Letter

Efficient representation for simulating U(1) gauge theories on digital quantum computers at all values of the coupling

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We derive a representation for a lattice U(1) gauge theory with exponential convergence in the number of states used to represent each lattice site that is applicable at all values of the coupling. At large coupling, this representation is equivalent to the Kogut-Susskind electric representation, which is known to provide a good description in this region. At small coupling, our approach adjusts the maximum magnetic field that is represented in the digitization as in this regime the low-lying eigenstates become strongly peaked around zero magnetic field. Additionally, we choose a representation of the electric component of the Hamiltonian that gives minimal violation of the canonical commutation relation when acting upon low-lying eigenstates. For $(2+1)$ dimensions with 4 lattice sites the expectation value of the plaquette operator can be calculated with only 7 states per lattice site with per-mille level accuracy for all values of the coupling constant.

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While massive theoretical and algorithmic developments in classical computing have allowed us to probe many aspects of the Standard Model (SM) of Particle Physics, there remain a plethora of open questions that are not amenable to these methods. With a fundamentally different computational strategy, quantum computers hold the promise to simulate the dynamics of quantum field theories from first principles, allowing access to *ab-initio* predictions of observables that are inaccessible using existing techniques on classical computers.[1] In order to harness the full potential of quantum computers, an efficient implementation of the Hamiltonian of gauge theories on quantum processors is a mandatory first step. For a review of various approaches, both analog and digital, see Refs. [3–9].

The Hilbert space of the field theories describing the SM are infinite dimensional, but in order to be implemented onto a digital quantum computer, the physical Hilbert space must be finite. This requires choosing a truncation and digitization scheme, as well as a finite-dimensional representation of the various operator components of the Hamiltonian. These schemes and representation must be chosen such that the discrete Hamiltonian reproduces the physics of the continuum theory with a sufficiently high fidelity and with quantifiable errors. There has been much effort in developing various methods and formulations. Techniques exist that enforce gauge invariance without not restricting to physical states (see for example [10–20]), but limited quantum resources make it preferable to define the Hamiltonian purely in terms of physical states. Possible formulations of gauge theories include magnetic or dual basis representations [21–24], prepotentials with a basis of loop, string and hadron excitations [25–31], discrete subgroups and group space decimation [32–35], mesh digitization [36], light-front formulations [37,38] and orbifold lattice methods [39,40]. For work on experimental realizations, see Refs. [41–46], and for a study of achieving the continuum limit of $1+1$ dimensional U(1) field theory, see Ref. [47].

For this work, we focus on Abelian lattice theories, particularly U(1) lattice gauge theories. One well-known implementation of such a theory is the Kogut-Susskind (KS) Hamiltonian [48–52], which is defined in terms of integer-valued electric fields, plus plaquettes that act as lowering operators. As this formulation is naturally written in the electric basis, it is easy to truncate the theory by truncating the electric field values. We generally refer to this truncated version as the KS representation, which gives

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[1]A classical technique called tensor networks has potential to compute dynamics of gauge theories as long as entanglement is small enough [1,2].

a highly efficient and accurate description at strong coupling, where electric fluctuations are small.

However, for gauge theories in two or less spatial dimensions, or asymptotically-free theories in three spatial dimensions, the continuum limit corresponds to the weak-coupling limit. In this limit, the widths of the eigenstate wave functions in the electric basis increase, such that a truncation at a fixed value of the electric field becomes inadequate. On the other hand, the support of the wave function in the magnetic basis decreases as the coupling decreases, indicating that these gauge theories are more efficiently represented in the magnetic basis.

In this work we derive a new digitized representation of a U(1) gauge theory that is efficient, regardless of the strength of the gauge coupling. The implementation of this representation proceeds in two steps. The first is determining the optimal digitization and truncation of the magnetic field values, as we always work in the magnetic basis. The second is determining the representation of the electric Hamiltonian in the magnetic basis. This results in a simple and analytic expression for the magnetic field digitization, as well as a choice for the electric Hamiltonian that allows for a maximally faithful representation of the lowest-lying states.

