# MSc Proseminar "Quantum Information: From Foundations to Algorithms": Simulations of lattice gauge theories

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# Introduction

This report contains a general overview of simulations of lattice gauge theories to discuss a theoretical setting that allows for quantum simulations. It will start by presenting Wilson's formalism, then apply it to define Wilson's Hamiltonian of quantum electrodynamics (QED). Afterwards, quantum link models are introduced and used to state a Hamiltonian for lattice quantum electrodynamics ($U(1)$ gauge symmetry) and a Hamiltonian for a $SU(N)$ lattice gauge theory. A short discussion on the symmetric properties of both theories is also included, which allows an interpretation of the physically realizable quantum states, based on the generators of the symmetry in each theory.

Finally, a discussion is included on how fermionic and bosonic quantum operators can be transformed into spin operators. In particular, an example of this with a quantum link model of QED is discussed.

# Lattice gauge theories

A lattice gauge theory corresponds to a physical system that lives on a lattice, where its dynamics are invariant upon local (gauge) transformations. These transformations form a symmetry group (also called gauge group), and the symmetry group has its set of generators, which can be used to construct a general gauge transformation belonging to the symmetry group. For the case of continuous symmetries, the symmetry groups are Lie groups, which can be Abelian (e.g. $U(1)$) or non-Abelian (e.g. $SU(N)$).

Two main gauge theories will be discussed throughout this report. One of which is QED, which is a theory with $U(1)$ gauge symmetry, so the symmetry has 1 generator. This generator corresponds to one bosonic degree of freedom, which in QED becomes the photon and mediates the interactions between spin$-1/2$ particles and antiparticles with an electric charge.

The other relevant gauge theory for this report is the one with $SU(N)$ gauge symmetry. This symmetry has $N^2 - 1$) generators. A physical example is QCD, which is a theory with $SU(3)$ gauge symmetry, so it has 8 generators that correspond to 8 bosonic degrees of freedom, i.e. 8 gluons mediating strong interaction between quarks with color charge.

## A classical gauge symmetry

A classical example where a gauge freedom seems physically irrelevant is in the case of classical electrodynamics, the equations that model this theory are Maxwell's equations:

$$\nabla \cdot E(t, \mathbf{x}) = \rho(t, \mathbf{x}), \tag{1}$$

$$\nabla \cdot B(t, \mathbf{x}) = 0, \tag{2}$$

$$\nabla \times E(t, \mathbf{x}) + \partial_t B(t, \mathbf{x}) = 0, \tag{3}$$

$$\nabla \times B(t, \mathbf{x}) - \partial_t E(t, \mathbf{x}) = j(t, \mathbf{x}). \tag{4}$$

The electric and magnetic fields are physical observables (consider an experiment with a test charge where the electric and magnetic fields can be inferred). However, it is convenient to define electromagnetic potentials $\Phi(t, \mathbf{x})$, $\mathbf{A}(t, \mathbf{x})$ by considering

$$E = -\nabla\Phi - \partial_t \mathbf{A}, \tag{5}$$

$$B = \nabla \times \mathbf{A}, \tag{6}$$

which by construction implies that (2), (3) are solved. Nevertheless, this convenient choice is introducing ambiguity to the theory: there is now a local (gauge) transformation that leaves Maxwell's equations invariant.

The gauge transformation the following:

$$\mathbf{A}(t,\mathbf{x}) \longmapsto \mathbf{A}(t,\mathbf{x}) - e\,\nabla\alpha(t,\mathbf{x}) \tag{7}$$

$$\Phi(t,\mathbf{x}) \longmapsto \Phi(t,\mathbf{x}) + e\,\partial_t\alpha(t,\mathbf{x}) \tag{8}$$

(or with a covariant notation)

$$A_\mu(x) \mapsto A'_\mu(x) = A_\mu(x) + e\,\partial_\mu\alpha(x), \tag{9}$$

where $e$ is the electron charge and $A_\mu$ is the gauge field. From this result, notice that the gauge field in classical electrodynamics is made up of the vector potential and the electric potential.

Inserting this local transformation $\alpha(x)$ into (5) and (6) via $(\Phi, \mathbf{A})$, the electric and magnetic fields are unaffected. Upon fixing the gauge by making a specific choice for $\alpha(x)$, the gauge redundancy is removed.

Although it seems that introducing the gauge field $A_\mu(x)$ is unnecessary for obtaining an accurate physical description, it is important to note that gauge fields are necessary when we go to the quantum context. In particular, in the path integral formulation, the electron interacts directly with the gauge field $A_\mu(x)$ through its Hamiltonian, and not via the electric and magnetic fields themselves. One relevant setup where the gauge field has observable physical consequences is when a thin solenoid with current is located in between the two slits of the double-slit experiment. The gauge field due to this thin solenoid implies a phase difference in the wave-function of an electron going through one slit or the other. This phase difference is $\Delta\phi = e\oint \mathbf{A}\cdot \mathrm{d}\mathbf{x}$ and it implies a shift in the interference pattern the electron produces (view Figure 1 for reference). This is known as the Aharonov-Bohm effect [1], which has been confirmed experimentally [2].

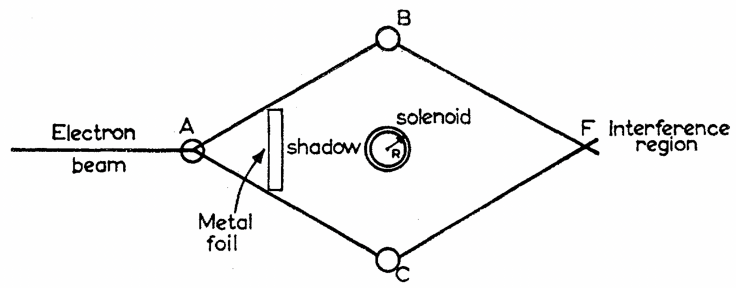


Figure 1: Reproduction of the Aharonov-Bohm effect diagram from the original paper by Aharonov and Bohm in 1959 [1]

## The Dirac free electron and the photon field

In the quantum relativistic context, wave functions do not describe point particles, but instead, particles are excitations of the underlying fields described by a quantum field theory. In particular, for the Dirac free electron, its dynamics are described by the Lagrangian density

$$\mathcal{L} = \overline{\psi}(x)(i\not{\partial} - m)\psi(x), \tag{10}$$

which has a global $U(1)$ symmetry that can be observed by doing the transformation

$$\psi(x) \mapsto \psi'(x) = \exp(ie\alpha)\psi(x). \tag{11}$$

Although here $\alpha$ is just a number, we want to see what would happen if $\alpha$ is a spacetime function $\alpha(x)$. In other words, what happens to the fields if we impose a local $U(1)$ symmetry?

