutions for both strong and weak coupling can be found by noticing that the eigenstates approach the electric eigenstates and the quantum harmonic oscillator eigenstates, respectively.

Figure 6: Derivation and numerical results for the mixed basis Hamiltonian

'physical links' and 'tree links'. Tree links are those links that form a tree, where a tree contains no closed loops. Additionally, the tree links form a *maximal tree*, meaning that adding any link into the tree would create a closed loop. Any link that is not a tree link is defined to be a physical link; these physical links will be denoted by κ . There is no unique choice for this partitioning. The convention used here, for a two-dimensional lattice, is shown in Figure 6a: tree links are links in the \hat{x} directions for y = 0 and all links in the \hat{y} direction. In order to gauge fix, every tree link is set to the identity by systematically carrying out gauge transformations on each site located on the tree, navigating outwards from the origin. It is possible to keep track of these gauge transformations by defining closed paths that originate at the origin of the lattice, traverse only tree links until reaching a physical link, traverse the physical link and then use only tree links to return to the origin; one such path is shown in Figure 6a. With this convention, each loop is uniquely associated with a single physical link.

With this gauge-fixing procedure in place, the Hamiltonian now needs to be rewritten in terms of only physical link variables and loop variables; new electric link variables need to be defined in order to preserve the commutation relations. In particular, the loop operator $\hat{X}(\kappa)$ is defined as the oriented product of link operators along the path $P(\kappa)$, namely

$$\hat{X}(\kappa) = \prod_{\ell \in P(\kappa)} \hat{U}(\ell)^{\sigma_{\ell}}, \qquad (13)$$

where $\sigma_{\ell} = \pm 1$, depending on whether the link ℓ is traversed in the positive or negative direction, respectively. The commutation relations between the original electric link operators and the new loop variables are quite complicated and I will not go into explicit detail about them; Figure 6a details the four cases that have to be considered. However, we define new electric link operators in terms of the old electric link operators that have been parallel transported. Defining these as $\mathcal{E}_{L,R}$,



Figure 7: Axis angle coordinates as hyperspherical coordinates.

the commutation relations are

$$[\hat{\mathcal{E}}_{L}^{a}(\kappa), \hat{X}(\kappa')] = T^{a}\hat{X}(\kappa)\delta_{\kappa,\kappa'} \qquad [\hat{\mathcal{E}}_{R}^{a}(\kappa), \hat{X}(\kappa')] = \hat{X}(\kappa)T^{a}\delta_{\kappa,\kappa'} \tag{14}$$

which are alagous to the canonical commutation relations of Eq. (8). The Hamiltonian is

$$H = \underbrace{\frac{g^2}{2a} \sum_{\ell} \left(\sum_{\kappa \in t_+(\ell)} \hat{\mathcal{E}}^a_{L\kappa} - \sum_{\kappa \in t_-(\ell)} \hat{\mathcal{E}}^a_{R\kappa} \right)^2}_{\text{Electric}} + \underbrace{\frac{1}{2g^2a} \sum_p Tr\left(I - \prod_{\kappa \in p} \hat{X}(\kappa)^{\sigma(\kappa)} \right) + \text{h.c.}}_{\text{Magnetic}}, \quad (15)$$

where $t_{\pm}(\ell)$ is the set of all physical links κ such that ℓ is contained in the path $P(\kappa)$ as a positive or negative link, respectively.

The next step is parameterizing the electric links and gauge loops in terms of coordinates that can be easily digitized and truncated. A convenient parameterization is axis-angle coordinates (ω, θ, ϕ) . These coordinates have the range

$$\theta \in [0,\pi] \qquad \phi \in [0,2\pi] \qquad \omega \in [0,2\pi] \tag{16}$$

and can be conceptualized as hyperspherical coordinates for S^3 , as shown in Figure 7. Using this coordinate system, each gauge link is given by

$$U = \begin{pmatrix} \cos\frac{\omega}{2} - i\sin\frac{\omega}{2}\cos\theta & -i\sin\frac{\omega}{2}\sin\theta e^{-i\phi} \\ -i\sin\frac{\omega}{2}\sin\theta e^{i\phi} & \cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\cos\theta \end{pmatrix}$$
(17)

while the electric link operators are differential operators, e.g.