In this representation the required number of states per lattice site is quite small for the degree of precision achieved. While we leave a detailed study for future work, we believe that the representation presented here can be implemented onto qubits with minimal modification, making this representation well-tailored for working near the continuum limit. Additionally, the representation works regardless of the strength of the coupling; in fact, at large coupling it is related to the well-known KS formulation via a simple Fourier transform. Magnetic-basis formulations have previously been considered for example in [21,23], with [23] focusing on creating a resource-efficient representation at weak coupling. A comparison to this work can be found in the Supplemental Material [53].

The pure gauge part of a U(1) gauge theory is given by the Hamiltonian

$$H = \frac{1}{2}\int \mathrm{d}^d x[\vec{E}(x)^2 + B(x)^2], \tag{1}$$

where, for simplicity, we will work in $(2+1)$ dimensions. The electric and magnetic field are related to the vector potential by $\vec{E}(x) = \mathrm{d}\vec{A}(x)/\mathrm{d}t$ and $B(x) = \vec{\nabla}\times\vec{A}(x)$, respectively, and we work in the $A_0(x) = 0$ gauge. Note that the curl of a vector field is a 2-form, which in $(2+1)$ dimensions is dual to a scalar.

Gauge invariance implies Gauss' law $[\vec{\nabla}\cdot\vec{E} - \rho]|\Psi\rangle = 0$, giving a constraint on physical states $|\Psi\rangle$. This constraint can be solved by writing [54] $\vec{E} = \vec{E}^L + \vec{E}^T$ with $\vec{\nabla}\cdot\vec{E}^L = \rho$ and $\vec{E}^T = \vec{\nabla}\times R$, where ρ denotes the charge density, and R is again a two-form. Thus, in the absence of electric charges, the Hamiltonian can be written in terms of the two scalar quantities, R (rotor field) and B (magnetic field), which satisfy the canonical commutation relations $[B(x), R(y)] = i\delta(x-y)$.

On a lattice there are two different formulations with the same continuum limit, but noticeably different behavior at finite lattice spacing. Using dimensionless variables and rescaling $A \to A/g$, $E \to gE$, the Hamiltonian for a noncompact theory with no net charge is given by

$$H^{\mathrm{NC}} \equiv H_E + H_B^{\mathrm{NC}} = \frac{1}{2a}\sum_p \left[g^2(\vec{\nabla}\times R_p)^2 + \frac{B_p^2}{g^2}\right], \tag{2}$$

where a is the lattice spacing, and g denotes the bare lattice coupling. The sum is over plaquettes p and $\vec{\nabla}\times R_p$ is the lattice curl, defined in [54]. The commutation relations on the lattice are given by $[B_p, R_{p'}] = i\delta_{p,p'}$.

Alternatively, the gauge field can be compactified, leading to the compact version of the theory with $H^{\mathrm{C}} = H_E + H_B^{\mathrm{C}}$. This changes the magnetic Hamiltonian to the compact form

$$H_B^{\mathrm{C}} = \frac{1}{2a}\sum_p \frac{1}{g^2}(2 - P_p - P_p^\dagger), \qquad P_p = e^{iB_p}, \tag{3}$$

reproducing the KS Hamiltonian. In the following, we will usually work with the compact version of the Hamiltonian, but our final results will also be applicable to the noncompact Hamiltonian.

Setting the convention to denote operators by upper case letters, their eigenvalues by the corresponding lower case ones, and states by bras and kets of lower case letters, the compact nature of the magnetic field immediately leads to an integer spectrum in the rotor fields with

$$R_p|r_p\rangle = r_p|r_p\rangle, \quad P_p|r_p\rangle = |r_p - 1\rangle, \quad r_p \in \mathbb{Z}. \tag{4}$$

Thus, the KS Hamiltonian is naturally represented in the electric (rotor) basis. One can switch to the magnetic basis through a Fourier transform

$$|b_p\rangle = \sum_{r=-\infty}^{\infty} e^{ib_p r_p}|r_p\rangle, \tag{5}$$

which immediately demonstrates the compact nature of the magnetic states $|b_p + 2\pi\rangle = |b_p\rangle$.