Trying naively to transform the Lagrangian density, we find

$$\psi(x) \mapsto \psi'(x) = \exp(ie\alpha(x))\psi(x), \tag{12}$$

$$\not{\partial}\psi(x) \mapsto e^{ie\alpha(x)}\not{\partial}\psi(x) + (\not{\partial}e^{ie\alpha(x)})\psi(x). \tag{13}$$

So it is convenient to define a "covariant derivative" that can absorb the extra terms, such that we can recover a gauge-invariant Lagrangian density. This covariant derivative can be defined in the simplest non-trivial case by adding a spacetime function $f_\mu(x)$

$$D_\mu = \partial_\mu + f_\mu(x), \tag{14}$$

subject to compliance with the local $U(1)$ symmetry

$$\not{D}\psi \mapsto e^{ie\alpha}\not{D}\psi. \tag{15}$$

This implies that we have

$$D'_\mu\psi' = e^{ie\alpha(x)}D_\mu\psi(x), \tag{16}$$
$$(\partial_\mu + f'_\mu(x))(e^{ie\alpha(x)}\psi(x)) = e^{ie\alpha(x)}(\partial_\mu + f_\mu(x))\psi(x), \tag{17}$$
$$(\partial_\mu e^{ie\alpha(x)})\psi(x) + f'_\mu(x)e^{ie\alpha(x)}\psi(x) = f_\mu(x)e^{ie\alpha(x)}\psi(x), \tag{18}$$
$$f'_\mu(x)\psi(x) = (f_\mu(x) - ie\partial_\mu\alpha(x))\psi(x), \tag{19}$$

or in other words, that the extra field $f_\mu(x)$ has to transform like

$$f_\mu(x) \mapsto f'_\mu(x) = f_\mu(x) - ie\,\partial_\mu\alpha(x). \tag{20}$$

By doing a re-scaling as $if_\mu(x) = A_\mu(x)$, our gauge field in QED transforms like the gauge field from classical electrodynamics:

$$A_\mu(x) \mapsto A'_\mu(x) = A_\mu(x) + e\,\partial_\mu\alpha(x). \tag{21}$$

Given that now the gauge theory is quantum, the gauge field corresponds to the photon field.

To complete the gauge theory, the photon field dynamics are added via the field tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, to define the Lagrangian density for QED:

$$\mathcal{L} = \overline{\psi}(i\not{D} - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{22}$$

# Defining the lattice

In a quantum field theory, scattering amplitudes are expectation values of the interactions between the particles involved in the theory. However, we often encounter that the integrals of these expectation values contain divergences that are systematically removed by renormalizing the theory, such that now the scattering amplitudes are finite and correspond to the experimentally observable values. One way to renormalize a theory is by introducing momentum cutoffs.

On the other hand, it is possible to define a gauge theory in a lattice and simulate this with computational methods to obtain numerical estimates of these scattering amplitudes. When properly discretized, the lattice gauge theory reproduces the continuous gauge theory when the lattice spacing $a \to 0$. Furthermore, defining a lattice theory introduces a natural momentum cutoff $\sim 1/a$, because the interaction length-scale is at least the size of the lattice spacing; so the regularization of a quantum field theory can be done via the lattice parameters [3].

## A staggered lattice

There is not a unique way of defining a lattice gauge theory. For example, two distinct lattice gauge theories correspond to different physical systems, but as long as in the continuous limit ($a \to 0$) both converge to the same continuous gauge theory, they represent the same quantum field theory[1] [3, 4].

[1] Converging to the same continuous gauge theory means obtaining the same **long-distance** physics.

One possible lattice definition consists of staggering particle-antiparticle fermionic sites in the lattice (a checkered pattern). In the case of Dirac's electron, this can be useful because we separate the spin-dependence (particle-antiparticle representation) from the fermionic fields, and instead the spin is incorporated by staggering particle and antiparticle sites in the lattice [3].

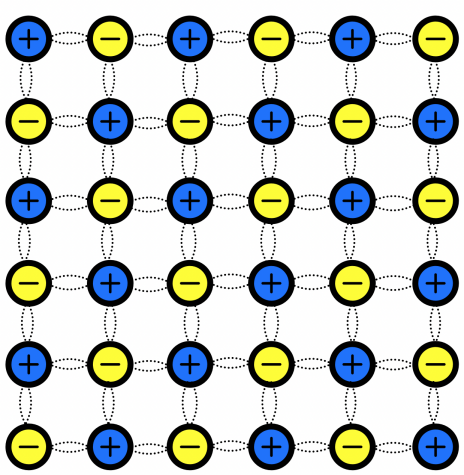

Figure 2: Pictorial view of what the staggered lattice looks like for a square lattice. The blue (+) sites represent fermion particles and the yellow (−) sites represent fermion anti-particles.

For the free Dirac's free electron, we can define a discrete version of the Lagrangian in a lattice as follows. Starting from the Lagrangian definition

$$S = \int \mathrm{d}^d x\, \overline{\psi}(x)(i\gamma_\mu \partial^\mu - m)\psi(x), \tag{23}$$

we can apply a finite differences scheme to perform a discrete derivative

$$\partial^\mu \psi(x) \mapsto \frac{1}{2a}\left[\psi(x + k^\mu a) - \psi(x - k^\mu a)\right] \equiv \frac{1}{2a}\left(\psi_{x+\mu} - \psi_{x-\mu}\right), \tag{24}$$

$$\implies \int \mathrm{d}^d x\, \overline{\psi}(x)(i\gamma_\mu \partial^\mu - m)\psi(x) \mapsto \sum_{x,\mu} a^d \left[\overline{\psi}_x \frac{i\gamma_\mu}{2a}\psi_{x+\mu} - \overline{\psi}_x \frac{i\gamma_\mu}{2a}\psi_{x-\mu} - m\overline{\psi}_x \psi_x\right], \tag{25}$$

where $d$ refers to the number of space-time dimensions in the lattice system, and $\mu$ indexes these dimensions. $\gamma^\mu$ are the elements of Dirac's algebra ($\{\gamma^\mu \gamma^\nu\} = 2g^{\mu\nu}\mathbb{1}$) for $g^{\mu\nu}$ being the metric. In principle, a discretized Lagrangian density can be defined and used to perform computational simulations on a lattice. For clarification purposes, a $d$-dimensional lattice in the Lagrangian formalism is made up of $d-1$ discrete spatial dimensions and 1 discrete time dimension.

