Quantum algorithm for calculating topological order parameter of a dimerized spin chain

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The present work is a summary of my personal research notes of the I concepts needed and learned during the first part of my AScI internship at Aalto University. I have set them up in a way which would have aided my past-self in swiftly learning the topic. I have added personal interpretations, comparisons, and figures to give myself, and hopefully any other reader, a better understanding.

CONTENTS

I. INTRODUCTION

The Heisenberg model describes magnetic interactions between spins fixed on a lattice. This model provides information on how macroscopic properties like magnetism emerge from quantum interactions. On the other hand, quantum computing leverages quantum mechanics to perform calculations, making it an adequate platform to simulate and analyze quantum matter. The present work focuses on calculating quantized Berry phases on a spin chain, which serve as a local topological order parameter, with the aid of a quantum algorithm. Intuitively, the aim is to characterize different states of a spin chain.

II. BERRY PHASE & TOPOLOGY

The following notes are taken & mixed from Solemn & Biedenharn[1] and Xiao et al[2].

The Berry phase is a "consequence of the unobservable nature of the phase space"[1]. It is also called the geometrical phase, as it depends on the "geometry" of the parameters that a Hamiltonian depends on. We will consider a Hamiltonian H which depends on parameters $\boldsymbol{q} = (q_1, q_2, ...)$. The Hamiltonian is slowly varied on a closed circuit in parameter space, from an initial time to a final time, such that $\boldsymbol{q}(0) = \boldsymbol{q}(T)$. The evolution of a vector is determined by the time-dependent Schrödinger equation:

$$H(\boldsymbol{q}(t))\,|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle\,. \tag{1}$$

At any time, there exists a basis set of eigenstates that are labeled by n at time t, such that they fulfill the time-independent Schrödinger equation:

$$H(\boldsymbol{q}(t))\,|\psi_n(\boldsymbol{q}(t))\rangle = E_n(\boldsymbol{q}(t))\,|\psi_n(\boldsymbol{q}(t))\rangle\,. \tag{2}$$

A typical result of adiabatic (slow) evolution, is that a system that starts in the n-th eigenvector will evolve adiabatically (slowly) with H, such that it stays labeled by n, and acquires a dynamical phase[3]:

$$|\psi(t)\rangle = \exp\left[\frac{-i}{\hbar}\int_0^t E_n(\boldsymbol{q}(t'))dt'\right]|\psi_n(\boldsymbol{q}(t))\rangle\,. \tag{3}$$

However, Equation 2 alone does not uniquely determine the statevector, as one can arbitrarily choose a phase that depends on the parameters (and time). Taking this into account, Equation 3 can be adjusted such that the evolution of a state takes into account the arbitrary phase:

$$|\psi(t)\rangle = \exp\left[\frac{-i}{\hbar}\int_0^t E_n(\boldsymbol{q}(t'))dt'\right]\exp(i\gamma_n(t))\,|\psi_n(\boldsymbol{q}(t))\rangle\,. \tag{4}$$

The first exponent of Equation 4 is called the dynamical phase, and the second exponent is called the geometrical (Berry) phase, we can rewrite as:

$$|\psi(t)\rangle = e^{i\theta_n(t)}e^{i\gamma_n(t)}\,|\psi_n(\boldsymbol{q}(t))\rangle\,. \tag{5}$$

where $\theta_n(t) = \frac{-1}{\hbar}\int_0^t E_n(\boldsymbol{q}(t'))dt'$. Let us understand some properties of the geometrical phase by inserting Equation 5 into Equation 1:

$$H|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\left(e^{i\theta_n(t)}e^{i\gamma_n(t)}|\psi_n\rangle\right) \tag{6}$$

