Gauss constrained basis for SU(N) Lattice Gauge Theory with Tensor Networks

Carlos Falquez
falquez@nuberisim.de

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Abstract

We construct a basis for $(d+1)$ dimensional SU(N) Kogut-Susskind Lattice Gauge Theory (LGT) with fundamental staggered fermions in which all gauge constraints are explicitly enforced by extending the lattice Hilbert space so that all degrees of freedom may be localized at the vertices, which allows the imposition of the Gauss law at each vertex. We present a tensor network formulation of $(1+1)$ SU(N) LGT using the Gauss constrained basis, and test our approach by calculating the ground state energy and entanglement entropy for $(1+1)$ SU(2). Our numerical results support recent discussions in the literature [3, 37, 56] that only the full entanglement entropy constructed on an extended lattice Hilbert space correctly recovers the vacuum entanglement of the continuum QFT.

Contents

1 Introduction

Gauge theories are a fundamental building block of the theoretical framework of modern physics, and a constitutional element of the Standard Model. A prime example is Quantum Chromodynamics (QCD), the

theory describing the strong interactions of quarks and gluons, a gauge theory with SU(3) symmetry group and 6 flavours of quarks. The introduction of Lattice Gauge Theory (LTG) by Wilson [65] made possible the numerical investigation of non-perturbative phenomena and allowed the implementation of modern Monte Carlo algorithms for precise simulations. In the case of QCD, results of hadron spectroscopy calculations, for example, show extraordinary agreement with experiment [20]. The study of the QCD phase structure, on the other hand, remains a challenging problem [1]. In the numerical Monte Carlo approach, the path integral is evaluated using importance sampling integration by interpreting the lattice action as a probability weight of the corresponding lattice configuration [21]. The probability interpretation however becomes untenable when the lattice action turns complex, which happens when introducting a nonzero chemical potential. The Monte Carlo integration method is then no longer applicable. This is the infamous sign problem (or complex-phase problem), and represents a serious hurdle for the numerical investigation of gauge theories at finite density. For a pedagogical discussion of the problem see [1].

The Hamiltonian formulation of Wilson's theory by Kogut and Susskind [35] offers an alternative approach to the lattice discretization of gauge field theory amenable to numerical implementation which is also free of the sign problem. This makes the Hamiltonian approach particularly interesting, specially since the advent of tensor network methods [43, 44]. Tensor network methods can be motivated from the observation that for gapped local Hamiltonians, low energy eigenstates obey an area law for the entanglement entropy [17]. Further, due to quantum entanglement, the manifold of states reachable from some fiducial state by time-evolution generated from a local Hamiltonian over a period of time polynomial in the system size is contained inside an exponentially small subspace of the total Hilbert space [45]. Employing a wavefunction Ansatz specifically targeting those states obeying appropiate entanglement area laws is therefore physically warranted, and should be much more advantegeous numerically than dealing with the total Hilbert space (since, as is well known, "there is lots of room left in Hilbert space"[1]). In the tensor network approach, the relevant Hilbert subspace is parametrized by a collection of local tensors connected together under some topology appropiate for the problem at hand. Corresponding numerical algorithms for eigenstate search or time evolution are based on the variational optimization of the Ansatz wavefunction and can be implemented very efficiently by exploting its tensor network structure [51, 55].

By taking advantage of tensor network methods, the Hamiltonian formulation of Kogut and Susskind enables the calculation of spectral properties, the characterization of the phase diagram at nonzero chemical potential and the direct observation of real-time and thermal phenomena of lattice gauge theories. For recent studies of non-abelian models see [7, 36, 52, 54], and for comprehensive reviews see [8, 15].

Moreover, the Kogut-Susskind formulation provides the foundation for many proposed implementations of analog and digital quantum simulations of lattice gauge theories. A quantum simulator is understood as the experimental realization of a *controllable quantum system* designed to emulate another quantum model of interest such that measurements on the system elucidate relevant aspects of the model under study which are very hard to access for classical simulations [22, 29]. The Schwinger model has already been sucessfully realized on a digital quantum computer [39, 40] allowing the direct measurement of real-time evolution phenomena which are not easily accesible by conventional numerical simulations such as pair creation, vacuum decay and entanglement generation. Analog simulations of the Schwinger model have also been proposed using trapped ions [67] and ultracold-atom platforms [32, 68]. For general gauge symmetry groups, a reformulation of the Kogut-Susskind Hamiltonian amenable to experimental realization was presented in [69, 70]. The prospect of implementing lattice gauge theories as table top quantum experiments is very exciting.

One of the main challenges for both quantum and classical simulation of the Kogut-Susskind Hamiltonian is the local imposition of the Gauss constraint (A.3) on the lattice, which in the Hamiltonian formalism is no longer a direct consequence of the equations of motion but must be enforced as a restriction on the physical Hilbert space of the theory (see Appendix A). Furthermore, for both classical and quantum computation implementations, the infinite dimensional Hilbert space of the gauge link operator must be constrained to a finite dimensional subspace while respecting the gauge invariance of the system. Various proposed solutions, such as exploiting the Gauss Law to integrate out the link degrees of freedom, or writing the link operators as spin operators, have found applications both in classical and quantum computational techniques, demostrating the significant interplay between both approaches. Quantum simulation efforts thus present a further motivation to advance and develop tensor network methods to the study of lattice gauge theories.

[1] Saunders Mac Lane, as quoted in [47]

In this note, we introduce an efficient basis for the numerical calculation of SU(N) lattice gauge theories using tensor network methods, and test our approach for the case of SU(2) symmetry group and $(1+1)$ dimensions, replicating the results by Bañuls et al. [7].

Following Robson and Webber [49] we construct a basis for $(d+1)$ dimensional SU(N) Kogut-Susskind lattice gauge theory with fundamental staggered fermions in which all gauge constraints are explicitly enforced. This is realized by embedding the Kogut-Susskind Hilbert space $\mathcal{H}_{\rm KS}$ onto an extended *computational* Hilbert space $\mathcal{H}_{\rm comp}$, with all the degrees of freedom localized on lattice vertices. This is analogous to the introduction of computational vertices coupling matter and rishon fields in Quantum Link models [53]. In our case, the extended Hilbert space arises from embedding the "quantum rigid rotator" Hilbert space of the link operator into the tensor product two independent configuration spaces carrying all irreducible SU(N) representations, which are assigned to each of the two link vertices. The computational space $\mathcal{H}_{\rm comp}$ allows the imposition of the Gauss law (A.20) at each lattice site, and demanding $G^\alpha = 0$ defines the *Gauss constrained* subspace $\mathcal{H}_G \subset \mathcal{H}_{\rm comp}$. Constraining to this subspace is numerically advantegeous since its algebraic dimension can be controlled by truncating a Clebsch-Gordan series to a maximally allowed $SU(N)$ irrep $\sigma_{\rm max}$, and is much lower than that of the original Kogut-Susskind space. Setting a maximal irrep $\sigma_{\rm max}$ corresponds to defining an energy cutoff for the gluons. The gauge invariant (physical) subspace $\mathcal{H}_{\rm phys}$ may be recovered by pulling back to the "quantum rigid rotator" subspace between neighbouring vertices with projection operators, and imposing boundary conditions.With the help of tensor network methods, we test the usefulness of our construction by replicating the results of Bañuls and collaborators [7] for the case of $(1+1)$ SU(2) Yang-Mills with fundamental staggered fermions.

The work is organized as follows. In section 2 we define and construnct a basis for the Gauss constrained subspace of the computational Hilbert space $\mathcal{H}_{\rm comp}$. In section 3 we present the tensor network formulation for $(1+1)$ dimensions, and in section 4 we discuss our results for the ground state energy and entanglement entropy for the $(1+1)$ SU(2) theory. We also quickly review the difficulties defining entanglement entropy for non-abelian gauge theories. In section 5 we summarize our results. In Appendix A we present a very short review of the Kogut-Susskind formalism, and in Appendix B we recall some definitions concerning SU(N) Clebsch-Gordan coefficients as a way to establish our notation.

2 SU(N) Gauss constrained basis

The total lattice Hilbert space $\mathcal{H}_{\rm KS}$ for the Kogut-Susskind Hamiltonian is the tensor product of fermionic and gauge degrees of freedom

$$\mathcal{H}_{\rm KS} = \otimes_{x\in\Lambda}\mathcal{H}^x_Q \otimes_{l\in \mathrm{L}_\Lambda} \mathcal{H}^l_{\mathbf{U}}\,, \tag{2.1}$$

where $\mathcal{H}^x_Q$ is the staggered fermion Hilbert space at site $x \in \Lambda$, and $\mathcal{H}^l_{\mathbf{U}}$ the gauge field Hilbert space at link $l \in \mathrm{L}_\Lambda$ (see Appendix A for a quick review of the Kogut-Susskind formulation). The Gauss operator G^α on the lattice is given by

$$G^\alpha(x) = \sum_i E^\alpha_i(x) + \sum_i F^\alpha_i(x) + Q^\alpha(x)\,. \tag{2.2}$$

The physical lattice Hilbert space $\mathcal{H}_{\rm phys}$ is then given by demanding the Gauss constraint $G^\alpha = 0$ for all lattice sites $x \in \Lambda$

$$\mathcal{H}_{\rm phys} \equiv \left\{ |\Psi\rangle \in \mathcal{H}_{\rm KS} \,\middle|\, G^\alpha(x)|\Psi\rangle = 0\, \forall x \in \Lambda \right\}. \tag{2.3}$$

Following Robson and Webber [49], we would like to construct a gauge covariant basis for the Hilbert space (2.1) comprised by the eigenstates of the Gauss operator (2.2), then project to the invariant subspace $G^\alpha = 0$ which satisfies the constraint (2.3). This is done in the following sections. In section 2.1 we relabel the fermion occupation basis into a representation basis, by reducing the tensor product structure of the fermion sector to a direct sum of SU(N) irreps. In section 2.2, we embed $\mathcal{H}_{\mathbf{U}}$ into the tensor product of local Hilbert spaces carrying all irreps of the gauge group. In section 2.3 we introduce a computational Hilbert space, which allows us to write a gauge covariant basis using the eigenstates of G^α, with the help of the Clebsch-Gordan coefficients for SU(N). One may then trivially project to the gauge invariant subspace $G^\alpha = 0$. In section 2.5 we compare our approach to previous work on the subject.