$$E_R^z = i \left(\cos \theta \frac{\partial}{\partial \omega} - i \cot \frac{\omega}{2} \sin \theta \frac{\partial}{\partial \theta} - \frac{1}{2} \frac{\partial}{\partial \phi} \right)$$
(18)

The last step is to digitize these coordinates in an efficient manner *i.e.* using a minimal number of qubits per coordinate system to achieve the desired precision. It turns out that a convenient and efficient way to do this is to use a spherical harmonic basis for the angular coordinates (θ, ϕ) , *i.e.* use $Y_{LM}(\theta, \phi)$ as an orthonormal and complete basis. The radial coordinate ω can be digitized using methods previously developed for Abelian Hamiltonians [29]. Therefore, the final basis states are given by $|\omega_{\kappa}, L_{\kappa}, M_{\kappa}\rangle$, with κ labeling the physical links. As an example of how this formulation works in practice, the Hamiltonian of one plaquette with open boundary conditions is given by

$$H_{[1]} = \frac{2g^2}{a} \frac{\hat{L}^2}{4\sin^2\frac{\omega}{2}} - \frac{\partial^2}{\partial^2\omega} - \cot\frac{\omega}{2}\frac{\partial}{\partial\omega} + \frac{2}{g^2a}\left(1 - \cos\frac{\omega}{2}\right)$$
(19)

where \hat{L} is the total charge of the system; the appearance of the total charge of the system is the result of maximal tree gauge not fixing global gauge transformations. The results of digitizing this simple system using four qubits for the radial coordinate and a cut-off of $\ell_{\text{max}} = 3$ for the angular momentum quantum numbers, is shown in Figure 6b.

5. Conclusions

Quantum computers have a fundamentally different computational strategy and will hopefully provide novel probes of fundamental questions in particle and nuclear physics. The last several years have seen a massive resurgence of interest in the Hamiltonian simulations of relativistic lattice field theories in the nuclear and high energy physics community. This renewal of interest has been largely driven by rapid hardware improvements for quantum computation, though significant hardware and algorithmic advancements must occur in order to move towards fault-tolerant quantum computers. In the meantime, there is much theoretical and algorithmic development to be done in order to implement lattice gauge theories onto quantum computers. There are many topics that I was not able to cover in this plenary, though there were many great parallel talks on these topics. These topics include

- *Initial State Preparation*: How do you initialize a simulation when you do not know the eigenstates of the target theory?
- *Finite-Temperature Simulations*: How do you simulate finite-temperature systems (mixed states) on a computer that is inherently limited to pure states?
- *Alternative Computational Approaches*: How can alternatives to the quantum circuit qubit approach, such as measurement-based quantum computing, be used for simulating physical systems of interest?
- *Error Mitigation and Error Correction*: How can we mitigate and correct quantum error and noise on the path towards fault-tolerant quantum computers?
- *Variational Quantum Methods*: Can we use variational approaches to learn about quantum field theories on NISQ-era hardware?
- *Scale Setting, Improved Hamiltonians and Renormalization*: How do you extract physically meaningful information from lattice Hamiltonian simulations?

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This is an incredibly exciting and vibrant time for this field. While we are well on our way towards phenomenologically-relevant simulations of the Standard Model, there is much exciting work ahead!

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References

- [1] J. Preskill, Quantum computing in the NISQ era and beyond, Quantum 2 (2018) 79.
- [2] J. B. Kogut and L. Susskind, Hamiltonian Formulation of Wilson's Lattice Gauge Theories, Phys. Rev. D 11 (1975) 395.
- [3] A. Y. Kitaev, A. H. Shen and M. N. Vyalyi, *Classical and Quantum Computation*. American Mathematical Society, USA, 2002.
- [4] A. Aspuru-Guzik, *Quantum Chemistry in the Age of Quantum Computing, Chem. Rev.* **119** (2019) 10856 [1812.09976].
- [5] J. Gambetta, "Ibm's roadmap for scaling quantum technology." https://research.ibm.com/blog/ibm-quantum-roadmap.
- [6] J. Gambetta, "The hardware and software for the era of quantum utility is here." https://research.ibm.com/blog/quantum-roadmap-2033.
- [7] P. Chapman, "Scaling ionq's quantum computers: The roadmap." https: //ionq.com/posts/december-09-2020-scaling-quantum-computer-roadmap.
- [8] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*. Cambridge University Press, 2000.
- [9] F. Liu, R. Lundgren, P. Titum, G. Pagano, J. Zhang, C. Monroe et al., Confined quasiparticle dynamics in long-range interacting quantum spin chains, Phys. Rev. Lett. 122 (2019) 150601.
- [10] W. L. Tan et al., Domain-wall confinement and dynamics in a quantum simulator, Nature Phys. 17 (2021) 742 [1912.11117].
- [11] U.-J. Wiese, Ultracold Quantum Gases and Lattice Systems: Quantum Simulation of Lattice Gauge Theories, Annalen Phys. 525 (2013) 777 [1305.1602].