For quantum simulations, it is convenient to define the lattice gauge theory instead in with a Hamiltonian in the second quantization formalism. This is because there is a straightforward relationship between the Hamiltonian and the time evolution of a system, each time step corresponds to applying gates in a quantum circuit. For clarification purposes, a $(d+1)$-dimensional lattice in the Hamiltonian formalism is made up of $d$ discrete spatial dimensions and 1 continuous time dimension.

The lattice Hamiltonian for a $(d+1)$ dimension system that in the continuous limit reproduces the Dirac's free electron[2] [3] is

$$H_{\text{free}} = -t \sum_{\langle xy \rangle} s_{xy}\left(\psi_x^\dagger \psi_y + \psi_y^\dagger \psi_x\right) + m \sum_x s_x \psi_x^\dagger \psi_y, \tag{26}$$

notice the similarities to the terms in (25): the hopping term comes from the finite difference derivatives,

[2]Notice that for $d > 1$ spatial dimensions, we encounter fermion doubling with the staggered lattice as $2^{d-1}$, which can be resolved by suitable modifying the Hamiltonian.

and now the Dirac's algebra is encoded to the lattice staggering via the $s_x$ and $s_{xy}$ elements

$$s_x = (-1)^{x_1+\cdots+x_d} \quad \text{for particles/anti-particles staggering,} \tag{27}$$

$$s_{xy} = (-1)^{x_1+\cdots+x_{k-1}} \quad \text{for links in the } k \text{ spatial direction.} \tag{28}$$

## Wilson's formulation

To start building a lattice QED Hamiltonian, it is necessary to define how the gauge field may interact with the fermion sites in the lattice. To achieve this, the Wilson formulation introduces parallel transporters that can be defined with the gauge field as follows [3].

$$U_{xy} = \exp\left\{ ie \int_{x_k}^{x_k+a=y_k} \mathrm{d}x A_k(x) \right\} \in U(1) \tag{29}$$

where a step $a$ in the $k^{\text{th}}$ direction goes from the site $x$ to the site $y$. Notice that this allows to write down a line integral of the gauge field via concatenation of parallel transporters. In the continuous limit, the transporter at all links recovers the continuous gauge field in all space. Moreover, the transporter is an element of the $U(1)$ symmetry group and transforms according to

$$U'_{xy} = \Omega_x U_{xy} \Omega_y^\dagger, \quad \text{for} \quad \Omega_x = e^{ie\alpha(x)} \in U(1) \tag{30}$$

Similarly to how adding the photon field we obtain (22), we need to incorporate the electromagnetic fields into the lattice Hamiltonian from (26).

The Hamiltonian density for the electromagnetic fields is

$$\mathscr{H} = \frac{1}{2}\left(\vec{E}(x)^2 + \vec{B}(x)^2\right), \quad H = \int \mathrm{d}^d x \mathscr{H}(x). \tag{31}$$

The electric field $\vec{E}$ and the vector potential $\vec{A}$ are canonical variables in the Hamiltonian formulation, so for the lattice Hamiltonian, we can write them as

$$E_k(x) = -i\frac{\partial}{\partial A_k(x)}, \quad k = \{1, 2, 3, \ldots, d\}, \tag{32}$$

Furthermore, due to them being canonical variables, we can perform a canonical quantization as follows:

$$-\{E_j(x), A_k(y)\} = i\delta_{jk}\delta(x-y) \implies \left[\hat{E}_j(x), \hat{A}_k(y)\right] = \delta_{jk}\delta(x-y) \tag{33}$$

where now the electromagnetic fields are quantum operators.

The main implication of this procedure is that now our transporter also becomes a quantum operator that only depends on a vector potential operator $A_{xy} = \int_{x_k}^{y_k} \mathrm{d}x \hat{A}_k(x)/a$ along direction $k$ (the direction is implicitly defined by $y - x$), so we redefine $U_{xy} = \exp(iea A_{xy})$. The electric field is also redefined to $E_{xy} = -i\,\partial/\partial a e A_{xy}$ where this field now is quantum and is assigned to each lattice link. $a, e$ are the lattice spacing parameter and the electron's charge respectively. The commutation relations of these quantum operators are

$$[E_{xy}, U_{x'y'}] = \delta_{xx'}\delta_{yy'}U_{xy}, \tag{34}$$

$$\left[E_{xy}, U^\dagger_{x'y'}\right] = -\delta_{xx'}\delta_{yy'}U^\dagger_{xy}, \tag{35}$$

$$\left[U_{xy}, U^\dagger_{x'y'}\right] = 0. \tag{36}$$

Moreover, now we can write down the contribution to the Hamiltonian from summing the electric field at

all the links:

$$\frac{e^2}{2}\sum_{\langle xy\rangle} E_{xy}^2. \tag{37}$$

For the contributions from the magnetic field, lattice plaquettes are defined as

$$U_\square = U_{wx}U_{xy}U_{zy}^\dagger U_{wz}^\dagger, \tag{38}$$

$$U_\square^\dagger = U_{wz}U_{zy}U_{xy}^\dagger U_{wx}^\dagger. \tag{39}$$

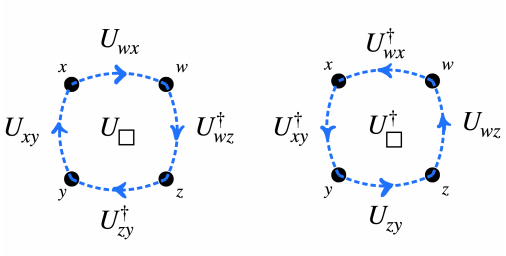


Figure 3: Physical picture of the plaquette operators.