	$\lvert\xi_{a_1\cdots}\rangle$	$\lvert Q\, s_3\rangle$
1	$\lvert 0\rangle$	$\lvert 0\rangle$
2	$\lvert\xi_1\rangle$	$\lvert\frac{1}{2}\ +\frac{1}{2}\rangle$
3	$\lvert\xi_2\rangle$	$\lvert\frac{1}{2}\ -\frac{1}{2}\rangle$
4	$\lvert\xi_{12}\rangle$	$\lvert B\rangle$

(a) SU(2)

	$\lvert\xi_{a_1\cdots}\rangle$	$\lvert Q\,(t_3, y)\rangle$
1	$\lvert 0\rangle$	$\lvert 0\rangle$
2	$\lvert\xi_1\rangle$	$\lvert 3\,(0, -\frac{2}{3})\rangle$
3	$\lvert\xi_2\rangle$	$\lvert 3\,(-\frac{1}{2}, +\frac{1}{3})\rangle$
4	$\lvert\xi_3\rangle$	$\lvert 3\,(+\frac{1}{2}, +\frac{1}{3})\rangle$
5	$\lvert\xi_{12}\rangle$	$\lvert\bar{3}\,(-\frac{1}{2}, -\frac{1}{3})\rangle$
6	$\lvert\xi_{23}\rangle$	$\lvert\bar{3}\,(0, +\frac{2}{3})\rangle$
7	$\lvert\xi_{31}\rangle$	$\lvert\bar{3}\,(+\frac{1}{2}, -\frac{1}{3})\rangle$
8	$\lvert\xi_{123}\rangle$	$\lvert B\,\rangle$

(b) SU(3)

Table 1: Occupation and corresponding representation basis for SU(2) and SU(3). The SU(3) Cartan operators are defined as $T_3 \equiv \frac{1}{2}(\hat{n}_3 - \hat{n}_2)$ and $Y \equiv \frac{1}{3}(\hat{n}_2 + \hat{n}_3 - 2\hat{n}_1)$.

2.1 Fermion representation basis

Consider the Grassman valued field operators ξ_a transforming under the fundamental representation of SU(N). Different states of the fermion Hilbert space $\mathcal{H}_Q$ are constructed by acting iteratively with creation operators $\xi^\dagger_a$ on the vacuum $|0\rangle \in \mathcal{H}_Q$, $|\xi_{a_1\ldots a_n}\rangle \equiv \xi^\dagger_{[a_1}\ldots\xi^\dagger_{a_n]}|0\rangle$, where $\xi^\dagger_{[a_1}\ldots\xi^\dagger_{a_n]} \equiv \frac{1}{n!}\sum_P (-1)^P \xi^\dagger_{\sigma(a_1)}\ldots\xi^\dagger_{\sigma(a_n)}$ is the sum over all possible permutations P of the n tensor indices a_i, with $(-1)^P = 1$ for even and $(-1)^P = -1$ for odd permutations. Since every totally antisymmetric tensor product of fundamental representations of $SU(N)$ defines an irreducible representation of the group, the $N-1$ subspaces $V_n \equiv \text{span}(\{|\xi_{a_1\ldots a_n}\rangle\})$, $n = 1\ldots N-1$ formed from the linear combination of totally antisymmetric n-tensor product states $|\xi_{a_1\ldots a_n}\rangle$ each furnish one of the $N-1$ fundamental irreps D^n of SU(N) [23]. The vacuum subspace $V_0 \equiv \text{span}\{|0\rangle\}$ carries SU(N) trivially. The N-tensor product $|\xi_{a_1\ldots a_N}\rangle$ also transforms under the trivial representation, we label this N-particle singlet state $|B\rangle$ (from "Baryon") to differentiate it from the vacuum $|0\rangle$. It follows that the $N+1$ subspaces $V_n \equiv \text{span}(\{|\xi_{a_1\ldots a_n}\rangle\})$, $n = 0\ldots N$ partition $\mathcal{H}_Q$ in $N+1$ SU(N) invariant subspaces,

$$\mathcal{H}_Q \equiv \left\{ |Q\, q\rangle \in \oplus_{n=0\ldots N} V_n \right\}, \tag{2.4}$$

where we have labeled $|Q\, q\rangle$ the basis states of V_n, and with some abuse of notation we have used Q to label the representation, and q to label the states. We may therefore relabel the occupation basis states $|\xi_{a_1\ldots a_n}\rangle$ as basis states $|Q\, q\rangle$ of an irreducible representation of SU(N). Table 1 lists the occupation and corresponding representation basis labels for SU(2) and SU(3).

2.2 Gauge Field extended space basis

Each positevely oriented lattice link $l \in \mathrm{L}_\Lambda$ carries a gauge field Hilbert space $\mathcal{H}^l_{\mathbf{U}}$. We may use the eigenstates $|U\rangle$ of the link operator $\mathbf{U}^J_{ab}$ as a basis of $\mathcal{H}^l_{\mathbf{U}}$,

$$\mathbf{U}^J_{ab}|U\rangle = D^J_{ab}\,(U)\,|U\rangle\,, \tag{2.5}$$

where $D^J_{ab}\,(U)$ is an SU(U) rotation matrix for the group element U in the J representation. Note that repeated action of the link operator $\mathbf{U}_{ab}$ results in higher order representations,

$$\mathbf{U}^{J_1}_{a_1b_1}\mathbf{U}^{J_2}_{a_2b_2} = \sum_{\substack{J\in J_1\otimes J_2\\ a,b\in J}} (-1)^{w(a)-w(b)}\,\dim J \begin{pmatrix} J_1 & J_2 & \bar{J} \\ a_1 & a_2 & \bar{a}\end{pmatrix}\begin{pmatrix} J_1 & J_2 & \bar{J} \\ b_1 & b_2 & \bar{b}\end{pmatrix}\mathbf{U}^J_{ab}\,, \tag{2.6}$$

where the *phase function* $w(a)$ is defined by some phase convention (see Appendix B). The problem with using the link operator eigenbasis $|U\rangle$ is the necessity of some continuous parametrization of the SU(N)

group manifold. One may expect the existence of a conjugate basis to $|U\rangle$ in which group elements may be expanded as a sum of discrete modes, similarly to a Fourier expansion on a compact domain. This is indeed the case for the electric eigenbasis, which can be constructed as follows [49]. Let the electric vacuum state $|000\rangle \in \mathcal{H}^l_{\mathbf{U}}$ be the state invariant under the gauge generators E^α and F^α,

$$E^\alpha|000\rangle = F^\alpha|000\rangle = 0\,. \tag{2.7}$$

Acting on the electric vacuum with the link operator defines the *electric eigenstates* $|Jmn\rangle$:

$$|Jmn\rangle \equiv (-1)^{w(\mu_J)-w(m)}\sqrt{\dim J}\;\mathbf{U}^J_{\bar{m}n}|000\rangle\,, \tag{2.8}$$

with $n \in J$, $\bar{m} \in J$ the conjugate state of $m \in \bar{J}$ and μ_J is the highest weight state of the irrep J. Together with (2.5), (2.7), and general properties of SU(N) generators, it can be shown that (2.8) define an orthonormal basis for $\mathcal{H}_{\mathbf{U}}$. The states (2.8) span the configuration space of a *quantum rigid rotator* with spherical symmetry [35]. The commutation relations (A.13) result in the linear transformations

$$\begin{aligned} E^\alpha|Jmn\rangle &= \sum_r \left(T^\alpha_{\bar{J}}\right)_{m'm}|Jm'n\rangle\,,\\ F^\alpha|Jmn\rangle &= \sum_r \left(T^\alpha_{J}\right)_{n'n}|Jmn'\rangle\,. \end{aligned} \tag{2.9}$$

From (2.9) we see that the electric eigenstate $|Jmn\rangle$ transforms separately as an eigenbasis of $\bar{J}$ under E^α, and as an eigenbasis of J under F^α. In particular, the electric eigenstates (2.8) are eigenvectors of both quadratic Casimir operators $\mathbf{E}^2 \equiv E^\alpha E^\alpha$, $\mathbf{F}^2 \equiv F^\alpha F^\alpha$ and the Cartan generators of the algebra.

Define the vector space $\mathbb{V}$ as the direct sum of all SU(N) irrep carrying vector spaces $\mathbb{V}_J = \mathrm{span}(\{|J\,m\rangle\})$, $\mathbb{V} \equiv \bigoplus_{J\in \mathrm{Irrep(SU}(N))}\mathbb{V}_J$. Motivated by the relations (2.9), introduce separate Hilbert spaces $\mathcal{H}^x_E$ at $x \in \Lambda$ and $\mathcal{H}^{x+\hat{e}_i}_F$ at $x+\hat{e}_i \in \Lambda$. Let both spaces be the direct sum of all irrep carrying spaces of SU(N), $\mathcal{H}_E \cong \mathcal{H}_F \cong \mathbb{V}$, upon which the generators E^α and F^α act. We define the extended gauge link Hilbert space $\mathcal{H}'^l_{\mathbf{U}}$ with tensor product structure

$$\mathcal{H}'^l_{\mathbf{U}} = \mathcal{H}^x_E \otimes \mathcal{H}^{x+\hat{e}_i}_F \cong \mathbb{V}\otimes\mathbb{V}\,, \tag{2.10}$$

and an *embedding* $\iota_{\mathbf{U}} : \mathcal{H}_{\mathbf{U}} \to \mathcal{H}'_{\mathbf{U}}$ with

$$\iota_{\mathbf{U}}\left(|Jmn\rangle\right) = |\bar{J}m\rangle|Jn\rangle\,. \tag{2.11}$$

The projection operator $\mathrm{P}^l_{\mathbf{U}}$ is defined on $\mathcal{H}'^l_{\mathbf{U}}$,

$$\mathrm{P}^l_{\mathbf{U}} \equiv \sum_{Jmn} |\bar{J}m\rangle|Jn\rangle\langle\bar{J}m|\langle Jn|\,. \tag{2.12}$$

The original gauge link Hilbert space $\mathcal{H}_{\mathbf{U}}$ is recovered as the range of $\mathrm{P}^l_{\mathbf{U}}$, $\mathcal{H}^l_{\mathbf{U}} = \mathrm{P}^l_{\mathbf{U}}\,\mathcal{H}'_{\mathbf{U}}$, and any observable $\hat{O}^l$ defined on $\mathcal{H}^l_{\mathbf{U}}$ can be extended to an observable on $\mathcal{H}'^l_{\mathbf{U}}$, $\hat{O}^l \to \hat{O}'^l = \mathrm{P}^l_{\mathbf{U}}\,\hat{O}\,\mathrm{P}^l_{\mathbf{U}}$.

