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Exploring different Formulations of non-Abelian Lattice Gauge Theories for Hamiltonian simulation

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Hamiltonian formulation of lattice gauge theories provides the natural framework for the purpose of quantum simulation, an area of research that is growing with advances in quantum-computing algorithms and hardware. It is therefore important to identify the most accurate, while computationally economic, Hamiltonian formulation(s) of lattice gauge theories along with necessary truncation imposed on the Hilbert space of gauge bosons for any finite computing resources. We report a study toward addressing this question in the case of non-Abelian lattice gauge theories that require the imposition of non-Abelian Gauss's laws on the Hilbert space.

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1. Introduction

In recent years, there has been a revived interest in the Hamiltonian formalism of gauge theories [1] that provides the natural framework when one aims at utilizing quantum computing technologies for the unsolved problems in QCD. From that motivation, the lattice gauge theory community throughout the globe is becoming increasingly interested in this research direction.

Given the fact that useful quantum computer [2] is yet to arrive for universal computation, we take the chance to study Hamiltonian simulation of gauge theories within the scope of classical computation using the different reformulations of the same available in the literature [3]. The motivation for this study is to see if one particular formulation or one particular choice of basis is more efficient for the purpose of Hamiltonian simulation, keeping in mind the fact that Hamiltonian analysis does call for imposing the Gauss' law constraints on the Hilbert space in order to keep the dynamics confined into the physical Hilbert space. For this study, instead of considering the theory of QCD (SU(3) gauge theory in 3 + 1 dimensions), we consider a theory with the simplest non-Abelian continuous gauge group, i.e. SU(2) defined on a 1 dimensional spatial lattice.

In this article, the different bases to work with the same theory are briefly introduced in section 2. In section 3, the computational complexities of the Hamiltonian simulation using different bases or representations are analyzed and finally, the most efficient basis to work with is identified.

2. Hamiltonian Lattice Gauge theory: different choice of basis vectors

In this section, we briefly describe four different bases (see figure 1) available in the literature to describe the Hilbert space Kogut-Susskind (KS) Hamiltonian for SU(2) [1], in 1 + 1 dimension, along with the form of the Hamiltonian in each basis that produces an identical spectrum.

The KS Hamiltonian is given by,

$$H^{(\mathrm{KS})} \;=\; H_I^{(\mathrm{KS})} + H_E^{(\mathrm{KS})} + H_M^{(\mathrm{KS})}. \tag{1}$$

Here, $H_I^{(\mathrm{KS})}$ denotes interactions among the fermionic and gauge fields as given in

$$H_I^{(\mathrm{KS})} \;=\; \frac{1}{2a}\sum_x \left[\psi^\dagger(x)\hat{U}(x)\psi(x+1) + \mathrm{h.c.}\right], \tag{2}$$

The mass and electric parts of the Hamiltonian are given by,

$$H_E^{(\mathrm{KS})} = \frac{g^2 a}{2}\sum_x \hat{\boldsymbol{E}}(x)^2 \quad , \quad H_M^{(\mathrm{KS})} = m\sum_x (-1)^x \psi^\dagger(x)\psi(x). \tag{3}$$

Here,g is a coupling and m is the mass of the two-component staggered fermionic fields considered. The electric field and the link operators act as the canonical conjugate variables of the theory and satisfy the canonical commutation relation:

$$[\hat{E}^a_{L/R}, \hat{E}^b_{L/R}] = -i\epsilon^{abc}\hat{E}^c_{L/R} \;\;,\;\; [\hat{E}^a_L, \hat{E}^b_R] = 0 \;\;,\;\; [\hat{E}^a_L, \hat{U}] = T^a\hat{U} \;\;,\;\; [\hat{E}^a_R, \hat{U}] = \hat{U}T^a, \tag{4}$$

where $T^a = \frac{1}{2}\tau^a$, and τ^a is the a^{th} Pauli matrix. The corresponding commutation relations for fields with different site indices vanish.