Then, by applying Stokes theorem in a single square loop in the lattice (view Figure 3 for reference),

$$\iint_S \mathrm{d}\vec{S}\cdot\vec{B} = \iint_S \mathrm{d}\vec{S}\cdot(\nabla\times\vec{A}) = \oint_{\partial S}\mathrm{d}\vec{r}\cdot\vec{A} = \oint_{wxyz}\mathrm{d}\vec{r}\cdot\vec{A}(x), \tag{40}$$

thus recovering the term in the exponent of $U_\square^\dagger$ (up to a change of sign). Using this relation between the plaquette terms and the magnetic field, the complete Hamiltonian in the lattice is written as [3]

$$H = -t\sum_{\langle xy\rangle} s_{xy}\left(\psi_x^\dagger U_{xy}\psi_y + \psi_y^\dagger U_{xy}^\dagger\psi_x\right) + m\sum_x s_x\psi_x^\dagger\psi_x + \frac{e^2}{2}\sum_{\langle xy\rangle}E_{xy}^2 - \frac{1}{4e^2}\sum_\square\left(U_\square + U_\square^\dagger\right), \tag{41}$$

which is a Hamiltonian that for $(a\to 0)$ recovers QED.

In summary, we have discussed the connection between the transporter (gauge field) and electromagnetic fields in the lattice. In particular, with the transporter, the gauge field can be discretized, and it gives the physical interpretation of the $A_k(x)$ gauge field living on the lattice links and mediating the fermion-fermion interaction from neighboring sites.

## Physical interpretation and symmetry remarks

One important property of gauge symmetry is that the symmetry group has generators, which due to gauge symmetry, commute with the Hamiltonian operator. For the lattice QED on Wilson's formulation, the generator $G_x$ can be defined as:

$$G_x = \psi_x^\dagger\psi_x + \sum_k\left(E_{x,x+\hat{k}} - E_{x-\hat{k},x}\right), \quad [H, G_x] = 0. \tag{42}$$

Furthermore, the operator resembles closely what a discrete Gauss' law would be because we have a term similar to a charge density at the lattice site, and a divergence of the electric field around a lattice site.

For completeness, we can use the generator to define a general gauge transformation as an operator $V$

$$V = \prod_x \exp(ie\alpha_x G_x), \tag{43}$$

where $\alpha_x$ are the weights to the gauge transformation at each lattice site, analogous to a general gauge transformation in the continuous gauge theory.

The transformations in the local elements of the Hamiltonian are thus

$$V\psi_x V^\dagger = \Omega_x \psi_x, \quad V\psi_x^\dagger V^\dagger = \psi_x^\dagger \Omega_x^\dagger, \quad V U_{xy} V^\dagger = \Omega_x U_{xy} \Omega_y^\dagger, \tag{44}$$

where $\Omega_z = \exp(ie\alpha_x)$. Substituting these transformations into the Hamiltonian in (41) proves its gauge invariance.

Wilson's formulation was introduced, and it allows defining lattice gauge theories. However, even in this lattice formulation, the Hilbert space of each lattice link is unbounded. This becomes a problem if we try to perform simulations of this quantum system with quantum resources with bounded Hilbert spaces (e.g. qubits).

# Quantum link models

Quantum link models are a generalization of the previous formulation that allows defining Hamiltonians whose operators have bounded Hilbert spaces. In basic terms, they are made of sites and links, whose properties and interactions are mediated by a Hamiltonian. Notice that the quantum link models still recover gauge invariance in the lattice and they can be sent to their continuous limit [3].

## U(1) quantum link model in (2+1) dimensions

To define a lattice with U(1) quantum link model, we can define the electric field $E_{xy}$ and the transporter $U_{xy}$ as spin$-1/2$ operators in the following way:

$$U_{xy} \mapsto S_{ij}^1 + iS_{ij}^2 = S_{ij}^+, \tag{45}$$

$$U_{xy}^\dagger \mapsto S_{ij}^1 - iS_{ij}^2 = S_{ij}^-, \tag{46}$$

$$E_{xy} \mapsto S_{ij}^3, \tag{47}$$

where $i$ and $j$ refer to the lattice sites that are linked. The spin commutation relations $\left[S_{jk}^a, S_{j'k'}^b\right] = i\delta_{jj'}\delta_{kk'}\epsilon^{abc}S_{jk}^c$ imply that in the quantum link model, we recover (34) and (35). Although we do not recover the analogous of (36):

$$\left[S_{jk}^+, S_{j'k'}^-\right] = 2\delta_{jj'}\delta_{kk'}S_{jk}^3. \tag{48}$$

The fermionic fields $\psi_x$ are rewritten as fermionic annihilation and creation operators at each site (they are the same object but now called $c_i$ and indexed by $i$)

$$\psi_x \equiv c_i \tag{49}$$

$$\psi_x^\dagger \equiv c_i^\dagger. \tag{50}$$

The Hamiltonian terms from (41) are rewritten respectively as

$$H_t = -t\sum_{\langle ij\rangle}\left[c_i^\dagger S_{ij}^+ c_j + \text{h.c.}\right], \tag{51}$$

$$H_m = m\sum_i (-1)^i c_i^\dagger c_i, \tag{52}$$

$$H_E = \kappa\sum_{\langle ij\rangle}(S_{ij}^3)^2, \tag{53}$$

$$H_\square = -J\sum_\square\left[S_{li}^+ S_{ij}^+ S_{kj}^- S_{lk}^- + \text{h.c.}\right], \tag{54}$$

such that the QED quantum link model in the $(2+1)$ dimensional lattice has the following Hamiltonian:

$$H = H_t + H_m + H_E + H_\square. \tag{55}$$

**Remarks about the U(1) quantum link model's Hilbert space**

Given that our Hamiltonian from (55) is now in the context of a quantum system, we can discuss further which states are physically allowed. In essence, the physical Hilbert space is the gauge-invariant Hilbert space, defined as

$$\mathcal{H}_G = \{|\psi\rangle \text{ s.t. } G_i |\psi\rangle = 0 \quad \forall i\}, \tag{56}$$

where $|\psi\rangle$ corresponds to the quantum state consisting of all fermions and spins in the lattice sites and links respectively. $G_i$ can be defined from (42). Recall that a physical interpretation of the generators of a gauge symmetry is that they are Gauss' laws, so our physical Hilbert space corresponds to all quantum many-body wave functions that comply with these laws. Moreover, given that the gauge symmetry for QED ($U(1)$ gauge theory) has only 1 generator, there is only 1 Gauss' law that separates the physical from the nonphysical quantum states.