- [12] E. Zohar, J. I. Cirac and B. Reznik, *Quantum Simulations of Lattice Gauge Theories using Ultracold Atoms in Optical Lattices, Rept. Prog. Phys.* 79 (2016) 014401 [1503.02312].
- [13] M. Dalmonte and S. Montangero, *Lattice gauge theory simulations in the quantum information era*, *Contemp. Phys.* 57 (2016) 388 [1602.03776].
- [14] M. Aidelsburger et al., Cold atoms meet lattice gauge theory, Phil. Trans. Roy. Soc. Lond. A 380 (2021) 20210064 [2106.03063].
- [15] G. Popkin, "Scientists are close to building a quantum computer that can beat a conventional one." https://www.science.org/content/article/ scientists-are-close-building-quantum-computer-can-beat-conventional-one.
- [16] M. Suzuki, Generalized Trotter's Formula and Systematic Approximants of Exponential Operators and Inner Derivations with Applications to Many Body Problems, Commun. Math. Phys. 51 (1976) 183.
- [17] N. Hatano and M. Suzuki, Finding Exponential Product Formulas of Higher Orders, Lect. Notes Phys. 679 (2005) 37 [math-ph/0506007].
- [18] J. B. Kogut, The lattice gauge theory approach to quantum chromodynamics, Rev. Mod. Phys. 55 (1983) 775.
- [19] J. C. Halimeh and P. Hauke, *Reliability of lattice gauge theories*, *Phys. Rev. Lett.* **125** (2020) 030503.
- [20] T. Byrnes and Y. Yamamoto, Simulating lattice gauge theories on a quantum computer, Phys. Rev. A 73 (2006) 022328 [quant-ph/0510027].
- [21] E. Zohar and M. Burrello, Formulation of lattice gauge theories for quantum simulations, Phys. Rev. D 91 (2015) 054506 [1409.3085].
- [22] Y. Ji, H. Lamm, S. Zhu, N. Collaboration et al., *Gluon field digitization via group space decimation for quantum computers*, *Physical Review D* 102 (2020) 114513.
- [23] E. J. Gustafson, H. Lamm, F. Lovelace and D. Musk, Primitive quantum gates for an su(2) discrete subgroup: Binary tetrahedral, Physical Review D 106 (2022) 114501.
- [24] E. Zohar, Quantum simulation of lattice gauge theories in more than one space dimension—requirements, challenges and methods, Phil. Trans. A. Math. Phys. Eng. Sci. 380 (2021) 20210069 [2106.04609].
- [25] S. Chandrasekharan and U. J. Wiese, Quantum link models: A Discrete approach to gauge theories, Nucl. Phys. B 492 (1997) 455 [hep-lat/9609042].
- [26] A. Bazavov, Y. Meurice, S.-W. Tsai, J. Unmuth-Yockey and J. Zhang, *Gauge-invariant implementation of the Abelian Higgs model on optical lattices*, *Phys. Rev. D* 92 (2015) 076003 [1503.08354].