In order to represent this field theory on digital (quantum) devices, the continuous magnetic field needs to be digitized. A standard way is to band-limit the electric representation by requiring $-L \leq r \leq L$. This samples the magnetic field through at $2L+1$ discrete equidistant points symmetric between $-\pi$ and π and introduces a spacing in the magnetic field given by $\delta b = 2\pi/(2L+1)$. Note that writing the theory in the electric basis with a bandlimit $-L \leq r \leq L$ corresponds to a $Z_{(2N+1)}$ gauge theory. There have also been investigations using digitizations that cover the range $-\pi < B < \pi$, but using a noninteger value of $2\pi/\delta b$ [55].

For the noncompact theory, the width of the wave function in the magnetic basis scales with the coupling constant as g. For the compact theory, this approximation still holds for small coupling (at large coupling, the support is over the full range $b_p \in [-\pi, \pi]$). Thus, at small coupling the magnetic wave functions become sharply peaked around 0 and to accurately represent them requires a small value of δb, which in turn necessities large L, making the representation very costly.

This work proposes a new efficient formulation that digitizes the magnetic field values directly, which is summarized in Fig. 1. As discussed, at small coupling the magnetic wave function only has support for $|b| < b_{\max} \sim g$. We therefore choose the magnetic field to only be defined in the range $|b| < b_{\max}$, and impose periodic boundary conditions identifying $b(-b_{\max}) = b(b_{\max})$. This samples the magnetic field at each plaquette at the values

$$b_p^{(k)} = -b_{\max} + \left(k + \frac{1}{2}\right)\delta b, \qquad \delta b = \frac{2b_{\max}}{2\ell+1}, \tag{6}$$

with $0 \leq k \leq 2\ell$. The magnetic field operator in the magnetic basis is simply

$$\langle b_p^{(k)} | B_p | b_{p'}^{(k')} \rangle = b_p^{(k)} \delta_{kk'} \delta_{pp'}. \tag{7}$$

This implies that the digitized conjugate rotor field satisfies

$$r_p^{(k)} = -r_{\max} + k\delta r, \tag{8}$$

with $0 \leq k \leq 2\ell$ and

$$\delta r = \frac{2\pi}{\delta b(2\ell+1)}, \qquad r_{\max} = \frac{\ell\pi}{b_{\max}}. \tag{9}$$

Note that for general $b_{\max}$ the spacing of the rotor fields δr is no longer equal to 1, unlike in the compact undigitized lattice theory. This deviation away from $\delta r = 1$ is key to having an efficient and accurate representation. As we will discuss below, in the limit $\ell \to \infty$ we recover the usual relation $\delta b = 2\pi/(2\ell+1)$ such that $\delta r = 1$.

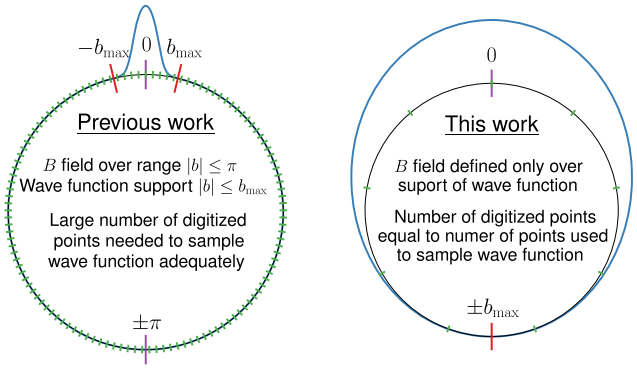

FIG. 1. Illustration of our representation of the magnetic field (right) compared to the previous work of [23] (left).