To illustrate this, consider the ground state of a quantum link model consisting of a chain. The ground state would consist of fermions in the anti-particle sites (yellow sites), and no fermions in the particle sites (blue sites). The number inside the sites are occupations on the number basis. The links are all in the same spin state (due to Gauss' law). The numbers below the sites are the site label ($i$). Then, the first energy excitation could be obtained by applying the hopping term as shown in Figure 4.

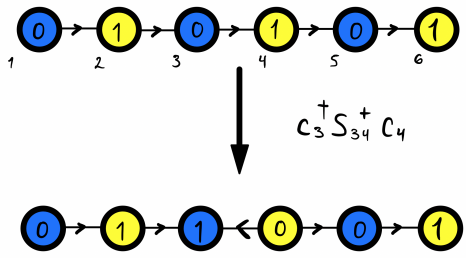


Figure 4: Application of a hopping term on the ground state.

The hopping term represents the creation of a particle-antiparticle pair, while the spin at the link flips to represent a change in the electric field. After the hopping, the Gauss' law is still valid.

## SU(N) quantum link model in (1+1) dimensions

In this section, the definition of a quantum link model with non-Abelian gauge symmetry is presented. Although there are generalizations to higher spatial dimensions, here we consider the case of a chain (1+1)-dimensional system. Without much discussion about its derivation, the theory consists of a chain of sites in which each site holds a pair of fermionic *rishon* operators with flavors ($m$) encoding the $SU(N)$ representation that we write the theory on.

$$c_{R;j}^{\alpha,(m)} \qquad \text{and} \qquad c_{L;j+1}^{\beta,(m)}, \tag{57}$$

where $\alpha$ and $\beta$ correspond to the color indices, and take values from 1 to $N$. The gauge field is made up of the following operator:

$$U_{j,j+1}^{\alpha\beta} = c_{R;j}^{\alpha} c_{L;j+1}^{\beta\dagger}, \tag{58}$$

and in the lattice sites, there are fermionic operators $\psi_j^\alpha$ corresponding to the matter fields.

The $N^2 - 1$ generators for the $SU(N)$ symmetry are

$$G_j^\gamma = \psi_j^{\alpha\dagger} \lambda_{\alpha\beta}^\gamma \psi_j^\beta + L_j^\gamma + R_j^\gamma, \tag{59}$$

for $\lambda^\gamma$ the SU(N) Gell-Mann matrices, and $L$, $R$ the non-Abelian flux operators (similar to the electric field terms in (42), they carry the flux of the bosons to the left and right lattice sites).

The flux operators are defined as

$$L_j^\gamma = c_{L;j}^{\alpha\dagger}\lambda_{\alpha\beta}^\gamma c_{L;j}^\beta, \tag{60}$$

$$R_j^\gamma = c_{R;j}^{\alpha\dagger}\lambda_{\alpha\beta}^\gamma c_{R;j}^\beta. \tag{61}$$

Finally, the Hamiltonian for a $SU(N)$ quantum chain model is defined as [4]

$$H_{SU(N)} = -t\sum_j \left[\left(\psi_j^{\alpha\dagger}c_{R;j}^\alpha\right)\left(c_{L;j+1}^{\beta\dagger}\psi_{j+1}^\beta\right) + \text{h.c.}\right] + m\sum_j (-1)^j\ \psi_j^{\alpha\dagger}\psi_j^\alpha + \frac{g^2}{2}\sum_j \left[L_j^\alpha L_j^\alpha + R_j^\alpha R_j^\alpha\right] + \epsilon\sum_j\left(\prod_{\kappa=1}^N c_{R;j}^{\kappa\dagger}c_{L;j+1}^\kappa + \text{h.c.}\right), \tag{62}$$

where the respective terms can be interpreted as energy coming from the interaction (hopping) of fermions between neighboring sites, the energy from the fermionic matter, the energy from the gauge field flux, and the energy from the gauge bosons.

#### Remarks about the SU(N) quantum link model's Hilbert space

Analogous to the case for the U(1) theory, the $N^2-1$ generators in this theory are symmetries of the Hamiltonian such that $\left[G_j^\gamma, H\right] = 0$ for $\gamma = \{1, 2, \dots N^2-1\}$. Each generator implies an independent Gauss' law, which restricts the physical Hilbert space to the space of quantum states that comply with

$$G_j^\gamma\,|\psi\rangle = 0, \quad \forall\, j\ \forall\gamma. \tag{63}$$

## Quantum simulations

To justify using quantum simulation algorithms in quantum computers instead of computational methods in classical computers, it is worth mentioning that classical computers may find it difficult to represent a quantum Hilbert space and perform estimates on it[3]. Two relevant problems related to this are the following:

#### Exponentially large Hilbert space

The exponentially growing Hilbert space with system size $n$ needs an exponential amount of classical computer memory to represent a quantum state. Consider for instance having a cubic lattice of $n = 5\times5\times5 = 125$ sites. It will also have $3n$ lattice links (periodic boundary conditions). At each lattice site and link, there is a qubit and for each qubit, we use 2 single-precision numbers to represent its wavefunction (2 angles in Bloch's sphere). This means that the total amount of memory (1 float = 4 bytes) needed to represent one wavefunction in this lattice is $4\cdot 2^{4n}$bytes $\approx 10^{151}$bytes.

#### Sign problem

One way of alleviating this problem in classical computation is by using Monte Carlo methods that sample accurately the system's Hilbert space. In this case, expectation values can be performed as

$$\langle O\rangle_p = \frac{\sum_{\{|\psi\rangle\}}\langle\psi|O|\psi\rangle\, p_{|\psi\rangle}}{\sum_{\{|\psi\rangle\}}\langle\psi|\psi\rangle\, p_{|\psi\rangle}}, \tag{64}$$

where as the notation suggests, the expectation value depends on the sampling function $p$. A choice for the sampling function is

$$p_{|\psi\rangle} = \exp\{-S(|\psi\rangle)\}. \tag{65}$$

Then the sign problem appears whenever $p_{|\psi\rangle}$ becomes negative (or, not a positive real number) [5].