2.3 Computational Lattice Hilbert Space and Gauss Invariant Subspace

We now extend the Kogut-Susskind lattice Hilbert space $\mathcal{H}_{\mathrm{KS}}$ (2.1) to a *computational* Hilbert space $\mathcal{H}_{\mathrm{comp}}$, which decomposes as the direct sum of locally covariant subspaces of G^α, i.e. subspaces carrying irreducible representations of the Gauss operator (2.2). Embedding the gauge link Hilbert space $\mathcal{H}^l_{\mathbf{U}}$ at each positevely oriented lattice link $l = (x, \hat{e}_i) \in \mathrm{L}_\Lambda$ into the extended space $\mathcal{H}'^l_{\mathbf{U}} = \mathcal{H}^x_{E_i} \otimes \mathcal{H}^{x+\hat{e}_i}_{F_i}$ would assign to each link vertex either local Hilbert space $\mathcal{H}^x_{E_i}$ or $\mathcal{H}^x_{F_i}$. Decomposition (2.10) thus motivates the introduction, analogous to the tensor network formulation of Quantum Link Models [53], of a *computational vertex space* $\mathcal{H}^x_V$ at each lattice site $x \in \Lambda$,

$$\mathcal{H}^x_V \equiv \otimes_{i=1\ldots d}\left(\mathcal{H}^x_{E_i}\otimes\mathcal{H}^x_{F_i}\right)\otimes\mathcal{H}^x_Q\,, \tag{2.13}$$

coupling fermion and gauge generator carrier spaces. A basis for $\mathcal{H}_V^x$ may be written as the tensor product of basis vectors,

$$|\{\sigma_i s_i\}\rangle \equiv |E_1\, m_1\rangle \otimes |F_1\, n_1\rangle \otimes \cdots \otimes |E_d\, m_d\rangle \otimes |F_d\, n_d\rangle \otimes |Q\, q\rangle \in \mathcal{H}_V^x\,, \tag{2.14}$$

for some sequence of irrep labels $\boldsymbol{\sigma} \equiv \{\sigma_i\} = \{E_1, F_1, \ldots, E_d, F_d, Q\}$ and corresponding carrier states $\{s_i\} = \{m_1, n_1, \ldots, m_d, n_d, q\}$. Note that the Gauss operator (2.2) is the total generator of gauge transformations on $\mathcal{H}_V^x$, and acts locally on each computational vertex as a tensor product operator. The local Gauss constraint $G^\alpha(x) = 0$ can thus be imposed separately for each $x \in \Lambda$.

Define the computational lattice Hilbert space $\mathcal{H}_{\text{comp}}$ as the tensor product over all lattice vertex spaces

$$\mathcal{H}_{\text{comp}} \equiv \otimes_{x\in\Lambda} \mathcal{H}_V^x\,. \tag{2.15}$$

It is clear that $\mathcal{H}_{\text{KS}} \subset \mathcal{H}_{\text{comp}}$, and we may recover $\mathcal{H}_{\text{KS}}$ as a constraint on $\mathcal{H}_{\text{comp}}$ by projecting each link tensor product $\mathcal{H}_{\mathbf{U}}^{ll}$ back to $\mathcal{H}_{\mathbf{U}}^{l}$ and eliminating the spurious degrees of freedom at the lattice boundaries. For each link $l = (x, \hat{e}_i) \in \mathrm{L}_\Lambda$, define the projection operator on $\mathcal{H}_{\text{comp}}$

$$\mathrm{P}_{\mathbf{U}}(l) \equiv \mathbf{1} \otimes \cdots \otimes \mathrm{P}_{\mathbf{U}}^{l} \otimes \cdots \otimes \mathbf{1}\,, \tag{2.16}$$

acting as the projection (2.12) on neighbouring sites $\mathcal{H}_{E_i}^x \otimes \mathcal{H}_{F_i}^{x+\hat{e}_i} \subset \mathcal{H}_{\text{comp}}$ and the identity everywhere else. Define further projection operators P_{F_i} and P_{E_i} acting on $|\Psi\rangle \in \mathcal{H}_{\text{comp}}$,

$$\mathrm{P}_{F_i}|\Psi\rangle = \begin{cases} |\Psi\rangle & \text{if } F_i^\alpha(x)|\Psi\rangle = 0\ \forall\, x \in \Lambda\,,\ x_i = 0, \\ 0 & \text{otherwise}\,, \end{cases} \tag{2.17a}$$

$$\mathrm{P}_{E_i}|\Psi\rangle = \begin{cases} |\Psi\rangle & \text{if } E_i^\alpha(x)|\Psi\rangle = 0\ \forall\, x \in \Lambda\,,\ x_i = L, \\ 0 & \text{otherwise}\,, \end{cases} \tag{2.17b}$$

which constrain the extra degrees of freedom at the boundaries. The Kogut-Susskind space $\mathcal{H}_{\text{KS}}$ is then recovered by the restriction

$$\mathcal{H}_{\text{KS}} = \Big\{ |\Psi\rangle \in \mathcal{H}_{\text{comp}} \,\Big|\, \mathrm{P}_{\mathbf{U}}(l)|\Psi\rangle = |\Psi\rangle\ \forall\, l \in \mathrm{L}_\Lambda\,, \tag{2.18a}$$

$$\mathrm{P}_{E_i}|\Psi\rangle = |\Psi\rangle\ \forall i \in \{1,\ldots,d\}\,, \tag{2.18b}$$

$$\mathrm{P}_{F_i}|\Psi\rangle = |\Psi\rangle\ \forall i \in \{1,\ldots,d\} \Big\}\,. \tag{2.18c}$$

Following Robson and Webber [49], we wish to construct a gauge covariant basis for $\mathcal{H}_{\text{comp}}$, then project to the invariant subspace $G^\alpha(x) = 0$ of the Gauss operator (2.2). First note that each of the spaces in the tensor product (2.13) decomposes as a direct sum of subspaces carrying some irreducible representation of the group. Given an irrep sequence $\boldsymbol{\sigma} \equiv \{\sigma_1, \ldots, \sigma_{2d+1}\}$ of $2d+1$ irreps $\sigma_i \in \mathrm{Irrep}(SU(N))$, the projection operator $\mathrm{P}_\sigma \equiv \sum_{s_i\in\sigma_i} |\{\sigma_i s_i\}\rangle\langle\{\sigma_i s_i\}|$ picks out a subspace $\mathcal{H}_\sigma^x \subset \mathcal{H}_V^x$ transforming under $G^\alpha(x)$ as the tensor product representation $\otimes_i \sigma_i$. The computational vertex space $\mathcal{H}_V^x$ then decomposes as the direct sum of all such subspaces, $\mathcal{H}_V^x = \oplus_\sigma \mathcal{H}_\sigma^x$, each subspace transforming separately under $G^\alpha(x)$. We call an irrep sequence $\boldsymbol{\sigma} = \{\sigma_i\}$ a *G-supported* irrep sequence, and G a *supported* irrep of $\boldsymbol{\sigma}$ with multiplicity $N_{\boldsymbol{\sigma}}^G$, iff the irrep G is contained within the direct sum decomposition of $\boldsymbol{\sigma}$ with outer multiplicity $N_{\boldsymbol{\sigma}}^G$, i.e. iff $\sigma_1 \otimes \sigma_2 \otimes \cdots = \underbrace{G \oplus \cdots \oplus G}_{N_{\boldsymbol{\sigma}}^G} \oplus \cdots = N_{\boldsymbol{\sigma}}^G\, G \oplus \cdots$. If G is not a supported irrep of $\boldsymbol{\sigma}$, let $N_{\boldsymbol{\sigma}}^G = 0$.

Then for any given irrep sequence $\boldsymbol{\sigma}$, the tensor product space $\mathcal{H}_\sigma^x$ can be further decomposed to a direct sum of invariant subspaces of the Gauss operator G^α carrying supported irreps G of $\boldsymbol{\sigma}$, each subspace occuring with multiplicity $N_{\boldsymbol{\sigma}}^G$ and identified with an index $\gamma = 1, \ldots, N_{\boldsymbol{\sigma}}^G$. The corresponding basis vectors $|G\, g, \gamma\rangle \in \mathcal{H}_\sigma^x$ are constructed as follows. Let $\{K_i\} = \{K_2, \ldots, K_{2d}\}$ be a sequence of $2d-1$ irreps $K_i \in \mathrm{Irrep}(SU(N))$. Given an irrep sequence $\boldsymbol{\sigma}$ and a $\boldsymbol{\sigma}$-supported irrep G, the sequence $\{K_i\}$ is called a *G-coupling* sequence of $\boldsymbol{\sigma}$ iff $K_2 \in \sigma_1 \otimes \sigma_2$, $K_i \in K_{i-1} \otimes \sigma_i$ for $2 < i < 2d+1$, and $G \in K_{2d} \otimes \sigma_{2d+1}$. For fixed $\boldsymbol{\sigma}$ and G, specifying the multiplicity index γ already determines the corresponding coupling sequence

$\{K_i\}$. The basis vectors $|G\, g, \gamma\rangle$ spanning the G-carrying subspace of $\mathcal{H}^x_\sigma$ with multiplicity index γ are then related to the computational basis (2.14) by the Clebsch-Gordan series

$$|G\, g, \gamma\rangle = \sum_{\substack{k_i \in K_i \\ s_i \in \sigma_i}} C^{k_2}_{s_1 s_2} C^{k_3}_{k_2 s_3} \dots C^{g,\gamma}_{k_{2d} s_{2d+1}} \, |\{\sigma_i\, s_i\}\rangle \ , \tag{2.19}$$

where the sum is over all states $s_i \in \sigma_i$ and $k_i \in K_i$ such that all Clebsch-Gordan coefficients are not zero, and the coupling sequence $\{K_i\}$ is specified by γ. The Clebsch-Gordan series (2.19) decomposes the vertex Hilbert space (2.13) as a direct sum *over all possible irrep sequences* $\boldsymbol{\sigma}$,

$$\mathcal{H}^x_V = \oplus_\sigma \mathcal{H}^x_\sigma \cong \oplus_\sigma \oplus_{G \in \otimes_i \sigma_\mathbf{i}} N^G_{\boldsymbol{\sigma}} \, \mathbb{V}_G . \tag{2.20}$$