Two key points need to be addressed. The first is determining the representation of the electric Hamiltonian in the magnetic basis, and the second is choosing a value for $b_{\max}$. Multiple representations of the electric Hamiltonian in the magnetic basis are possible, such as using a finite difference representation of the relation $R = -i\partial_b$, or the representation in [23], which we review in the Supplemental Material [53]. We choose, however, to follow [56] and represent the electric Hamiltonian by its exact eigenvalues through a Fourier transform

$$\begin{aligned} |r_p^{(k)}\rangle &= \frac{1}{\sqrt{2\ell+1}} \sum_{k'=0}^{2\ell} e^{i\frac{2\pi}{2\ell+1}(k-\ell)(k'-\ell-\frac{1}{2})} |b_p^{(k')}\rangle \\ &\equiv \sum_{k'=0}^{2\ell} (\mathrm{FT})_{kk'} |b_p^{(k')}\rangle. \end{aligned} \tag{10}$$

This allows us to write

$$\langle b_p^{(k)} | R_p | b_{p'}^{(k')} \rangle = \sum_{n=0}^{2\ell} r_p^{(n)} (\mathrm{FT})_{kn}^{-1} (\mathrm{FT})_{nk'} \delta_{pp'}. \tag{11}$$

To choose the optimal value of $b_{\max}$ we demand that the optimal digitization for the quantum harmonic oscillator violates the canonical commutation relation minimally [57,58] (suppressed exponentially in the dimension of the Hilbert space). To find the optimal value of $b_{\max}$ for both the noncompact and compact theory,[2] we define the "canonical commutator expectation value"

[2]While the compact and noncompact theory are different, we show in the Supplemental Material [53] that this condition works for a weakly coupled compact version of the harmonic oscillator.

$$\langle C_p^{(\ell)}\rangle[b_{\max}] \equiv 1 + i\langle\Omega^{(\ell)}|[B_p, R_p]|\Omega^{(\ell)}\rangle, \tag{12}$$

where the ground state and the spectrum of the operators also depend on the value of $b_{\max}$, g and ℓ. The value of $b_{\max}$ is now defined by minimizing $\langle C_p^{(\ell)}\rangle[b_{\max}]$,

$$b_{\max}^{(p)}(g,\ell) = \arg\min[\langle C_p^{(\ell)}\rangle[b_{\max}]], \tag{13}$$

and we indicated the dependence of $b_{\max}$ on the values of g and ℓ. Note that in general the condition in (13) gives a different value of $b_{\max}$ for each plaquette. However these differences are quite small and our final analytic expression uses a universal $b_{\max}$.

For a quantum harmonic oscillator (QHO), the condition that the canonical commutation relation be minimally violated has been previously used to derive analytically the optimal value of $b_{\max}(\ell) = \sqrt{(2\ell+1)\pi/2}$ [57,58]. The noncompact U(1) Hamiltonian is a three-dimensional QHO which can be reduced to three one-dimensional QHOs by neglecting terms that couple different lattice sites together. The optimal value of $b_{\max}$ for these one-dimensional QHOs is

$$b_{\max}^{\mathrm{NC}}(g,\ell) = g\sqrt{\frac{(2\ell+1)\pi}{\sqrt{2}}}. \tag{14}$$

For the compact theory, one needs to include the finite maximum range of the magnetic field to give

$$b_{\max}^{\mathrm{C}}(g,\ell) = \min\,[b_{\max}^{\mathrm{NC}}, \pi]. \tag{15}$$

At sufficiently large values of ℓ, $b_{\max}^{C}$ will always be equal to π and therefore $\delta r = 1$. With this final step, we now have a fully defined representation of a $2+1$ dimensional U(1) lattice gauge theory that is valid at all values of the coupling.

We conclude this manuscript by presenting two numerical tests of this formulation. We focus on the smallest possible system in $2+1$ dimensions, namely four lattice sites and periodic identification of the boundaries. Imposing Gauss's law and constraining to the trivial topological sector, the degrees of freedom are three rotors and three plaquettes. This system was previously derived and studied in [23] for the compact gauge group.