[3] However, there are classical computations that would be very hard to outperform with a quantum computer.

These problems do not become relevant in the quantum simulations realm, because quantum computing inherent can access a Hilbert space exponential with the system size $n$, and performing expectation values correspond to doing measurements at the end of a quantum algorithm (not susceptible to the sign problem).

## Transformations for different quantum platforms

To adapt our Hamiltonian between different operator statistics, we can make use of two transformations: the Holstein-Primakoff transformation to approximate spin operators via bosonic operators, and the Jordan-Wigner approximation to transform between spin and fermionic operators.

### Holstein-Primakoff transformation

This is a transformation that considers we can reproduce expectation values of bosonic wavefunctions with $N = 2s + 1$ spin$-s$ states, by truncating the bosonic Hilbert space to the first $N$ bosonic functions ($\{|0\rangle, |1\rangle, \ldots, |N-1\rangle$ in the number basis). The transformation requires us to establish an equivalence between the vacuum state $|0\rangle_B$ and the state $|s, m_s = +s\rangle$ of a spin$-s$ particle, and then the action of the creation operators acts analogous to lowering the spin $z$ projection number:

$$|s, s-n\rangle \mapsto \frac{1}{\sqrt{n!}} \left(a^\dagger\right)^n |0\rangle_B . \tag{66}$$

Then, the operators are equivalent in the following way:

$$S^+ = S^1 + iS^2 = \sqrt{2s}\sqrt{1 - \frac{a^\dagger a}{2s}}\, a, \tag{67}$$

$$S^- = S^1 - iS^2 = \sqrt{2s}\, a^\dagger \sqrt{1 - \frac{a^\dagger a}{2s}}, \tag{68}$$

$$S^3 = (s - a^\dagger a). \tag{69}$$

Thus, in principle we can transform the spin terms into a bosonic representation and perform a quantum simulation in a bosonic lattice (e.g. cold atoms).

Notice that fundamentally, both operators are different because bosonic creation/annihilation operators span an infinite dimensional Hilbert space (Fock space), while each spin$-s$ operator spans only a finite dimensional Hilbert space of size $2s + 1$. Nevertheless, the bosonic commutation relations imply:

$$\left[S^+, S^-\right] = 2S^3, \tag{70}$$

$$\left[a, a^\dagger\right] = 1, \tag{71}$$

$$[a, a] = \left[S^+, S^+\right] = 0, \tag{72}$$

which are the expected commutation relations for spin operators. More details can be found in the appendices to this report.

### Jordan–Wigner transformation

The Jordan-Wigner transformation allows us to change from spin$-s$ operators to fermionic creation and annihilation operators and viceversa. For a spin lattice, where all the sites are indexed by a single number $i$ (only 1 index even in higher dimensional lattices), to properly recover the fermionic anti-commutation relations

$$\{a_i, a_j^\dagger\} = \delta_{ij}, \tag{73}$$

$$\{a_i, a_j\} = 0, \tag{74}$$

$$\{a_i^\dagger, a_j^\dagger\} = 0, \tag{75}$$

we can make the following definition via spin$-1/2$ operators:

$$a_j^\dagger = \exp\left[+i\pi \sum_{k=1}^{j-1} S_k^+ S_k^-\right] S_j^+, \tag{76}$$

$$a_j = \exp\left[-i\pi \sum_{k=1}^{j-1} S_k^+ S_k^-\right] S_j^-, \tag{77}$$

$$a_j^\dagger a_j = S_j^+ S_j^-. \tag{78}$$

Inversely, we can write spin operators via fermionic operators:

$$S_j^+ = \exp\left[-i\pi \sum_{k=1}^{j-1} a_k^\dagger a_k\right] a_j^\dagger, \tag{79}$$

$$S_j^- = \exp\left[+i\pi \sum_{k=1}^{j-1} a_k^\dagger a_k\right] a_j, \tag{80}$$

$$S_j^3 = 2a_j^\dagger a_j - 1. \tag{81}$$

## Digital quantum simulation

Given that now we can define a lattice Hamiltonian in terms of convenient operators for our quantum computing platform, we shall discuss how we proceed and split up the Hamiltonian evolution of our system. Although the simulations that can be done experimentally still need much progress in error control and the number of qubits that can be used, algorithms are already developed to perform digital quantum simulations. These algorithms in principle allow for a large-scale simulation of a lattice gauge theory with a quantum computer.

The algorithms are based on decomposing the Hamiltonian operator and evolving in discrete time steps. The decomposition can be done by product formulas, discrete-time quantum walks, linear decomposition of unitaries, etc. [6] The performance that we can expect in a quantum simulation depends on the specific algorithm used and the number of qubits in the simulation. As a general rule, to achieve a lower error bound or to simulate a larger system, we require more gates. An advantage that digital quantum simulations offer is that it is possible to obtain theoretical asymptotic bounds to the gate complexity (amount of gates) required to achieve a given error $\epsilon$ or a given amount of qubits $n$ [6].

### Product formula algorithm

The product formula is a way to approximate the exponential of a sum of operators. Although this might be trivial for an exponential of a sum of numbers, this decomposition becomes complicated for non-commuting operators. Nevertheless, the terms coming from the commutation of the operators can be made to be small in a limit. To motivate the approximation, let us look at Zassenhaus' result:

$$e^{t(X+Y)} = e^{tX}\, e^{tY}\, e^{-t^2[X,Y]/2}\, e^{t^3(2[Y,[X,Y]]+[X,[X,Y]])/6} \cdots. \tag{82}$$

Naively, we can thus write down the first order approximation as

$$\exp\left(-it\sum_{j=1}^{L}\alpha_j H_j\right) \approx \left[\prod_{j=1}^{L}\exp\left(-\frac{it}{r}\alpha_j H_j\right)\right]^r. \tag{83}$$

The asymptotic error at this order can be found to be

$$\left\|\exp\left(-it\sum_{j=1}^{L}\alpha_j H_j\right) - \left[\prod_{j=1}^{L}\exp\left(-\frac{it}{r}\alpha_j H_j\right)\right]^r\right\| = \mathcal{O}\left(\frac{L\,t\,\alpha_{\max}}{\sqrt{r}}\right)^2, \tag{84}$$

where $\alpha_{\max} = \max_j \alpha_j$. To higher order, the approximation is the $(2k)^{\text{th}}$-order Suzuki formula, which gets a polynomial suppression in the error for each subsequent higher order.