The *Gauss invariant* subspace $\mathcal{H}^x_\mathbf{0} \subset \mathcal{H}^x_V$ results from restricting the direct sum (2.20) to the subspace $G = 0$

$$\mathcal{H}^x_\mathbf{0} \cong \oplus_\sigma N^0_{\boldsymbol{\sigma}} \, \mathbb{V}_0 \, . \tag{2.21}$$

All states $|\phi\rangle \in \mathcal{H}^x_\mathbf{0}$ belong to the singlet representation of G^α and satisfy the Gauss Law $G^\alpha(x)\,|\phi\rangle = 0$ trivially. Given a $0-$supported irrep sequence $\boldsymbol{\sigma}$, the linear transformation (2.19) targeting the singlet representation $G = 0$ forms a basis for a $N^0_{\boldsymbol{\sigma}}$-dimensional invariant subspace of $\mathcal{H}^x_V$,

$$|\boldsymbol{\sigma}, \gamma\rangle \equiv \sum_{k_i, s_i} C^{k_2}_{s_1 s_2} C^{k_3}_{k_2 s_3} \dots C^{0,\gamma}_{k_{2d} s_{2d+1}} \, |\{\sigma_i\, s_i\}\rangle \ . \tag{2.22}$$

For all $0-$supported irrep sequences $\boldsymbol{\sigma}$ the states (2.22) define a complete orthonormal basis for $\mathcal{H}^x_\mathbf{0}$, and the problem of constructing an orthonormal basis for the invariant subspace $\mathcal{H}^x_\mathbf{0}$ reduces to finding all possible $0-$supported irrep sequences $\boldsymbol{\sigma}$.

2.4 Gauss Constrained Basis and Truncated Subspace

Define the *Gauss constrained* computational tensor product space $\mathcal{H}_G \subset \mathcal{H}_\text{comp}$ on the lattice,

$$\mathcal{H}_G \equiv \otimes_{x \in \Lambda} \mathcal{H}^x_\mathbf{0} \, . \tag{2.23}$$

Since $\mathcal{H}_\text{phys}$ is just $\mathcal{H}_\text{KS}$ restricted by the Gauss constraint (2.3), we rewrite (2.18) as

$$\mathcal{H}_\text{phys} = \Big\{ |\Psi\rangle \in \mathcal{H}_G \,\Big|\, \mathrm{P}_\mathbf{U}(l)|\Psi\rangle = |\Psi\rangle \, \forall \, l \in \mathrm{L}_\Lambda \, , \tag{2.24a}$$

$$\mathrm{P}_{E_i} \, |\Psi\rangle = |\Psi\rangle \ \forall i \in \{1, \dots, d\} \, , \tag{2.24b}$$

$$\mathrm{P}_{F_i} \, |\Psi\rangle = |\Psi\rangle \ \forall i \in \{1, \dots, d\} \Big\} \, . \tag{2.24c}$$

A basis for $\mathcal{H}_G$ is just the tensor product of states (2.22), $|\{\boldsymbol{\sigma}_x\}\rangle \equiv \otimes_{x \in \Lambda} |\boldsymbol{\sigma}_x\rangle \in \mathcal{H}_G$, where we have left the multiplicity index γ implicit and made the lattice site index explicit. Such tensor product states are easily implemented working with the tensor network formalism, which makes it numerically convenient to work with the constrained basis. To recover the physical subspace (2.24), apply projection operators $\mathrm{P}_\mathbf{U}(l)$ on all neighbouring vertices and P_{E_i}, P_{F_i} at the boundaries.

The infinite dimensional subspace $\mathcal{H}_G$ must of course be truncated in some way for numerical implementation. Recall that every irrep $\sigma_i \in \mathrm{Irrep}(\mathrm{SU}(N))$ can be uniquely characterized by its *irrep weight*, which is a sequence of N non-negative integers. A bijection can be defined between all irreducible representations of $\mathrm{SU}(N)$ and the set of nonnegative integers $\mathbb{N}_0$, inducing a total ordering on $\mathrm{Irrep}(\mathrm{SU}(N))$ [2]. The ordering then allows for a straightforward truncation procedure: define a maximal representation σ_max, and consider only those $0-$supported irrep sequences $\{\sigma_i\}$ with $\sigma_i < \sigma_\text{max} \, \forall i$. The states (2.22) then generate a truncated space $\mathcal{H}^x_\mathbf{0}|_{\sigma_\text{max}} \subset \mathcal{H}^x_\mathbf{0}$ with finite dimension $d_\mathbf{0} = d_\mathbf{0}(\sigma_\text{max})$ polynomial in σ_max. The numerical dimension $d_\mathbf{0}$ can then be adapted for efficiency by adjusting σ_max. The basis for $\mathcal{H}^x_\mathbf{0}|_{\sigma_\text{max}}$ then generates a basis for the truncated Gauss constrained subspace $\mathcal{H}_G|_{\sigma_\text{max}}$.

	E	F	Q
1	0	0	0
2	0	0	B
3	$\frac{1}{2}$	0	$\frac{1}{2}$
4	$\frac{1}{2}$	$\frac{1}{2}$	0
5	$\frac{1}{2}$	$\frac{1}{2}$	B
6	0	$\frac{1}{2}$	$\frac{1}{2}$
7	1	$\frac{1}{2}$	$\frac{1}{2}$
8	1	1	0
9	1	1	B
10	$\frac{1}{2}$	1	$\frac{1}{2}$

(a) $SU(2)$

	E	F	Q
1	0	0	0
2	0	0	B
3	$\overline{3}$	0	3
4	3	0	$\overline{3}$
5	$\overline{3}$	3	0
6	$\overline{3}$	3	B
7	3	3	3
8	$\overline{6}$	3	3
9	0	3	$\overline{3}$
10	8	3	$\overline{3}$
11	3	$\overline{3}$	0
12	3	$\overline{3}$	B
13	0	$\overline{3}$	3
14	8	$\overline{3}$	3
15	$\overline{3}$	$\overline{3}$	$\overline{3}$
16	6	$\overline{3}$	$\overline{3}$
17	$\overline{6}$	6	0
18	$\overline{6}$	6	B
19	8	6	3
20	$\overline{3}$	6	$\overline{3}$
21	6	$\overline{6}$	0
22	6	$\overline{6}$	B
23	3	$\overline{6}$	3
24	8	$\overline{6}$	$\overline{3}$
25	8	8	0
26	8	8	B
27	$\overline{3}$	8	3
28	6	8	3
29	3	8	$\overline{3}$
30	$\overline{6}$	8	$\overline{3}$

(b) $SU(3)$

Table 2: $(1+1)$ Gauss constrained basis $|EFQ\rangle$ for SU(2) with $\sigma_{\max}=1$ and SU(3) with $\sigma_{\max}=8$. Note that in both cases no multiplicity index is necessary.

This truncation method is also "gauge invariant" in the following sense. Since the set of possible representations for the fermionic degrees of freedom is already limited, the truncation only affects the link degrees of freedom. The link operator acts as a creation and annihilation operator on the electric basis states (2.8), and trough equation (2.6) connects between different representations produced by the tensor product decomposition. Algorithmically, the tensor product of irreps is decomposed by generating new integer sequences which result from some bounded linear function of the irrep weights of the product (for details see [2]). For some sensible total ordering prescription, the tensor product of "small enough" irreps should decompose into representations which are "close enough" in the ordering. The kinetic energy of the quantum rigid rotator states (2.22) is proportional to the eigenvalues of the quadratic Casimir operator $\mathbf{E}^2 \equiv E^\alpha E^\alpha$. The Casimir eigenvalues are a polinomial function of the state irrep weights, and low energy states are states transforming under "low enough" representations. A truncation $\sigma_{\max}$ is then in effect an energy cutoff, and choosing a "large enough" $\sigma_{\max}$ truncation should leave low energy physics unperturbed, all interactions remaining within the truncated subspace.

In our work we use an algorithm by Alex et al. [2], which allow us to systematically generate $0-$supported irrep sequences $\boldsymbol{\sigma}$ with cutoff $\sigma_{\max}$. Table 2 shows an example for $(1+1)$ dimensions and gauge groups SU(2) and SU(3).

2.5 Comparison with previous work

Recent research applying tensor network methods to the study of gauge theories is based mainly on two formulations, Quantum Link Models (QLM) [15, 48, 53] and Quantum Simulation Models [69, 70].

The introduction of Quantum Link Models for gauge theories [10, 11, 14] was motivated by the correspondence between classical and quantum statistical field theory. The action in the path integral which is defined over classical field configurations is promoted to an operator acting on a discrete Hilbert space. It is argued that the continuum limit exists and is arrived at by dimensional reduction. In the *rishon* formulation of QLM, anticommuting creation and annihilation operators called rishons are introduced as the fundamental degrees of freedom from which gauge transformation generators and link operators are constructed. The rishons allow the definition of a computational lattice vertex so that the Gauss constraint can be imposed locally, and a gauge invariant basis can be constructed for use with tensor network algorithms [15, 48, 53].

Lattice Gauge Theory for Quantum Simulations was motivated by the exciting possibility of implementing Yang Mills theories using cold atoms in optical lattices [69, 70]. In the quantum simulation formulation, the electric states are realized as excitations on a Fock space, and bosonic creation and annihilation operators are introduced as the fundamental degrees of freedom. The Fock space formulation allows for straightforward truncation to a maximal group representation.

Both of these approaches introduce a new set of creation/annihilation operators and degrees of freedom in order to construct the gauge link operator. In the procedure we describe, no auxiliary operators are introduced. Insted, the gauge field Hilbert space $\mathcal{H}_{\mathbf{U}}$ is expanded to a product space $\mathcal{H}'_{\mathbf{U}}$ as a computational device. The link operator $\mathbf{U}_{ab}$ is only supported on $\mathcal{H}_{\mathbf{U}}$, and the spurious degrees of freedom are removed by projecting to $\mathcal{H}_{\mathbf{U}}$. This projection can be done without extra computational effort by applying it beforehand to the Hamiltonian.

3 Tensor Network Formulation for $(1+1)$ dimensions

In order to study the Hamiltonian (3.1) numerically we make use of tensor network methods. See [43, 44] for an introductory review and [51, 55] for a pedagogical description of the algorithms. In section 3.1 we recall the $(1+1)$ Kogut-Susskind Hamiltonian, in section 3.2 we write a basis for the Gauss constrained subspace $\mathcal{H}_G|_{\sigma_{\max}}$ in $(1+1)$ dimensions, and write the Hamiltonian as a Matrix Product Operator.