The Hilbert space of this system is spanned by three magnetic fields, which we choose to denote as $|b^{(\boldsymbol{k})}\rangle = |b_1^{(k_1)} b_2^{(k_2)} b_3^{(k_3)}\rangle$, where $\boldsymbol{k}$ is the vector of state labels for the magnetic operators. The magnetic Hamiltonian for the compact theory is diagonal with

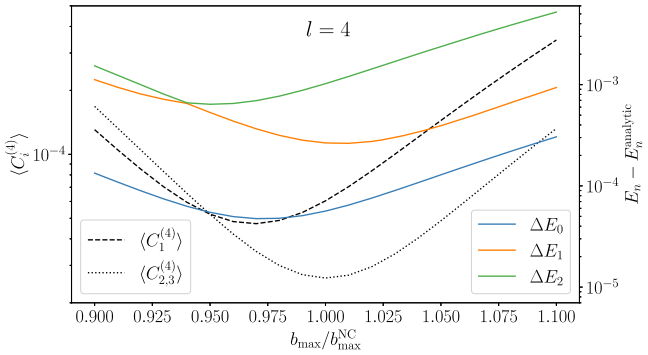

FIG. 2. Dependence of the noncompact theory on the value of $b_{\max}$ for two values of $\ell = 4$. The dashed and dotted lines show the commutator expectation value for the first and second/third lattice plaquette. In the solid lines we show the results for energy difference compared to the analytical result. All curves are minimized for values of $b_{\max} \approx b_{\max}^{\mathrm{NC}}$.

$$\langle b^{(\boldsymbol{k})}|H_B^{\mathrm{C}}|b^{(\boldsymbol{k}')}\rangle = \frac{1}{a}\frac{1}{g^2}\left(4 - \sum_{p=1}^{3}\cos b_p^{(k_p)} - \cos\left[\sum_{p=1}^{3} b_p^{(k_p)}\right]\right)\delta_{\boldsymbol{k}\boldsymbol{k}'}, \tag{16}$$

while for the noncompact theory one replaces each $\cos(b)$ by $1 - b^2/2$. The matrix elements of the electric Hamiltonian are given by

$$\langle b^{(\boldsymbol{k})}|H_E|b^{(\boldsymbol{k}')}\rangle = -\frac{2g^2}{a}\sum_{n_i=0}^{2\ell}(\mathbf{FT})^{-1}_{\boldsymbol{k}\boldsymbol{n}}(\mathbf{FT})_{\boldsymbol{n}\boldsymbol{k}'} \times\left(r_1^{(n_1)}(r_2^{(n_2)} + r_3^{(n_3)}) - \sum_{p=1}^{3}\left(r_p^{(n_p)}\right)^2\right), \tag{17}$$

where we have used the notation $(\mathbf{FT})_{\boldsymbol{k}\boldsymbol{k}'} = \prod_i (\mathrm{FT})_{k_i k_i'}$.

In Fig. 2 we show the dependence of the theory on the value of $b_{\max}$ for the noncompact theory with $\ell = 4$. The values of the $\langle C_p\rangle[b_{\max}]$ are shown by the dashed and dotted lines. The solid lines show the difference of the energies of the first three eigenstates of the Hamiltonian when compared to the exact value in the continuum limit. One can see that all curves have a minimum at very similar locations, and that these minima are very close to the analytical value $b_{\max}^{\mathrm{C}}$ given in (15). The method to solve the nondigitized theory is presented in the Supplemental Material [53].

As a second result, we present the expectation of the plaquette operator

$$\langle\square\rangle = -\frac{g^2a^2}{V}\langle\Psi_0|H_B|\Psi_0\rangle, \tag{18}$$