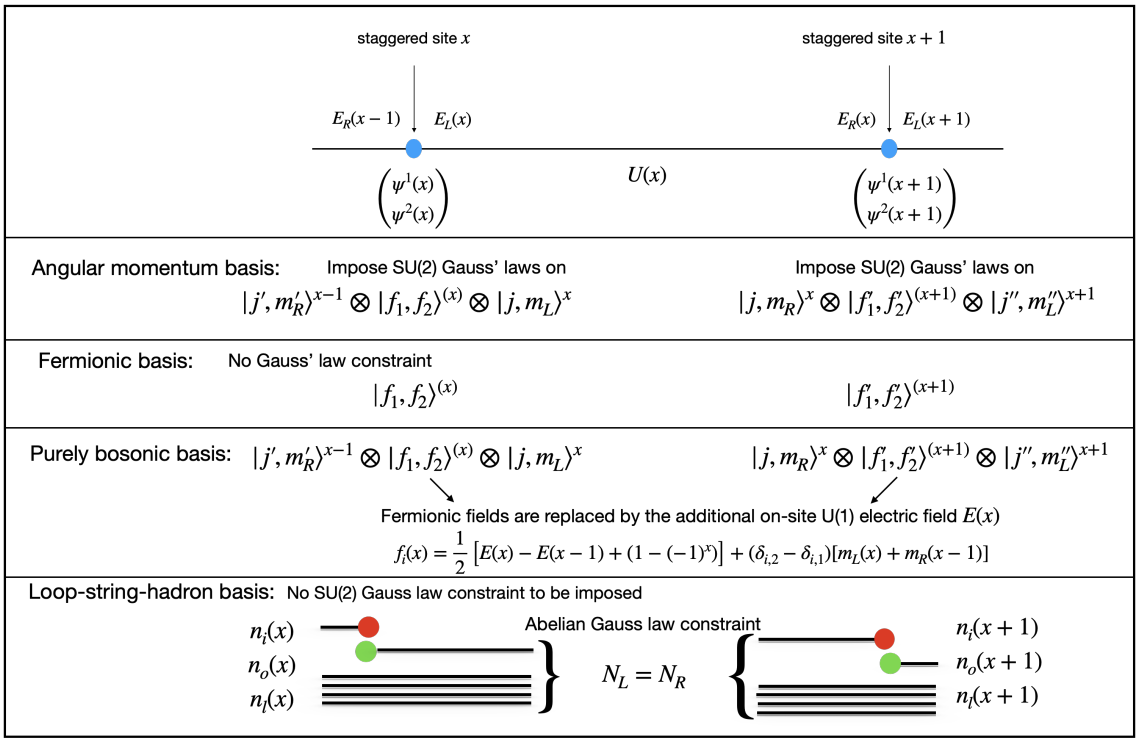

Figure 1: Different basis for KS Hamiltonian that produces an identical spectrum

The states in the physical Hilbert space are constrained as:

$$\hat{G}^a(x)|\Psi_{\text{phys}}\rangle = 0 \;\; \forall x \quad \text{with, } \hat{G}^a(x) = -\hat{E}^a_L(x) + \hat{E}^a_R(x-1) + \psi^\dagger(x)T^a\psi(x). \tag{5}$$

The strong coupling vacuum $|0\rangle$ is defined as the state that is annihilated by the electric part of the Hamiltonian and also eigenstate for the mass part of the Hamiltonian with the minimum eigenvalue. The strong coupling basis is built up by the action of the link operator on the strong coupling vacuum state. A general state consisting of gauge and matter fields is only physical when it satisfies (5).

2.1 Angular momentum basis

The most well known basis to describe SU(2) gauge theories is the angular momentum basis that acts as strong coupling eigenstates of the Kogut-Susskind Hamiltonian given in (1). The eigenstates of the electric part of the Hamiltonian is given by the rigid rotor states [1] for each link characterized by $|j,m_L,m_R\rangle$, where j counts the electric flux on the link and m_L/m_R are the left/right magnetic quantum number for the angular momentum representation. The (anti)matter content of the theory is represented by two component fermionic fields (in the fundamental representation of SU(2)) residing locally at each lattice site. The strong coupling basis states for the KS Hamiltonian are thus given by,

$$|\Phi\rangle^{(x)}_{(\text{KS})} = |J_R,m_R\rangle^{(x-1)}\otimes|f_1,f_2{}^{(x)}\rangle\otimes|J_L,m_L\rangle^{(x)}, \tag{6}$$

for each site x. Here, f_1 and f_2 are the fermionic occupation number of the two components of the (anti)matter field, ψ^1 and ψ^2, each taking values 0 and 1, corresponding to the absence and presence

of (anti)matter. The gauge-link operator acting on the rigid rotor basis creates a state with modified electric flux that comes with suitable coefficients [3] as per the angular momentum addition rules.