Let's work first on the right-hand side by expanding the time derivative:

$$\frac{\partial}{\partial t}\left(e^{i\theta_n(t)}e^{i\gamma_n(t)}\right)|\psi_n\rangle + e^{i\theta_n(t)}e^{i\gamma_n(t)}\frac{\partial}{\partial t}|\psi_n\rangle \tag{7}$$

$$= \left(e^{i\gamma_n}\frac{\partial}{\partial t}e^{i\theta_n} + e^{i\theta_n}\frac{\partial}{\partial t}e^{i\gamma_n} + e^{i\gamma_n}e^{i\theta_n}\frac{\partial}{\partial t}\right)|\psi_n\rangle$$

Let's work on some individual parts, starting with the derivative of the dynamical phase:

$$\frac{\partial}{\partial t}e^{i\theta_n} = e^{i\theta_n}\frac{\partial}{\partial t}i\theta_n \tag{8}$$

$$= e^{i\theta_n}\frac{\partial}{\partial t}\frac{-i}{\hbar}\int_0^t E_n(\boldsymbol{q}(t'))dt' = \frac{-i}{\hbar}e^{i\theta_n}E_n(\boldsymbol{q}(t)).$$

Now the derivative of the geometrical phase:

$$\frac{\partial}{\partial t}e^{i\gamma_n} = ie^{i\gamma_n}\frac{\partial}{\partial t}\gamma_n. \tag{9}$$

Lastly the derivative of the eigenvector (using the chain rule):

$$\frac{\partial}{\partial t}|\psi_n\rangle = \frac{\partial|\psi_n\rangle}{\partial q_1}\frac{\partial q_1}{\partial t} + \frac{\partial|\psi_n\rangle}{\partial q_1}\frac{\partial q_2}{\partial t} + ... \tag{10}$$

$$= \nabla_{\boldsymbol{q}}|\psi_n\rangle\cdot\frac{\partial \boldsymbol{q}}{\partial t}.$$

Inserting the parts into Equation 7:

$$e^{i\gamma_n}e^{i\theta_n}\left(\frac{-i}{\hbar}E_n + i\frac{\partial}{\partial t}\gamma_n + \frac{\partial \boldsymbol{q}}{\partial t}\cdot\nabla_{\boldsymbol{q}}\right)|\psi_n\rangle. \tag{11}$$

Returning to Equation 6, we put in the reduced right-hand side Equation 11:

$$H|\psi(t)\rangle = e^{i\gamma_n}e^{i\theta_n}\left(E_n - \hbar\frac{\partial}{\partial t}\gamma_n + i\hbar\frac{\partial \boldsymbol{q}}{\partial t}\cdot\nabla_{\boldsymbol{q}}\right)|\psi_n\rangle. \tag{12}$$

$$\left(e^{i\theta_n}e^{i\gamma_n}\right)H|\psi_n(t)\rangle = e^{i\gamma_n}e^{i\theta_n}\left(E_n - \hbar\frac{\partial}{\partial t}\gamma_n + i\hbar\frac{\partial \boldsymbol{q}}{\partial t}\cdot\nabla_{\boldsymbol{q}}\right)|\psi_n\rangle.$$

$$H|\psi_n(t)\rangle = \left(E_n - \hbar\frac{\partial}{\partial t}\gamma_n + i\hbar\frac{\partial \boldsymbol{q}}{\partial t}\cdot\nabla_{\boldsymbol{q}}\right)|\psi_n\rangle.$$

Dotting with the same eigenstate:

$$\langle\psi_n|H|\psi_n\rangle = \langle\psi_n|\left(E_n - \hbar\frac{\partial}{\partial t}\gamma_n + i\hbar\frac{\partial \boldsymbol{q}}{\partial t}\cdot\nabla_{\boldsymbol{q}}\right)|\psi_n\rangle. \tag{13}$$

$$E_n = E_n - \hbar\frac{\partial}{\partial t}\gamma_n + i\hbar\frac{\partial \boldsymbol{q}}{\partial t}\cdot\langle\psi_n|\nabla_{\boldsymbol{q}}|\psi_n\rangle \tag{14}$$

$$\frac{\partial}{\partial t}\gamma_n = i\langle\psi_n|\nabla_{\boldsymbol{q}}|\psi_n\rangle\cdot\frac{\partial \boldsymbol{q}}{\partial t} \tag{15}$$

We arrive at the conclusion that the Berry phase fulfilling Equation 15 is a valid solution to Schrödinger's equation. This means that during adiabatic evolution, a system will gain in addition to the normal dynamical phase, a geometrical phase.