3.1 $(1+1)$ SU(N) Kogut-Susskind Hamiltonian

The Kogut-Susskind Hamiltonian for $(1+1)$ Yang-Mills with gauge group SU(N) and staggered fermions in the fundamental representation is given by [26, 27],

$$H = \frac{ag^2}{2}\sum_x \mathbf{E}^2(x) + \frac{1}{2a}\sum_x \Big(\xi_a^\dagger(x)\mathbf{U}_{ab}(x,x+1)\xi_b(x+1) + \text{h.c.}\Big) + m\sum_x (-1)^x \xi_a^\dagger(x)\xi_a(x)\,, \tag{3.1}$$

where a is the lattice spacing, g the coupling constant and m the fermion mass (see Appendix A). Using the fermion number operator $N(x) \equiv \sum_a \xi_a^\dagger(x)\xi_a(x)$, and defining dimensionless parameters $\hat{g} \equiv ag$, $\hat{r} \equiv \frac{m}{g}$, we can write the lattice Hamiltonian (3.1) as a dimensionless operator W

$$W \equiv \frac{2}{ag^2}H = \sum_x W_1(x) + \frac{1}{\hat{g}^2}\sum_x W_2(x,x+1)\,, \tag{3.2}$$

with the one-particle operator W_1 and next-neighbour operator W_2 defined as

$$W_1(x) \equiv \mathbf{E}^2(x) + (-1)^x \frac{2\hat{r}}{\hat{g}} N(x)\,, \tag{3.3}$$

$$W_2(x,x+1) \equiv \xi_a^\dagger(x)\mathbf{U}_{ab}(x,x+1)\xi_b(x+1) + \text{h.c.}\,. \tag{3.4}$$

Usually the fermionic operators $\xi_a^\dagger, \xi_a$ are converted to bosonic spin operators by means of a generalized Jordan Wigner transformation [31, 60], in order to account for the correct field statistics. For SU(2) we can directly calculate the W_2 matrix elements using the gauge invariant basis described in the next section.

3.2 Gauss constrained basis and MPO representation

For (1+1) dimensions each computational vertex is the tensor product of 3 irreps, the fermion representation Q and the neighbouring link generators E and F. The basis states (2.22) are labeled $|E\,F\,Q\,\gamma\rangle$, and the singlet subspace can be easily projected using the SU(N) Wigner 3-j symbols (B.3)

$$|\boldsymbol{\sigma},\gamma\rangle = |E\,F\,Q\,\gamma\rangle \equiv \sum_{m,n,q} \left(\begin{smallmatrix} E & F & Q_\gamma \\ m & n & q \end{smallmatrix}\right) |Em\,Fn\,Q_\gamma q\rangle\ . \tag{3.5}$$

Note that the requirement that $\boldsymbol{\sigma}$ be 0−supported is equivalent to the requirement that the corresponding Wigner 3-j symbols be nonzero for some combination of m,n,q. For SU(2) this is the triangle condition $|E-F| \le Q \le E+F$. The tensor product of states $|EFQ\gamma\rangle$ with cutoff $\sigma_{\max}$ then build a basis for the Gauss constrained subspace $\mathcal{H}_G|_{\sigma_{\max}}$. In the following the multiplicity index γ will be left implicit. An example of the basis $|EFQ\rangle$ for SU(2) and SU(3) is listed in Table 2.

The Hamiltonian operators (3.3) and (3.4) are defined on the Kogut-Susskind lattice $\mathcal{H}_{\rm KS}$, which is embedded in the computational lattice $\mathcal{H}_{\rm comp}$. To evaluate matrix elements of operators $\hat{O}$ supported on $\mathcal{H}_{\rm KS} \subset \mathcal{H}_{\rm comp}$, use relations (3.5),

$$\begin{aligned}\langle \boldsymbol{\sigma}'|\hat{O}|\boldsymbol{\sigma}\rangle &= \langle E'\,F'\,Q'|\hat{O}|E\,F\,Q\rangle \\ &= \sum_{m',n',q'}\sum_{m,n,q} \begin{pmatrix} E' & F' & Q' \\ m' & n' & q' \end{pmatrix}\begin{pmatrix} E & F & Q \\ m & n & q \end{pmatrix} \langle E'm'\,F'n'\,Q'q'|\,\hat{O}\,|Em\,Fn\,Qq\rangle\ .\end{aligned} \tag{3.6}$$

The 1-body operator $W_1(x)$ acts diagonally on the Gauss invariant subspace,

$$W_1^{\sigma'_x\sigma_x} \equiv \langle \boldsymbol{\sigma}'_x|W_1|\boldsymbol{\sigma}_x\rangle = \left(E_x^2 + (-1)^x\frac{2\hat{r}}{\hat{g}}N_x\right) I^{\sigma'_x\sigma_x}\,, \tag{3.7}$$

where with some abuse of notation we have denoted the quadratic Casimir eigenvalue of irrep E with E^2, and $I^{\sigma'_x\sigma_x}$ is the unit matrix in the Gauss constrained basis. To evaluate the 2-body operator $W_2(x,x+1)$ we must first project back to the quantum rotator space $\mathcal{H}_{\mathbf{U}}$ with the help of projection operator $\mathrm{P}_{\mathbf{U}}(l)$ (2.16). Further, to take advantage of tensor network algorithms, the 2-body operator is written as a Kronecker product of 1-body operators U_k, V_k by finding the singular value decomposition (SVD) of a specific permutation of the matrix elements of W_2 [38].

$$\begin{aligned}W_2^{\sigma'_x\sigma'_{x+1}\sigma_x\sigma_{x+1}} &\equiv \langle \boldsymbol{\sigma}'_x\boldsymbol{\sigma}'_{x+1}|\,\mathrm{P}_{\mathbf{U}}(l)W_2\,\mathrm{P}_{\mathbf{U}}(l)|\boldsymbol{\sigma}_x\boldsymbol{\sigma}_{x+1}\rangle = \delta_{\overline{E'}_x,F'_{x+1}}\delta_{\overline{E}_x,F_{x+1}}\langle \boldsymbol{\sigma}'_x\boldsymbol{\sigma}'_{x+1}|W_2|\boldsymbol{\sigma}_x\boldsymbol{\sigma}_{x+1}\rangle \\ &= \sum_k \langle \boldsymbol{\sigma}'_x|U_k|\boldsymbol{\sigma}_x\rangle \otimes \langle \boldsymbol{\sigma}'_{x+1}|V_k|\boldsymbol{\sigma}_{x+1}\rangle = \sum_k U_k^{\sigma'_x\sigma_x}\otimes V_k^{\sigma'_{x+1}\sigma_{x+1}}\ .\end{aligned} \tag{3.8}$$

The dimensionless Hamiltonian matrix $W^{\boldsymbol{\sigma}'\boldsymbol{\sigma}}$ (3.2) can then be decomposed as a series of Matrix Product Operators (MPOs) [51],

$$\begin{aligned}W^{\boldsymbol{\sigma}'\boldsymbol{\sigma}} \equiv \langle\{\boldsymbol{\sigma}'_x\}|W|\{\boldsymbol{\sigma}_x\}\rangle &= \sum_{x=1}^{L}\left(E_x^2 + (-1)^x\frac{2\hat{r}}{\hat{g}}N_x\right) I^{\sigma'_x\sigma_x} + \frac{1}{\hat{g}^2}\sum_{x=1}^{L-1}\sum_k U_k^{\sigma'_x\sigma_x}\otimes V_k^{\sigma'_{x+1}\sigma_{x+1}} \\ &= W^{[1]\sigma'_1\sigma_1}W^{[2]\sigma'_2\sigma_2}\ldots W^{[L]\sigma'_L\sigma_L}\ .\end{aligned} \tag{3.9}$$

The state vector $|\Psi\rangle \in \mathcal{H}_G|_{\sigma_{\max}}$ written as a Matrix Product State (MPS) serves as variational ansatz for the groundstate search

$$|\Psi\rangle = A^{[1]\sigma_1}A^{[2]\sigma_2}\ldots A^{[L]\sigma_L}|\boldsymbol{\sigma}_1\rangle\,|\boldsymbol{\sigma}_2\rangle\ldots|\boldsymbol{\sigma}_L\rangle\,. \tag{3.10}$$

4 Results for $(1+1)$ dimensional SU(2) Lattice Gauge Theory

In this section we present numerical calculations using the Gauss constrained basis constructed in the previous sections. We calculate the ground state energy and entanglement entropy for $(1+1)$ dimensional SU(2) LGT, replicating the results by Bañuls et al. [7]. We also briefly summarize the difficulties defining entanglement entropy for lattice gauge theories. As was already argued by various authors [3, 37, 56], we find that only the full entanglement entropy formula (4.6) delivers the expected results in the continuum limit.

For this work, we have developed a proof of concept tensor network library [19] which implements the standard variational optimization algorithm for Matrix Product States with two-site tensor update, as described in [51, 55]. The SU(2) irrep sequences and Clebsch-Gordan phases are determined numerically using an algorithm by Alex and collaborators [2]. The eigenvalue problem is solved with the help of PRIMME [59] and the singular value decomposition is computed using the open-source BLAS implementation OpenBLAS [66]. Tensor contraction and transposition is done using the libraries TCL and HPTT [57, 58]. The nonlinear regression is done with LMFIT [41].

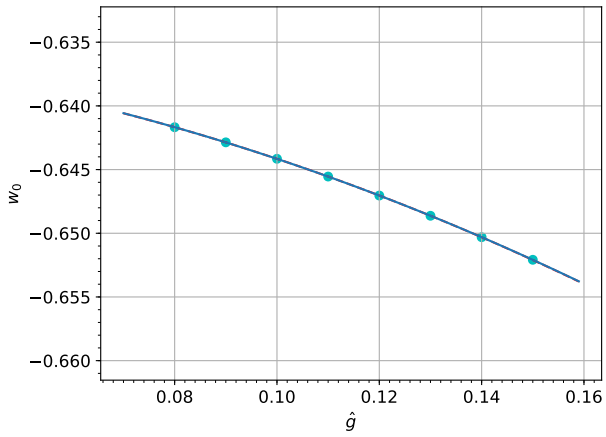

Figure 1: Continuum extrapolation of the ground state energy density w_0 for $\hat{r} = 0.8$.