The physical Hilbert space, that satisfies (5) is explicitly constructed in the angular momentum basis. Despite the fact that, for the non-Abelian gauge theories, there exists a set of mutually non-commuting constraints, there exist certain states that solve all of the Gauss' law constraints. For angular momentum representation, such a state can be identified as a combination of angular momentum states (and also matter field state, where a presence of a single matter field is equivalent to angular momentum flux $J = 1/2$) at each site where the total angular momentum adds up to zero following angular momentum addition rules. Such a local gauge-invariant state is thus a linear combination of states as given in (6) with proper Clebsch Gordon coefficients. This construction is discussed in detail in [3]. Note that, absence of a fermion at a site, or the presence of two fermions at a site, is independent of any gauge flux and yield states in the physical Hilbert space.

2.2 Purely fermionic basis

As a characteristic for any one dimensional gauge theory, the KS Hamiltonian in (1) combined with the Gauss's law constraints on the Hilbert space, leaves no dynamical gauge degrees of freedom. For a SU(2) gauge theory in 1+1 D with the open boundary condition (OBC), where the incoming flux of the (right) electric field is set to a fixed value, the value of electric-field excitations throughout the lattice gets fixed by the global fermionic distribution on the lattice. As a result, one can work with a purely fermionic Hilbert space for 1 + 1 dimensional SU(2) gauge theory. This was first discussed in [4] and is used in recent tensor-network simulations of the SU(2) LGT in [5].

As derived in [3], with the choice of pure gauge fixing[1], the mass, interaction and electric parts of the original KS Hamiltonian is obtained in the form:

$$H_M^{(\mathrm{F})} = m \sum_{x=0}^{N-1} (-1)^x \psi^{\dagger'}(x)\psi'(x) \quad , \quad H_I^{(\mathrm{F})} = \frac{1}{2a} \sum_{x=0}^{N-2} \left[\psi^{\dagger'}(x)\psi'(x+1) + \mathrm{h.c.}\right]$$
$$H_E^{(\mathrm{F})} = \frac{g^2 a}{2} \sum_{x=0}^{N-1} \sum_{a=1}^{3} \left[\epsilon_0^a + \sum_{y=0}^{x} \psi^{\dagger'}(y) T^a \psi'(y)\right]^2 , \tag{7}$$

Note, the electric part of the purely fermionic Hamiltonian contains long-range interaction between fermions. In the context of the Schwinger model, this same feature arises and has been utilized to a great extent for the purpose of both classical and quantum simulation.

In this formulation, any explicit dependence on the gauge link and electric fields are eliminated and any state can be written in terms of a complete fermionic occupation-number basis,

$$|\Phi\rangle_{(\mathrm{KS,F})} = \prod_{x=0}^{N-1} |f_1, f_2\rangle^{(x)}, \tag{8}$$

where as before, f_1 and f_2 refer to the occupation number of the two components of the (anti)matter field, ψ_1 and ψ_2, respectively, each taking values 0 or 1.

[1] consisting of the following gauge transformation: $U(x) \to U'(x) = \left[\prod_{y<x} U(y)\right] U(x) \left[\prod_{z<x+1} U(z)\right]^\dagger$, and choosing $U' = \mathbb{I}$.

2.3 Purely bosonic basis

One can obtain a purely fermionic theory only in 1+1 D, as in higher dimensions the number of constraints at each lattice site is not sufficient to eliminate the gauge DOF in all spatial directions. One could reversely consider eliminating the fermionic DOF with the use of Gauss's laws, as proposed in Ref. [6], to obtain a fully bosonic theory. This protocol works in all dimensions but requires enlarging the gauge group to accommodate a sufficient number of constraints needed to eliminate the fermions. One further needs to keep track of the fermionic statistics by encoding in the purely bosonic interactions, the nontrivial signs associated with the anti-commuting nature of the fermions [7].

The bosonized form of the SU(2) LGT in 1+1 D is derived in [3], following the procedure outlined in Ref. [6] for general dimensions. For the SU(2) gauge theory in 1 + 1-dimension, the extended theory has an extra U(1) symmetry, of which Z_2 is a subgroup that takes care of translating fermionic statistics to hardcore bosons. The on-site Hilbert space is described in Figure. 1. The physical Hilbert spaces of the SU(2) theory and the U(2) theory are isomorphic, meaning that in the limit where the U(1) gauge link approaches unity, the Hamiltonian matrix elements in the original theory is recovered from those in the extended theory. The extended Hamiltonian involves nearest-link interactions but is otherwise local [6].