In fact, it is possible to derive upper bounds for the error. For the $1^{\text{st}}$ order:

$$\left\| \exp\left( -it \sum_{j=1}^{L} H_j \right) - \left[ \prod_{j=1}^{L} \exp\left( -\frac{it}{r} H_j \right) \right]^r \right\| \leq \frac{(L\Lambda t)^2}{r} \exp\left( \frac{L\Lambda |t|}{r} \right), \tag{85}$$

where $\Lambda = \max_j \|H_j\|$. Therefore, we can define the minimum $r$ values to achieve the desired maximum norm error $\epsilon$

$$r_1 = \left\lceil \max\left\{ L\Lambda|t|,\ \frac{e(L\Lambda t)^2}{\epsilon} \right\} \right\rceil . \tag{86}$$

$$\tag{87}$$

While the Product formula algorithm might seem simple to understand conceptually, other algorithms make use of more powerful quantum resources, like ancillary states, to reduce the complexity of the final routine, while also being able to keep a desired bound on the error [6].

## Concluding remarks

Some gauge theories are useful for modeling the fundamental processes in nature. As discussed in this report, there is a procedure that allows discretizing them into lattice gauge theories: Wilson's formulation. This formulation involves quantum operators with unbounded Hilbert spaces, so quantum link models were introduced, which can be made up of only quantum operators with bounded Hilbert spaces, and thus are convenient for simulation purposes.

A discussion on how to model lattice gauge theories using these quantum link models was presented for a $U(1)$ gauge theory and a $SU(N)$ gauge theory. Furthermore, the Holstein-Primakoff and the Jordan-Wigner transformations were introduced, which allow relating bosonic or fermionic operators to spin operators. In principle, a quantum link model can thus be made with a lattice of spins.

Finally, a short review of the product-formula algorithm was presented, which allows in principle to study lattice gauge theories via quantum link models.

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# Holstein-Primakoff transformation commutation relations

To observe directly the relationship between the commutation relationships of spin operators and bosonic operators, let us prove that we recover the spin commutation relations from bosonic commutation relations when we apply the Holstein-Primakoff transformation.

The transformation is defined as

$$S^+ = S^1 + iS^2 = \sqrt{2s}\sqrt{1 - \frac{a^\dagger a}{2s}}\, a, \tag{88}$$

$$S^- = S^1 - iS^2 = \sqrt{2s}\, a^\dagger \sqrt{1 - \frac{a^\dagger a}{2s}}, \tag{89}$$

$$S^3 = (s - a^\dagger a). \tag{90}$$

Moreover, the bosonic creation and annihilation operators have the following commutation relations

$$\left[a, a^\dagger\right] = 1, \tag{91}$$

$$[a, a] = 0, \tag{92}$$

$$\left[a^\dagger, a^\dagger\right] = 0. \tag{93}$$

Now, let us compute the commutation relationship of the operators defined in (88), (89), (90):

$$\begin{aligned}
\left[S^+, S^-\right] &= S^+S^- - S^-S^+, \\
&= 2s\left(\sqrt{1 - \frac{a^\dagger a}{2s}}aa^\dagger\sqrt{1 - \frac{a^\dagger a}{2s}} - a^\dagger\sqrt{1 - \frac{a^\dagger a}{2s}}\sqrt{1 - \frac{a^\dagger a}{2s}}a\right), \\
&\text{taking } aa^\dagger = 1 + a^\dagger a, \\
&= 2s\left(\sqrt{1 - \frac{a^\dagger a}{2s}}(1 + a^\dagger a)\sqrt{1 - \frac{a^\dagger a}{2s}} - a^\dagger\left(1 - \frac{a^\dagger a}{2s}a\right)\right), \\
&\text{now expanding the product terms,} \\
&= 2s\left(1 - \frac{a^\dagger a}{2s} + \cancel{a^\dagger a} - \frac{a^\dagger a\, a^\dagger a}{2s} \cancel{a^\dagger a} + \frac{a^\dagger a^\dagger a\, a}{2s}\right) \\
&= 2s\left(1 - \frac{a^\dagger a}{2s} - \cancel{\frac{a^\dagger a^\dagger a a}{2s}} - \frac{a^\dagger a}{2s} + \cancel{\frac{a^\dagger a^\dagger a a}{2s}}\right) \\
&= 2\left(s + a^\dagger a\right) = 2S^3, \\
\left[S^+, S^-\right] &= S^+S^- - S^-S^+ = 2S^3.
\end{aligned}$$

This is precisely the commutation relationship for spin$-s$ operators. The transformation is thus valid because the commutation relations are consistent, however, notice that in any case, the Holstein-Primakoff transformation is only an approximate transformation, because the bosonic Hilbert space is unbounded, while the spin$-s$ Hilbert space is of dimension $2s + 1$.

## Jordan-Wigner commutation relations

For the Jordan-Wigner transformation, we can use spin$-1/2$ operators and prove that the commutation relations are consistent. Starting from the definition of the transformation

$$a_j^\dagger = \exp\left[+i\pi \sum_{k=1}^{j-1} S_k^+ S_k^-\right] S_j^+, \tag{94}$$

$$a_j = \exp\left[-i\pi \sum_{k=1}^{j-1} S_k^+ S_k^-\right] S_j^-, \tag{95}$$

$$a_j^\dagger a_j = S_j^+ S_j^-, \tag{96}$$

we can prove that the anti-commutation relations of the fermionic creation and annihilation operators are a consequence of the commutation relations of spin operators

$$\{a_i, a_j^\dagger\} = \delta_{ij}, \tag{97}$$

$$\{a_i, a_j\} = 0, \tag{98}$$

$$\{a_i^\dagger, a_j^\dagger\} = 0. \tag{99}$$

Let us start by computing $\{a_l, a_m^\dagger\}$

$$\begin{aligned}
\{a_l, a_m^\dagger\} &= a_l\, a_m^\dagger + a_m^\dagger a_l, \\
&= \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] S_l^- \exp\left[+i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] S_m^+ \\
&\quad + \exp\left[+i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] S_m^+ \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] S_l^-, \\
&\text{w.l.o.g., assume } l \geq m, \\
&= \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] \exp\left[+i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] S_l^- S_m^+ \\
&\quad + \exp\left[+i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] \exp\left[-i\pi \sum_{k=1,k\neq m}^{l-1} S_k^+ S_k^-\right] S_m^+ \exp\left[-i\pi S_m^+ S_m^-\right] S_l^-,
\end{aligned}$$