4.1 Ground state energy

We compute the ground state of the dimensionless Hamiltonian (3.2) written as an MPO (3.9), using the MPS Ansatz (3.10) on the truncated subspace with $\sigma_{\max} = 3/2$, for the parameter range $L \in \{100, 200\}$, $\hat{r} \in \{0.4, 0.8, 1.2\}$, $\hat{g} \in \{0.08, 0.09, \ldots, 0.15\}$, $D \in \{60, 100, 140, 200\}$. We follow the extrapolation methods and error estimation described in [7]. From the results at various bond dimensions the limit $1/D \to 0$ is calculated. The thermodynamic limit is found by fitting to a polynomial in $1/L$ [25]. Finally the continuum limit is extrapolated by fitting to a polynomial in $\hat{g}$. Figure 1 shows the result for $\hat{r} = 0.8$.

In the continuum limit $\hat{g} \to 0$ the W_2 operator (3.4) dominates, the Hamiltonian (3.2) becomes the XY antiferromagnetic spin model for 2 massless fermions, and the expected energy density is [27]

$$w_0 = \lim_{\substack{L\to\infty \\ \hat{g}\to 0}} \frac{\hat{g}^2}{2}\frac{E_0}{L} = -\frac{2}{\pi} = -0.6366. \tag{4.1}$$

The computed results are shown in table 3.

$\hat{r}$	w_0	δw_0	$w_0 + 2/\pi$
0.40	−0.6366	$1.2 \cdot 10^{-5}$	$6.5 \cdot 10^{-5}$
0.80	−0.6356	$8.3 \cdot 10^{-5}$	$9.9 \cdot 10^{-4}$
1.20	−0.6340	$1.5 \cdot 10^{-4}$	$2.6 \cdot 10^{-3}$

Table 3: Fitted value of w_0 with estimated error δw_0.

4.2 Entanglement entropy

Entanglement is a fundamental property of composite quantum systems [64], see [42] for a review from the perspective of quantum field theory. In the context of gauge theories, the proper definition of entanglement entropy is a subtle problem [4, 13, 16, 37, 56, 62]. Given a spatial bipartition of the lattice degrees of freedom into a connected region A and its complement B, let $\mathcal{A}_A$, $\mathcal{A}_B$ be the algebra of gauge invariant operators supported on A and B respectively. The center $\mathcal{Z}_A$ of the algebra $\mathcal{A}_A$, $\mathcal{Z}_A = \mathcal{A}_A \cap \mathcal{A}_B$, is in general not trivial, so that the physical (gauge invariant) Hilbert space $\mathcal{H}_{\text{phys}}$ of the theory does not factorize as a tensor product of gauge invariant subspaces $\mathcal{H}^A_{\text{phys}} \otimes \mathcal{H}^B_{\text{phys}}$.

A natural approach to the problem is to consider an *extended* Hilbert space $\mathcal{H}$ defined as a tensor product over all degrees of freedom i on the lattice (vertices, links, etc.), $\mathcal{H} = \otimes_i \mathcal{H}_i$. The physical Hilbert space is then given by an embedding, $\mathcal{H}_{phys} \to \mathcal{H}$, and the extended Hilbert space does trivially factorize as a tensor product $\mathcal{H} = \mathcal{H}^A \otimes \mathcal{H}^B$ of sublattices $\mathcal{H}^A = \otimes_{i\in A}\mathcal{H}_i$ and $\mathcal{H}^B = \otimes_{i\in B}\mathcal{H}_i$. The *reduced density matrix* (RDM) ρ^A for sublattice A can then be unambiguously constructed from a density matrix ρ defined on

the extended space $\mathcal{H}$ by tracing over all degrees of freedom in B, $\rho^A \equiv \mathrm{Tr}_{\mathcal{H}^B}\,\rho$. The corresponding *full entanglement entropy* S^A is the von Neumann entropy

$$S^A = -\,\mathrm{Tr}_{\mathcal{H}^A}\;\rho^A \log\left(\rho^A\right)\,. \tag{4.2}$$

For a discussion on the extended Hilbert space construction see [16, 37, 56, 62]. Here we recall the main results. Denote with ∂A the boundary of sublattice A, containing $|\partial A|$ lattice degrees of freedom. Let each simplex $i \in \partial A$ carry a representation $r_i \in \mathrm{Irrep}\,G$ of the group. The choice of $|\partial A|$ such representations defines a *superselection sector* $\vec{r} = (r_1, \ldots, r_{|\partial A|})$, and the extended Hilbert subspace decomposes as a direct sum over all possible sectors $\vec{r}$, $\mathcal{H}^A = \oplus\mathcal{H}^A_{\vec{r}}$. The superselection sector partitioning $\vec{r}$ cannot be modified by gauge invariant operators acting locally on A, and state superposition is allowed only within each partition. It follows that the reduced density matrix ρ^A has block diagonal structure, $\rho^A = \oplus_{\vec{r}}\,\rho^A_{\vec{r}}$. Further, for each superselection sector $\vec{r}$, the corresponding Hilbert space $\mathcal{H}^A_{\vec{r}}$ decomposes to a tensor product $\mathcal{H}^A_{\vec{r}} \cong (\otimes_i \mathbb{V}_{r_i}) \otimes \bar{\mathcal{H}}^A_{\vec{r}}$ of boundary spaces $\mathbb{V}_{r_i}$ carrying group irreps r_i and a *bulk* space $\bar{\mathcal{H}}^A_{\vec{r}}$. Any gauge invariant operator can act non-trivially only on the bulk space $\bar{\mathcal{H}}^A_{\vec{r}}$. The reduced density matrix ρ^A may then be written as

$$\rho^A = \bigoplus_{\vec{r}} \rho^A_{\vec{r}} = \bigoplus_{\vec{r}} p^A_{\vec{r}} \left(\bigotimes_{r_i} \frac{\mathbf{1}_{r_i}}{\dim r_i}\right) \otimes \bar{\rho}^A_{\vec{r}}\,. \tag{4.3}$$

with the superselection sector probabilities $p^A_{\vec{r}}$ defined as $p^A_{\vec{r}} \equiv \mathrm{Tr}_{\mathcal{H}^A_{\vec{r}}}\,\rho^A_{\vec{r}}$. The full entanglement entropy (4.2) is then given as the sum of *classical*, *boundary* and *bulk* contributions,

$$S^A = -\sum_{\vec{r}} p^A_{\vec{r}}\,\log\left(p^A_{\vec{r}}\right) + \sum_{\vec{r}} p^A_{\vec{r}}\,\log\left(\dim\,\vec{r}\right) - \sum_{\vec{r}} p^A_{\vec{r}}\,\mathrm{Tr}_{\bar{\mathcal{H}}^A_{\vec{r}}}\,\bar{\rho}^A_{\vec{r}}\log\left(\bar{\rho}^A_{\vec{r}}\right)\,, \tag{4.4}$$

with $\dim\,\vec{r} = \prod_i \dim\,r_i$. Since the probabilities $p^A_{\vec{r}}$ and representation dimensions $\dim\,r_i$ are fixed for each partitioning $\vec{r}$, the classical and boundary terms in (4.4) cannot be manipulated using gauge invariant operators. Only the bulk entanglement is physically extractable by LOCC, hence it is also called *extractable* or *distillable* entanglement entropy [56, 62]. Further, if the trace (4.2) is restricted to the *physical* subspace $\mathcal{H}^A_{\mathrm{phys}} \subset \mathcal{H}^A$, it can be shown that the resulting entanglement entropy does not include the boundary term present in (4.4) [37, 56]. The degrees of freedom at the boundaries must couple to form a singlet representation of the group, and are determined by the degrees of freedom in the bulk. Such a restriction defines the *electric center* entanglement entropy S^A_{ec},

$$S^A_{\mathrm{ec}} = -\sum_{\vec{r}} p^A_{\vec{r}}\,\log\left(p^A_{\vec{r}}\right) - \sum_{\vec{r}} p^A_{\vec{r}}\,\mathrm{Tr}_{\bar{\mathcal{H}}^A_{\vec{r}}|_{\mathrm{phys}}}\,\bar{\rho}^A_{\vec{r}}\log\left(\bar{\rho}^A_{\vec{r}}\right)\,. \tag{4.5}$$

Projecting to the singlet subspace $G = 0$ and using basis (2.22) we recover from our calculations only the electric center entanglement entropy (4.5). In order to reconstruct the full entanglement entropy (4.4), the boundary term $\log\dim r_i$ must be added to (4.5),

$$S^A = S^A_{\mathrm{ec}} + \sum_{\vec{r}} p^A_{\vec{r}}\,\log\left(\prod_i \dim\,r_i\right)\,. \tag{4.6}$$

The question immediately arises of which definition of the entanglement entropy is the correct one to use in calculations, and what significance if any may be attributed to the physically inaccesible boundary components of the entropies (4.4) and (4.5) [2]. Soni and Trivedi [56] calculated the topological entanglement entropy for a class of non-abelian toric codes and showed that the correct result is given by the full entanglement entropy (4.4). Aoki et al. [3] established that all three components of the full entanglement entropy (4.4) appear in the hopping parameter expansion for a $(1+1)$ $SU(N)$ Yang-Mills theory with matter in the fundamental representation, and argued that this should hold in the continuum theory. Lin and Radičević [37] conjecture that precisely the full entanglement entropy correctly computes universal terms of a CFT.

Our own results show that only the full entanglement entropy (4.6) accurately estimates the expected value of the CFT central charge for $(1+1)$ SU(2) Yang-Mills with fundamental matter.

[2] Compare this problem with a recent discussion on the basis dependence of holographic complexity [28].

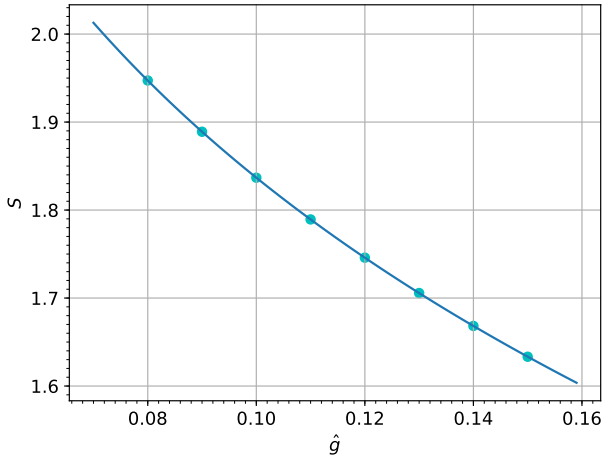

Figure 2: Continuum extrapolation of the full entanglement entropy for $L = 200$ and $\hat{r} = 0.8$.