2.4 Loop-String-Hadron basis

An alternate reformulation of KS Hamiltonian formalism in terms of Schwinger bosons, known as the prepotential formalism, has been developed over the past decade [8–16]. In a recent work [17], the prepotential formalism of the SU(2) LGT has been made complete to construct the loop-string-hadron (LSH) formalism to include staggered fermions, explicit Hamiltonian, and the associated Hilbert space.

Exploiting the most important feature of the prepotential formalism, namely splitting a link into its left and right parts, those are weaved together by one Abelian Gauss law (AGL) defined on the link, the LSH formalism describes the manifestly gauge invariant operators and states at each site, denoting the local snap-shots of the gauge invariant Wilson loops and string states weaved by the AGL across the links. This particular description for the Hilbert space for SU(2) gauge theory on a 1-D spatial lattice is spanned by local basis vectors characterized by the following integer valued quantum numbers:

$$|\Phi\rangle_{(LSH)} = \prod_x |n_l, n_i, n_o\rangle^{(x)}; \quad \text{where, } 0 \leq n_l < \infty \ \ \& \ \ 0 \leq n_i, n_o \leq 1 \ \ \forall x. \tag{9}$$

The local LSH quantum numbers at the neighboring lattice sites must satisfy the AGL, that in the LSH formulation reads as,

$$\hat{n}_l(x) + \hat{n}_o(x)(1 - \hat{n}_i(x)) = \hat{n}_l(x+1) + \hat{n}_i(x+1)(1 - \hat{n}_o(x+1)). \tag{10}$$

Note that, the states $|\Phi\rangle_{(LSH)}$ are already the physical states of the theory without explicitly imposing the complicated SU(2) Gauss law constraints.

The LSH Hamiltonian, as given in [3, 17] contains electric, mass and interaction terms expressed in terms of the operators $\hat{n}_l, \hat{n}_i, \hat{n}_o$, those are the number operators corresponding to the

LSH quantum numbers for each state define at each x. Additionally, the interaction Hamiltonian contains the string creation-annihilation operators, which are composite operators constructed out of the ladder operators in the loop-string-hadron basis and are presented in detail in [3, 17]. The LSH Hamiltonian, albeit looks very much different from the KS Hamiltonian, produces an identical spectrum and exhibits identical cut-off effects to establish itself as a fully reliable reformulation of the original formalism without any loss of generality.

3. Choosing the most efficient basis: study of the cost of simulation in different basis

Hamiltonian simulation, in general, involves four steps, namely: 1) state preparation or building up the Hilbert space, 2) construction of the Hamiltonian, 3) Finding the spectrum of the Hamiltonian and 4) computing the dynamics of the system. The cost of performing each of the steps for each of the formalism are different and are analyzed in detail in [3]. Here, we briefly quote the conclusion of this analysis performed in [3].

Angular momentum representation:

This basis is mathematically well understood and describes the most general case of SU(2) gauge theory. However, the most expensive part of using this basis is to impose the Gauss's law constraints on the angular momentum states throughout the lattice in order to build up the physical Hilbert space of the theory. In this process, the physical states come up as a linear combination of angular momentum basis states. With increasing lattice size, the number of terms in such linear combinations grows exponentially [3]. The cost of the next step, i.e. forming the Hamiltonian matrix is hugely affected by the fact just stated. To appreciate that, one may think about the algorithm one uses while forming the Hamiltonian: a physical state is considered and marked as the initial state $|i\rangle$, the Hamiltonian acts on it to yield another state, a scan through all the states of the physical Hilbert space would identify this state to be the state $|j\rangle$, so that the (i, j) element of the Hamiltonian matrix is fixed. Now, given the fact all of the physical states are a linear combination of a large number of angular momentum states, that grows exponentially, also increases the cost of forming the Hamiltonian exponentially. Once the Hamiltonian is formed, it is quite sparse in nature and the sparsity also increases with system size. One can use standard and most efficient exact diagonalization techniques to find the spectrum and dynamics of the system. One must note that the dimension of the Hilbert space depends on the cut-off on the angular momentum Casimir that we choose and so is the cost of Hamiltonian simulation. However, for a lattice with open boundary condition, there exists a saturated value of cut-off (equal to twice the system size, for a system with zero incoming flux) beyond which the Hilbert space does not grow and hence the bosonic Hilbert space remains finite-dimensional.