commuting $S^+$ with $\exp[-i\pi S^+ S^-]$ can be illustrated by considering the first non-trivial term in the expansion

$$\begin{aligned}
S^+ e^{-i\pi S^+ S^-} \approx S^+\left(1 - i\pi S^+ S^-\right) &= S^+ - i\pi S^+ S^+ S^-, \\
&\text{notice that } \left[S^+, S^-\right] = 2S^3, \text{ such that} \\
&= S^+ - i\pi S^+ S^- S^+ - i\pi S^+ 2S^3, \\
&= S^+ - i\pi S^+ S^- S^+ - i\pi S^+, \\
&= \left(1 - i\pi S^+ S^- - i\pi\right) S^+, \\
&\approx e^{-i\pi S^+ S^-} e^{-i\pi} S^+, \\
S^+ e^{-i\pi S^+ S^-} &= e^{-i\pi S^+ S^-} e^{-i\pi} S^+.
\end{aligned}$$

Going back to computing $\{a_l, a_m^\dagger\}$:

$$\begin{aligned}
\{a_l, a_m^\dagger\} &= \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] \exp\left[+i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] S_l^- \, S_m^+ \\
&\quad - \exp\left[+i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] S_m^+ \, S_l^-, \\
&= \exp\left[-i\pi \sum_{k=m}^{l-1} S_k^+ S_k^-\right] \left[S_l^-, S_m^+\right], \\
&= \exp\left[-i\pi S_m^+ S_m^-\right] (-2S_m^3)\delta_{ml}. \\
&= (-2S_m^3) \cdot (-2S_m^3)\, \delta_{ml} \\
\{a_l, a_m^\dagger\} &= \mathbb{1}\, \delta_{ml}.
\end{aligned}$$

The other commutation relation can be computed similarly

$$\begin{aligned}
\{a_l, a_m\} &= a_l \, a_m + a_m \, a_l, \\
&= \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] S_l^- \, \exp\left[-i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] S_m^- \\
&\quad + \exp\left[-i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] S_m^- \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] S_l^-, \\
&\text{w.l.o.g., assume } l \geq m, \\
&= \exp\left[-i\pi \sum_{k=1}^{l-1} S_k^+ S_k^-\right] \exp\left[-i\pi \sum_{k=1}^{m-1} S_k^+ S_k^-\right] \left[S_l^-, \, S_m^-\right], \\
&= (\dots) \cdot 0.
\end{aligned}$$

Analogously, $\{a_l^\dagger, a_m^\dagger\} = 0$. In conclusion, the commutation relations due to the spin operators imply the anticommutation relations of the fermionic operators (and vice versa) via the Jordan-Wigner transformation. Furthermore, the transformation conserves the full Hilbert space, because both the fermionic and the spin$-1/2$ operators' Hilbert spaces are of the same dimension. Nevertheless, the transformation is non-local.

# Writing down a quantum link model in terms of qubits

Here, the Hamiltonian for a U(1) gauge invariant quantum link model is written down in terms of only spin$-1/2$ operators. This is to illustrate a use of the transformation to translate the Hamiltonian for a given quantum computing platform.

Recall the definition of the Hamiltonian from (55):

$$H = -t \sum_{\langle ij \rangle} \left[ c_i^\dagger S_{ij}^+ c_j + \text{h.c.} \right] + m \sum_i (-1)^i c_i^\dagger c_i + \kappa \sum_{\langle ij \rangle} (S_{ij}^3)^2 - J \sum_{\square} \left[ S_{li}^+ S_{ij}^+ S_{kj}^- S_{lk}^- + \text{h.c.} \right]. \tag{100}$$

From here, the necessary transformation is to write down the fermionic operators in terms of spin$-1/2$ operators, such that

$$H = -t \sum_{\langle ij \rangle} \left[ \left\{ \exp\left( +i\pi \sum_{k=1}^{i-1} S_k^+ S_k^- \right) S_i^+ \right\} S_{ij}^+ \left\{ \exp\left( -i\pi \sum_{k=1}^{j-1} S_k^+ S_k^- \right) S_j^- \right\} + \text{h.c.} \right] + m \sum_i (-1)^i S_i^+ S_i^- \tag{101}$$

$$+ \kappa \sum_{\langle ij \rangle} (S_{ij}^3)^2 - J \sum_{\square} \left[ S_{li}^+ S_{ij}^+ S_{kj}^- S_{lk}^- + \text{h.c.} \right]. \tag{102}$$

Finally,

$$H = -t \sum_{\langle ij \rangle} \left[ S_{ij}^+ S_i^+ \exp\left( +i\pi \sum_{k=1}^{i-1} S_k^+ S_k^- \right) \exp\left( -i\pi \sum_{k=1}^{j-1} S_k^+ S_k^- \right) S_j^- + \text{h.c.} \right] + m \sum_i (-1)^i S_i^+ S_i^- \tag{103}$$

$$+ \kappa \sum_{\langle ij \rangle} (S_{ij}^3)^2 - J \sum_{\square} \left[ S_{li}^+ S_{ij}^+ S_{kj}^- S_{lk}^- + \text{h.c.} \right]. \tag{104}$$

Notice that $ij$ labels the links, while $i$ or $j$ alone label the sites. Therefore, the physical system consists of qubits on each lattice site and on each lattice link. The sites represent electrons/positrons, and the links the photon field. Notice there is a "string" joining two sites in order to reproduce the fermionic anti-commutation relations (the operator between $S_i^+$ and $S_j^-$). Relating the system to the ground state example in Figure 4, the ground state is now in a spin chain (Figure 5).

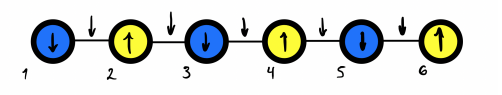


Figure 5: Quantum link model with spins.