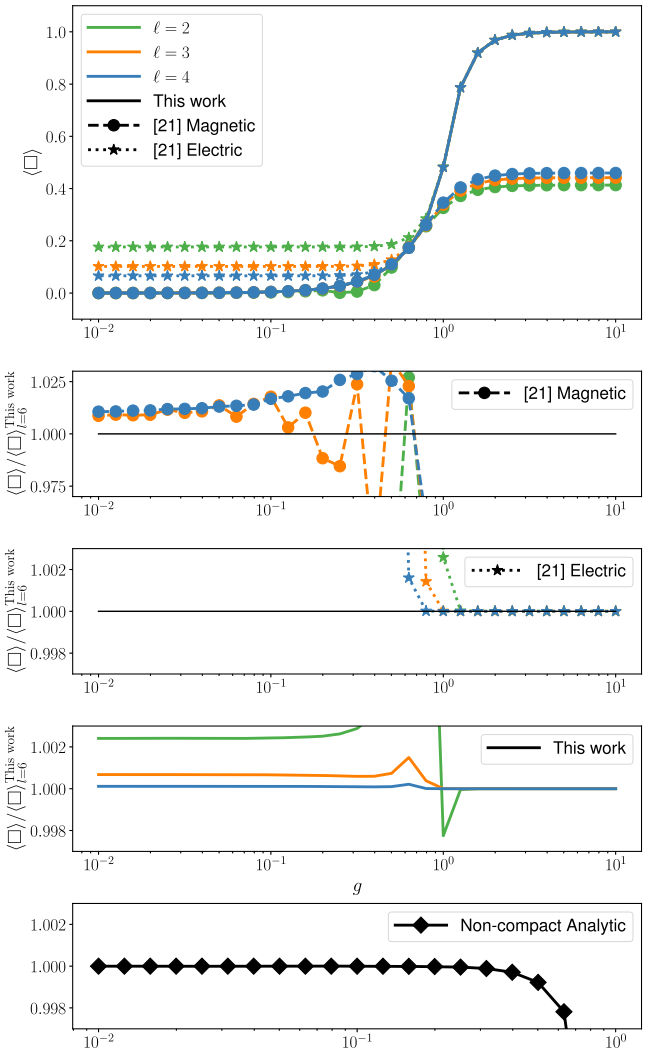

FIG. 3. Expectation value of the plaquette operator for $\ell = 2$ (red), $\ell = 3$ (green), $\ell = 4$ (blue). The solid lines show the results of this work, while the dashed lines (circles) and dotted lines (crosses) denote the results of [23] in the magnetic and electric basis, respectively. The ratios to the result of our work with $\ell = 6$ are shown below, while the bottom plot shows the analytical solution of the noncompact theory, which should give the correct result at low values of g.

where $|\Psi_0\rangle$ is the ground state of the theory and V is the number of plaquettes in the system. This matrix element has been considered in the past [59], and allows for comparisons to [23]. The result is shown in Fig. 3, where the solid lines correspond to the result of this work, while the dashed lines with circles and dotted lines with crosses correspond to the results of [23] in the magnetic and electric basis, respectively, making the same choices as in the original paper, including the choice of the optimal value of L given ℓ. We can see that our results have very good convergence over the entire range of the coupling constant, and already with $\ell = 3$ we have per-mille level accuracy for all values of g. As discussed before, the magnetic (electric) basis of [23] only works at small (large) couplings, and one can see that at small coupling the magnetic basis is only able to reach percent-level accuracy, even for larger ℓ.

In this manuscript we presented a novel formulation of $(2+1)$-dimensional $U(1)$ lattice gauge theories. This formulation is able to reproduce the low-lying spectrum of the theory for all values of the coupling with per-mille or better accuracy while utilizing minimal resources. It digitizes a Hamiltonian that only contains physical states, utilizing an analytic expression to estimate the optimal maximum field value based on the gauge coupling and the available resources for each lattice site. We believe that this procedure can be extended to larger systems in $(2+1)$-dimensions, and a similar procedure should be applicable to $(3+1)$ dimensions, though an additional constraint will likely complicate the procedure [24]. Dynamical fermions can be included in a straightforward way by including a longitudinal electric field $\vec{E}^L$. Extensions of this work to important case of non-Abelian gauge theories is in progress. We close by noting that this work focused on a formulation of U(1) gauge theories that was efficient in the overall dimension of the Hilbert space. While we believe our representation also allows for an efficient implementation on digital quantum computers, we leave a detailed study of the implementation in terms of quantum circuits in future work.

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