Purely fermionic representation:

The most complicated part of Hamiltonian gauge theory simulation, namely the Hilbert space formation is trivial in this formulation and one gets all possible fermionic states on the system without any significant cost as there is no Gauss law constraint for this gauge fixing condition. Unlike the angular momentum basis, the fermionic states are one sparse and hence the cost of Hamiltonian formation is exponentially cheaper than that of the angular momentum basis. Moreover, being only

fermionic, no cut-off needs to be specified for this formulation. However, although being extremely efficient, this formulation is not valid beyond one spatial dimension and open boundary condition, and hence one cannot think of utilizing this for the ultimate goal of simulating gauge theories in real 3 + 1 dimensions.

Purely bosonic formulation:

This particular formulation involves some extra steps of removing the fermionic degrees of freedom at the cost of extending the gauge symmetry with one extra U(1) gauge degrees of freedom. This extra U(1) gauge symmetry, exhibits extra cut off ($\Lambda_{U(1)}$) dependence on this formulation and only for $\Lambda_{U(1)} \to \infty$ the original Kogut-Susskind Hamiltonian is retrieved. One can then choose the angular momentum basis for the SU(2) part of the gauge group and the computational complexity is exactly the same as that for the angular momentum basis described above.

LSH formulation:

The Hilbert space for this formulation is described by a hybrid boson-fermion basis, defined at each lattice site that is free from any SU(2) gauge redundancy. Hence, there is no extra cost of solving the Gauss law constraints. However, solving for the on-link Abelian constraint (10) makes the Hilbert space construction more expensive compared to the purely fermionic formalism, but it is still costs less than the same with angular momentum representation as shown in Figure. 2. The physical LSH basis states, being 1-sparse, significantly reduces the cost of the Hamiltonian construction as compared with the angular momentum representation. Once the Hamiltonian is constructed it turns out to be exactly the same as in the angular momentum representation and one can perform any calculation, like finding the spectrum and studying the static as well as dynamics of the theory as demonstrated in [3].

It is also possible to identify different global symmetry sectors of the theory for which the Hamiltonian is block diagonal as it is really convenient to perform calculations for each block of the Hamiltonian matrix. In terms of the LSH Hilbert space, identifying these global symmetry sectors are very much intuitive. For example, forSU(2) gauge theory in 1+1 dimension, one can define the following global charges: $Q = (n_i(x) + n_o(x)) \equiv \nu N$, $q = \sum_x (n_o(x) - n_o(x))$. where $Q \in (0, 2N)$ denotes the total number of fermions on the lattice and $q \in (0, N)$ denotes the electric flux on the last link of the lattice of length N. Each values of them defines a superselection sector of the theory. The SU(2) gauge theory Hamiltonian also exhibits charge conjugation symmetries, that allow one to identify the global charge sector Q with the $2N - Q$ sector that exhibits the same spectrum and dynamics.

4. Summary and Discussions

In this work, we have performed a comparative analysis of the different Hamiltonian formulations available in the literature that describes a SU(2) gauge theory in 1+1 dimension from the perspective of Hamiltonian simulation using a classical computer. Albeit the exponential growth of the Hilbert space, it is possible to identify the global symmetry sectors of the theory and perform calculations both for statics and dynamics of the theory within each superselection sector. We have demonstrated that one particular choice of basis, namely the purely fermionic basis costs the

least for Hamiltonian simulation as shown in Figure. 2. However, this basis works only in one spatial dimension and open boundary condition. The convenient yet general framework suitable for Hamiltonian simulation for non-Abelian gauge theories is the LSH framework as demonstrated in Figure. 2.

A similar study in higher dimension as well as for other relevant gauge theories, such as SU(3) gauge theory would be more useful. Works in these directions are in progress and will be reported in near future. It is also important to note that the exact diagonalization technique for classical Hamiltonian simulation is extremely limited due to the exponential growth of the Hilbert space. However, there exist recent Hamiltonian simulation techniques such as using tensor network ansatz [18–20]. The present study also sheds light on choosing a suitable framework for the tensor network constructed for a gauge theory, that also leads to obtain a quantum algorithm. Following this direction, follow-up of the present work aims to construct quantum algorithms and estimate resources for simulating non-Abelian gauge theories on an analog or a digital quantum computer.