- [27] D. B. Kaplan and J. R. Stryker, *Gauss's law, duality, and the hamiltonian formulation of u(1) lattice gauge theory, Phys. Rev. D* **102** (2020) 094515 [1806.08797].
- [28] J. F. Haase, L. Dellantonio, A. Celi, D. Paulson, A. Kan, K. Jansen et al., A resource efficient approach for quantum and classical simulations of gauge theories in particle physics, *Quantum* 5 (2021) 393 [2006.14160].
- [29] C. W. Bauer and D. M. Grabowska, Efficient Representation for Simulating U(1) Gauge Theories on Digital Quantum Computers at All Values of the Coupling, 2111.08015.
- [30] D. M. Grabowska, C. Kane, B. Nachman and C. W. Bauer, Overcoming exponential scaling with system size in Trotter-Suzuki implementations of constrained Hamiltonians: 2+1 U(1) lattice gauge theories, 2208.03333.
- [31] C. Kane, D. M. Grabowska, B. Nachman and C. W. Bauer, *Efficient quantum implementation* of 2+1 U(1) lattice gauge theories with Gauss law constraints, 2211.10497.
- [32] N. Klco, J. R. Stryker and M. J. Savage, SU(2) non-Abelian gauge field theory in one dimension on digital quantum computers, Phys. Rev. D 101 (2020) 074512 [1908.06935].
- [33] A. Ciavarella, N. Klco and M. J. Savage, *Trailhead for quantum simulation of SU(3)* Yang-Mills lattice gauge theory in the local multiplet basis, *Phys. Rev. D* 103 (2021) 094501
 [2101.10227].
- [34] Y. Y. Atas, J. Zhang, R. Lewis, A. Jahanpour, J. F. Haase and C. A. Muschik, SU(2) hadrons on a quantum computer via a variational approach, Nature Commun. 12 (2021) 6499 [2102.08920].
- [35] R. C. Farrell, I. A. Chernyshev, S. J. M. Powell, N. A. Zemlevskiy, M. Illa and M. J. Savage, Preparations for quantum simulations of quantum chromodynamics in 1+1 dimensions. I. Axial gauge, Phys. Rev. D 107 (2023) 054512 [2207.01731].
- [36] R. C. Farrell, I. A. Chernyshev, S. J. M. Powell, N. A. Zemlevskiy, M. Illa and M. J. Savage, Preparations for quantum simulations of quantum chromodynamics in 1+1 dimensions. II. Single-baryon β-decay in real time, Phys. Rev. D 107 (2023) 054513 [2209.10781].
- [37] M. Mathur, Harmonic oscillator prepotentials in SU(2) lattice gauge theory, J. Phys. A 38 (2005) 10015 [hep-lat/0403029].
- [38] M. Mathur, Loop states in lattice gauge theory, Physics Letters B 640 (2006) 292.
- [39] M. Mathur, Loop approach to lattice gauge theories, Nuclear Physics B 779 (2007) 32.
- [40] R. Anishetty, M. Mathur and I. Raychowdhury, Prepotential formulation of SU(3) lattice gauge theory, J. Phys. A 43 (2010) 035403 [0909.2394].
- [41] I. Raychowdhury and J. R. Stryker, Solving Gauss's Law on Digital Quantum Computers with Loop-String-Hadron Digitization, Phys. Rev. Res. 2 (2020) 033039 [1812.07554].

- [42] I. Raychowdhury and J. R. Stryker, *Loop, string, and hadron dynamics in SU(2) Hamiltonian lattice gauge theories*, *Phys. Rev. D* 101 (2020) 114502 [1912.06133].
- [43] R. Dasgupta and I. Raychowdhury, Cold Atom Quantum Simulator for String and Hadron Dynamics in Non-Abelian Lattice Gauge Theory, 2009.13969.
- [44] S. V. Kadam, I. Raychowdhury and J. R. Stryker, *Loop-string-hadron formulation of an* SU(3) gauge theory with dynamical quarks, 2212.04490.
- [45] S. V. Kadam, I. Raychowdhury and J. R. Stryker, Loop-string-hadron formulation of an su(3) gauge theory with dynamical quarks, Phys. Rev. D 107 (2023) 094513.
- [46] M. Kreshchuk, W. M. Kirby, G. Goldstein, H. Beauchemin and P. J. Love, *Quantum Simulation of Quantum Field Theory in the Light-Front Formulation*, 2002.04016.
- [47] H. Singh and S. Chandrasekharan, *Qubit regularization of the O*(3) *sigma model*, *Phys. Rev.* D 100 (2019) 054505 [1905.13204].
- [48] T. V. Zache, D. González-Cuadra and P. Zoller, *Quantum and Classical Spin-Network Algorithms for q-Deformed Kogut-Susskind Gauge Theories*, *Phys. Rev. Lett.* 131 (2023) 171902 [2304.02527].
- [49] C. W. Bauer, I. D'Andrea, M. Freytsis and D. M. Grabowska, A new basis for Hamiltonian SU(2) simulations, 2307.11829.
- [50] M. Creutz, Gauge fixing, the transfer matrix, and confinement on a lattice, Phys. Rev. D 15 (1977) 1128.