L	$\hat{r}$	c	δc	$2 - c$
100	0.40	1.963	$2.9 \cdot 10^{-3}$	$3.7 \cdot 10^{-2}$
200	0.40	2.007	$3.3 \cdot 10^{-3}$	$-7.5 \cdot 10^{-3}$
100	0.80	1.975	$3.3 \cdot 10^{-3}$	$2.5 \cdot 10^{-2}$
200	0.80	1.978	$3.9 \cdot 10^{-3}$	$2.2 \cdot 10^{-2}$
100	1.20	1.938	$1.7 \cdot 10^{-3}$	$6.2 \cdot 10^{-2}$
200	1.20	1.939	$1.7 \cdot 10^{-3}$	$6.1 \cdot 10^{-2}$

Table 4: Values of the central charge c obtained from a least squares fit to the the function (4.7) for different values of L and $\hat{r}$.

As described in [7], the ground state entanglement entropy for a partition along the center of the lattice should display a logarithmic functional dependence on $\hat{g}$ for small coupling constant g [12], with linear corrections due to lattice effects

$$S^A(\hat{g}) = -\frac{c}{6}\log(\hat{g}) + c_2\hat{g} + c_3 + O\left(\hat{g}^2\right) , \tag{4.7}$$

with the central charge expected to correspond to the number of fermionic degrees of freedom $c = 2$. Within the MPS formalism the entanglement entropy is directly accesible from a singular value decomposition. Since we already work using the Gauss constrained subspace, the SVD gives the electric center entanglement entropy S^A_{ec}. For $(1+1)$ dimensions, label the superselection sectors with $j \in \text{Irrep}(G)$, then the full entanglement entropy is given by

$$\begin{aligned} S^A &= -\sum_j p_j^A \log\left(p_j^A\right) - \sum_j p_j^A \,\text{Tr}_{\bar{\mathcal{H}}_j^A}\, \bar{\rho}_j^A \log\left(\bar{\rho}_j^A\right) + \sum_j p_j^A \log(\dim\, j) \\ &= S^A_{\text{ec}} + \sum_j p_j^A \log(\dim\, j) \ . \end{aligned} \tag{4.8}$$

From the ground state MPS calculated in section 4.1 we calculate the half chain RDMs $\rho_j^{L/2}$ for each superselection sector j by projecting to the j subspace. For each sector we compute the log dim boundary term and using equation (4.8) recover the full entanglement entropy $S^{L/2}$ for a partition along the center of the chain and for different values of the coupling constant g and parameters L, $\hat{r}$. Results of the least squares fit to function (4.7) for various values of L and $\hat{r}$ are given in Table 4. Figure 2 shows an example for $L = 200$ and $\hat{r} = 0.8$. Only the full entanglement formula (4.8) delivers values of c near 2, as discussed previously.

5 Conclusion and future work

We have shown how to construct a basis for the Gauss constrained subspace of the computational lattice Hilbert space $\mathcal{H}_G \subset \mathcal{H}_{\text{comp}}$ by finding all $0-$supported irrep sequences σ at each vertex $x \in \Lambda$. All such sequences σ together with a multiplicity index γ label an orthonormal basis of the gauge invariant subspace $\mathcal{H}^x_{\mathbf{0}}$. We have algorithmically constructed such a basis for SU(2) and SU(3) using a routine by Alex et al. [2]. We write the $(1+1)$ SU(N) Kogut-Susskind Hamiltonian with fundamental fermions in this basis, and decompose it as a Matrix Product Operator. For $(1+1)$ SU(2) we find the ground state energy and entanglement entropy at half-lenght. We check that the right energy density and entanglement entropy functional dependence is found, comparing our results with [7], from which the extrapolation and numerical error estimation procedures are taken. We also find that only the full entanglement entropy formula (4.4) gives the correct estimation for the CFT central charge.

This work has served to demostrate the viability of the constrained Gauss basis. Generalizing to $N > 2$ and higher fermion representations will be the subject of future investigations.

A Kogut-Susskind Formulation of Yang-Mills Theory

In order to set up our notation let us quickly review here the Kogut-Susskind Hamiltonian formulation of $(d+1)$ Yang-Mills Theory on the lattice [33–35] with staggered fermions [61].

A.1 Hamiltonian Formalism and Gauss Law

The Yang-Mills Lagrangian $\mathscr{L}$ for a semisimple Lie group G (the *gauge* group) and N_f matter fields ψ_n in the fundamental representation is given by [63]

$$\mathscr{L} = -\frac{1}{2}\operatorname{Tr} F^{\mu\nu}F_{\mu\nu} - \sum_{n=1}^{N_f}\overline{\psi}_n\left(i\not{D} - m_n\right)\psi_n\,, \tag{A.1}$$

where $F_{\mu\nu} \equiv F^\alpha_{\mu\nu}T^\alpha \equiv \frac{i}{g}\left[D_\mu, D_\nu\right]$, $D_\mu \equiv \partial_\mu - igA^\alpha_\mu T^\alpha$, $\not{D} \equiv \gamma^\mu D_\mu$, γ^μ the Dirac matrices, g the coupling constant of the theory, m_n the fermion masses, and T^α are the hermitian generators of the algebra $\mathfrak{g}$ of G in the fundamental representation, with commutation relations $[T^\alpha, T^\beta] = if^{\alpha\beta\gamma}T^\gamma$ and norm $\operatorname{Tr}(T^\alpha T^\beta) = \frac{1}{2}\delta^{\alpha\beta}$. Note that from (A.1) follows $\frac{\partial\mathscr{L}}{\partial A^\alpha_0} = 0$, which represents a primary constraint [24, 50]. The canonical Hamiltonian density $\mathscr{H}$ corresponding to (A.1) is then given by

$$\mathscr{H} = \frac{1}{2}\left(\mathbf{E}\cdot\mathbf{E} + \mathbf{B}\cdot\mathbf{B}\right) - \sum_{n=1}^{N_f}\bar{\psi}_n\left(i\not{\mathbf{D}} - m_n\right)\psi_n - A^\alpha_0\left(\mathbf{D}^{\alpha\beta}\cdot\mathbf{E}^\beta + gQ^\alpha\right)\,, \tag{A.2}$$

with the electric field operator $E^\alpha_i \equiv F^\alpha_{0i}$, magnetic field operator $B^\alpha_i \equiv \frac{1}{2}\epsilon_{ijk}F^\alpha_{jk}$, ϵ_{ijk} the 3-dim Levi-Civita symbol, spatial covariant derivative $D^{\alpha\beta}_i \equiv \partial_i\delta^{\alpha\beta} + gf^{\alpha\beta\gamma}A^\gamma_i$, and charge operator $Q^\alpha \equiv \sum_{n=1}^{N_f}\psi^\dagger_n T^\alpha\psi_n$. This is a generalized Hamiltonian system with first class constraints [18], and we may interpret A^α_0 as a Lagrange multiplier which when the system is quantized in the Weyl gauge $A^\alpha_0 = 0$ imposes upon the physical Hilbert space $\mathcal{H}_{\text{phys}}$ the Gauss Law

$$G^\alpha \equiv \mathbf{D}^{\alpha\beta}\cdot\mathbf{E}^\beta + gQ^\alpha = 0\,. \tag{A.3}$$

In the Hamiltonian quantum formulation, the Gauss Law (A.3) is no longer an automatic consequence of the equations of motion but has to be enforced as a restriction on the Hilbert space [30].

A.2 Kogut-Susskind Lattice Gauge Theory

Introduce a finite $d-$dimensional spatial lattice Λ

$$\Lambda \equiv \left\{ x = (x_1, \ldots, x_d) \,\middle|\, x_i \in a\mathbb{Z}\,,\, 0 \leq x_i \leq L \right\}, \tag{A.4}$$

with lattice spacing a and side-lenght L. Allow the time variable t to remain continuous. For convenience we also define the set L_Λ of positevely oriented links of Λ,

$$\mathrm{L}_\Lambda \equiv \left\{ (x, \hat{e}_i) \middle| x, x + \hat{e}_i \in \Lambda \right\}, \tag{A.5}$$

where $\hat{e}_i$ is a unit lattice vector (in lattice units a) in the positive i direction.

On each lattice site $x \in \Lambda$ define a fermionic field operator $\xi_a(x)$ obeying anticommutation relations

$$\{\xi_a(x), \xi_b(y)\} = 0\,,\, \left\{\xi_a^\dagger(x), \xi_b(y)\right\} = \delta_{ab}\delta_{xy}\,, \tag{A.6}$$

transforming locally under the fundamental representation of a gauge symmetry group G:

$$\xi_a(x) \to \Omega_{ab}(x)\xi_b(x)\,,\, \Omega_{ab}(x) \in G\,. \tag{A.7}$$

The corresponding generator (conserved Noether charge) of local gauge transformations $Q^\alpha(x)$ at x can be infered by considering an infinitesimal gauge transformation $\delta_\epsilon \xi_a(x) = i\left[\epsilon^\alpha Q^\alpha(x), \xi_a(x)\right] = i\epsilon^\alpha T^\alpha_{ab}\xi_b(x)$. It follows that Q^α may be expressed as a bilinear in the fields

$$Q^\alpha(x) = \xi_a^\dagger(x) T^\alpha_{ab} \xi_b(x)\,, \tag{A.8}$$

and obeys the commutation relations for G

$$\left[Q^\alpha(x), Q^\beta(y)\right] = \delta_{xy} i f^{\alpha\beta\gamma} Q^\gamma(x)\,. \tag{A.9}$$

Demanding *local* gauge invariance for the fermionic fields $\xi_a(x)$ at each $x \in \Lambda$ requires the introduction of an oriented gauge connection operator $\mathbf{U}_{ab}(x, \hat{e}_i)$ for each lattice link $(x, \hat{e}_i) \in \mathrm{L}_\Lambda$ transforming as

$$\mathbf{U}_{ab}(x, \hat{e}_i) \to \Omega_{ac}(x)\mathbf{U}_{cd}(x, \hat{e}_i)\Omega^{-1}_{db}(x + \hat{e}_i)\,. \tag{A.10}$$