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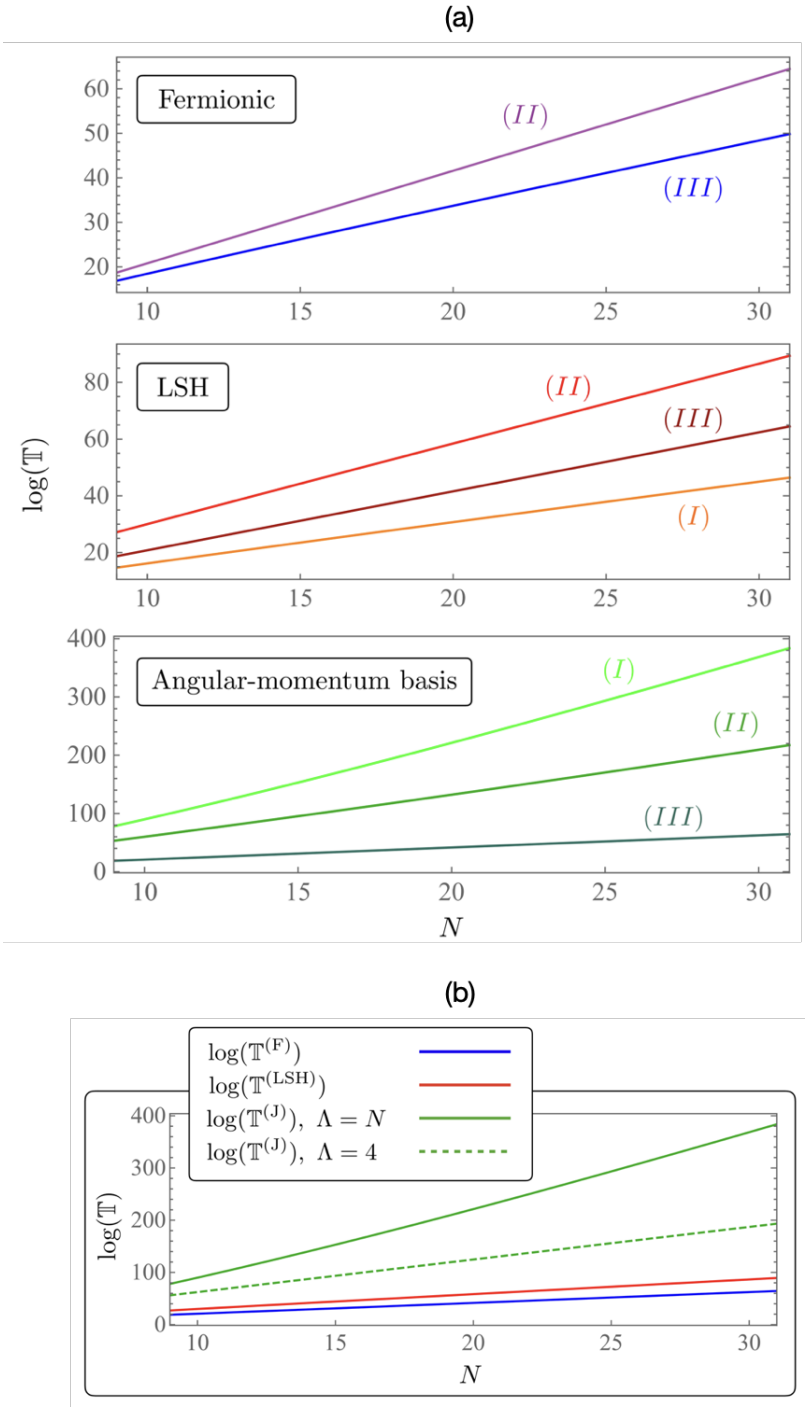

Figure 2: (a) The asymptotic cost of each step and (b) cumulative cost of all the steps of given classical algorithms for Hamiltonian simulation of the KS SU(2) LGT in 1+1 D with the fermionic formulation (F), LSH formulation, and the angular-momentum basis in the physical sector (J), as a function of the lattice size N for large N. Step (I) refers to Hilbert-space construction, step (II) refers to Hamiltonian generation and step (III) denote observable computation. The step (I) for the fermionic formulation is of O(1).