The oriented link operator $\mathbf{U}_{ab}(x, \hat{e}_i)$ therefore connects local gauge transformations between x and $x + \hat{e}_i$. The negative orientation is defined as the inverse operator

$$\mathbf{U}_{ab}(x, -\hat{e}_i) \equiv \mathbf{U}^{-1}_{ab}(x - \hat{e}_i, \hat{e}_i)\,. \tag{A.11}$$

Note from (A.10) that left and right indices of the link operator $\mathbf{U}_{ab}$ transform independently under gauge transformations, as required by local gauge invariance. These left and right link transformations are induced by local generators $E^\alpha(x, \hat{e}_i) \equiv E^\alpha_i(x)\hat{e}_i$ and $F^\alpha(x, \hat{e}_i) \equiv F^\alpha_i(x)\hat{e}_i$ of the Lie algebra $\mathfrak{g}$ at each site $x \in \Lambda$. In contrast to the link operator $\mathbf{U}_{ab}$, the gauge generators transform locally at each site [46]

$$E_{ab}(x, \hat{e}_i) \to \Omega_{ac}(x) E_{cd}(x, \hat{e}_i)\Omega^{-1}_{db}(x)\,, \tag{A.12}$$

They satisfy the commutation relations

$$\left[E^\alpha_i(x), E^\beta_j(y)\right] = \delta_{xy}\delta_{ij} i f^{\alpha\beta\gamma} E^\gamma_i(x)\,,\, \left[F^\alpha_i(x), F^\beta_j(y)\right] = \delta_{xy}\delta_{ij} i f^{\alpha\beta\gamma} F^\gamma_i(x)\,,\, \left[E^\alpha_i(x), F^\beta_j(y)\right] = 0\,. \tag{A.13}$$

The commutations relations with $\mathbf{U}_{ab}(x, \hat{e}_i)$ follow directly from (A.10)

$$[E^\alpha_i(x), \mathbf{U}_{ab}(y, \hat{e}_j)] = -\delta_{xy}\delta_{ij} T^\alpha_{ac}\mathbf{U}_{cb}(x, \hat{e}_i)\,,\, [F^\alpha_i(x + \hat{e}_i), \mathbf{U}_{ab}(y, \hat{e}_j)] = \delta_{xy}\delta_{ij}\mathbf{U}_{ac}(x, \hat{e}_i) T^\alpha_{cb}\,. \tag{A.14}$$

Define the link operator $\mathbf{U}_{ab}(x, \hat{e}_i)$ in terms of a lattice vector potential $A^\alpha(x, \hat{e}_i) \equiv A^\alpha_i(x)\hat{e}_i$,

$$\mathbf{U}(x, \hat{e}_i) \equiv \exp\left(iagT^\alpha A^\alpha(x, \hat{e}_i)\right). \tag{A.15}$$

Writing $\delta_a(x-y) \equiv \frac{1}{a}\delta_{x,y}$, it follows from (A.14)

$$\left[gE_i^\alpha(x), A_j^\beta(y)\right] = i\delta^{\alpha\beta}\delta_{ij}\delta_a(x-y)\,. \tag{A.16}$$

Equation (A.16) identifies the rescaled generator $gE_i^\alpha(x)$ as the canonical operator conjugate to $A_i^\alpha(x)$. In the continuum limit, (A.16) becomes the familiar canonical commutation relation for the electric field $E_\mu(x)$ and vector potential $A_\mu(x)$ in the Weyl gauge [30]. Note that the lattice field $F_i^\alpha(x)$ is not an extra degree of freedom, but is related to $E_i^\alpha(x)$ trough parallel transport,

$$F^\alpha(x+\hat{e}_i, \hat{e}_i) = -M^{\alpha\beta}(x, \hat{e}_i)E^\beta(x, \hat{e}_i)\,, \tag{A.17}$$

with the lattice parallel transport operator $M^{\alpha\beta}(x, \hat{e}_i)$ defined as [35, 49]

$$M^{\alpha\beta}(x, \hat{e}_i) \equiv 2\,\mathrm{Tr}\left(\mathbf{U}(x, \hat{e}_i)T^\alpha\mathbf{U}^{-1}(x, \hat{e}_i)T^\beta\right)\,. \tag{A.18}$$

The Hilbert space $\mathcal{H}_{KS}$ for the Kogut-Susskind lattice formulation can be written as the tensor product of fermionic and gauge degrees of freedom,

$$\mathcal{H}_{KS} \equiv \otimes_{x\in\Lambda}\mathcal{H}_Q^x \otimes_{l\in \mathrm{L}_\Lambda} \mathcal{H}_{\mathbf{U}}^l\,, \tag{A.19}$$

where $\mathcal{H}_Q^x$ is the staggered fermion Hilbert space at lattice site $x \in \Lambda$, and $\mathcal{H}_{\mathbf{U}}^l$ the gauge field Hilbert space at lattice link $l \in \mathrm{L}_\Lambda$. The continuum Gauss operator $G^\alpha(x)$ when discretized becomes the lattice operator

$$G^\alpha(x) = \sum_i E_i^\alpha(x) + \sum_i F_i^\alpha(x) + Q^\alpha(x)\,. \tag{A.20}$$

The physical lattice Hilbert space $\mathcal{H}_{phys}$ is then given by imposing (A.20) on $\mathcal{H}_{KS}$,

$$\mathcal{H}_{phys} \equiv \left\{ |\Psi\rangle \in \mathcal{H}_{KS} \,\middle|\, G^\alpha(x)|\Psi\rangle = 0\,\forall x \in \Lambda \right\}. \tag{A.21}$$

B SU(N) Clebsch-Gordan coefficients

We recall here some definitions regarding the irreducible representations of SU(N) as a way to introduce our notation. A texbook introduction to the theory of Lie groups is found in [23], a pedagogical exposition of SU(N) representation theory is given in [2]. See also [5, 6, 9].

Let Irrep(SU(N)) be the index set of all irreducible representation (irreps) of SU(N). We label irreps with capital latin letters $E, F, G, \ldots$ or the lowercase greek letter σ. Given an irrep $J \in \mathrm{Irrep}(\mathrm{SU}(N))$, denote with T_J^α the hermitian generators of infinitesimal SU(N) transformations, carrying Lie algebra index $\alpha = 1, \ldots, N^2-1$ and acting on the *carrier space* $\mathbb{V}_J$ of J with dimension $\dim J = \dim \mathbb{V}_J$.

Each irrep $J \in \mathrm{Irrep}(\mathrm{SU}(N))$ is uniquely characterized by a set of N non-negative integers, called the *irrep weight* of J. Further, the orthonormal basis vectors spanning $\mathbb{V}_J$ can be labeled uniquely with the help of triangular arrangements of non-negative integers satisfying some constraints, called *Gelfand-Tsetlin* (GT) patterns [2, 5]. The top row of a valid GT pattern is always the irrep weight of some irrep J, so that each valid GT pattern corresponds exclusively to one single irrep, and one single irrep can produce many valid GT patterns. We label GT patterns with lowercase latin letters $m, n, \ldots$ and write $m \in J$ to denote that the GT pattern m corresponds to an irrep J. Each pattern $m \in J$ is uniquely associated to an orthonormal basis vector $|m\rangle$ of the carrier space $\mathbb{V}_J$, so that the linear span of the set of all vectors $\{|m\rangle | m \in J\}$ is $\mathbb{V}_J$ and the number of all possible valid GT patterns m for a given irrep J is $\dim J$.

The matrix elements of any operator $\hat{O}$ acting on $\mathbb{V}_J$ are written as $(\hat{O})_{mn} \equiv \langle m|\hat{O}|n\rangle$. In particular the matrix elements of the SU(N) generators T^α in the J representation are $(T_J^\alpha)_{mn} \equiv \langle m|T_J^\alpha|n\rangle$.

The label $m \in J$ thus simultaneously denotes a valid GT pattern of J, a specific vector of the carrier space basis, and the corresponding matrix elements. When necessary, we sometimes make the irrep J of m explicit and write $|m\rangle = |Jm\rangle$.

Given an irrep $J \in \mathrm{Irrep}(\mathrm{SU}(N))$, the *weights* $\mu_m = (\mu_m^\beta)$ for each state $|m\rangle$ are the sets of eigenvalues of the $N-1$ Cartan generators H^β of the algebra, $H^\beta|m\rangle = \mu_m^\beta|m\rangle$. For some ordering convention, a *highest weight* $\mu_J = (\mu_J^\beta)$ can be defined for every representation J. We abuse our notation somewhat and also use μ_J to label the highest weight state of J, so that $H^\beta|\mu_J\rangle = \mu_J^\beta|\mu_J\rangle$.

The *conjugation operation* for $\mathrm{SU}(N)$ uniquely assigns to each irrep $J \in \mathrm{Irrep}(\mathrm{SU}(N))$ a corresponding *conjugate representation* $\bar{J} \in \mathrm{Irrep}(\mathrm{SU}(N))$. Further, each GT pattern $m \in J$ is uniquely assigned a corresponding *conjugate pattern* $\bar{m} \in \bar{J}$, and each basis state $|m\rangle$ is uniquely assigned a corresponding *conjugate state* $|\bar{m}\rangle$,

$$|m\rangle \to (-1)^{w(\mu_J)-w(m)}\,|\bar{m}\rangle\ . \tag{B.1}$$

The scalar function $w(m)$ depends solely on the GT pattern $m \in J$, and in effect specifies a *phase convention* for the conjugation operation (B.1) [6].

We write $J \in J_1 \otimes J_2$ to denote that J is included in the product representation $J_1 \otimes J_2$, that is $J_1 \otimes J_2 = N^J_{J_1 J_2}\, J \oplus \cdots$. The multiplicity index $\gamma = 1 \cdots N^J_{J_1 J_2}$ serves to distinguish between multiple instances of irrep J in the decomposition.

The $\mathrm{SU}(N)$ Clebsch-Gordan coefficients are written

$$C^m_{m_1 m_2} \equiv \langle m_1, m_2 | m\rangle\,. \tag{B.2}$$

The $\mathrm{SU}(N)$ Wigner 3-j symbols are defined as

$$\left(\begin{smallmatrix} J_1 & J_2 & J \\ m_1 & m_2 & m \end{smallmatrix}\right) \equiv \frac{(-1)^{w(\mu_J)-w(m)}}{\sqrt{\dim J}} \langle m_1, m_2 | \bar{m}\rangle\,. \tag{B.3}$$

where we have left the irrep labels explicit, and the phase convention is the same as in (B.1).

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