A. Berry vector potential & gauge dependence

We define the Berry vector potential (often called the Berry connection) as:

$$\boldsymbol{A}_n(\boldsymbol{q}) = i\langle\psi_n|\nabla_{\boldsymbol{q}}|\psi_n\rangle. \tag{16}$$

Thus the Berry phase can be obtained as an integral dependent only on the path of the parameters during adiabatic evolution:

$$\frac{d}{dt}\gamma_n(t) = \boldsymbol{A}_n(\boldsymbol{q})\cdot\frac{\partial \boldsymbol{q}}{\partial t} \tag{17}$$

$$\gamma_n(t) = \int_0^t \boldsymbol{A}_n(\boldsymbol{q}(t))\cdot\frac{\partial \boldsymbol{q}}{\partial t}dt$$

$$\gamma_n = \int_C \boldsymbol{A}_n\cdot d\boldsymbol{q},$$

where C denotes the curve of the parameters. We can now see that the Berry phase is completely determined by the path that the parameters take, hinting at the geometric properties.

The Berry potential is gauge dependent. Taking a gauge transform using smooth functions $f(\boldsymbol{q})$:

$$|\psi_n\rangle \to e^{f(\boldsymbol{q})}|\psi_n\rangle. \tag{18}$$

the Berry potential then changes accordingly:

$$\boldsymbol{A}_n \to i\langle\psi_n|e^{-if}\nabla_{\boldsymbol{q}}e^{if}|\psi_n\rangle \tag{19}$$

$$= i\langle\psi_n|e^{-if}\left(e^{if}\nabla_{\boldsymbol{q}}|\psi_n\rangle + ie^{if}|\psi_n\rangle\nabla_{\boldsymbol{q}}f\right)$$

$$= i\langle\psi_n|\nabla_{\boldsymbol{q}}|\psi_n\rangle - \nabla_{\boldsymbol{q}} f(\boldsymbol{q})$$

$$\therefore \boldsymbol{A}_n \to \boldsymbol{A}_n - \nabla_{\boldsymbol{q}} f(\boldsymbol{q}). \tag{20}$$

The geometrical phase is then also affected by a gauge transformation:

$$\gamma_n \to \int_C (\boldsymbol{A}_n - \nabla_{\boldsymbol{q}} f(\boldsymbol{q}))\cdot d\boldsymbol{q} \tag{21}$$

$$= \gamma_n - \int_C \nabla_{\boldsymbol{q}} f(\boldsymbol{q})\cdot d\boldsymbol{q} = \gamma_n - (f(\boldsymbol{q}_f) - f(\boldsymbol{q}_0))$$

$$= \gamma_n - \Delta f$$

It was then believed that one could choose a suitable transform $f(\boldsymbol{q})$ that would always cancel out the geometrical phase. The gauge dependence implies that the Berry phase is not observable, which explains why for a long time it did not affect experiments. However, Michael Berry challenged this remark by considering a closed loop in parameters, i.e a cyclic evolution:

$$\boldsymbol{q}(0) = \boldsymbol{q}(T). \tag{22}$$

The gauge transform $f(\boldsymbol{q})$ is smooth and must map uniquely eigenstates with one set of parameters to another. It must also be single-valued in the range $[0, 2\pi)$. This means that the Berry phase in a closed loop can only be changed in multiples of 2π:

$$e^{if(\boldsymbol{q}(0))}|\psi_n\rangle = e^{if(\boldsymbol{q}(T))}|\psi_n\rangle \tag{23}$$

$$e^{i(f(\boldsymbol{q}(T))-f(\boldsymbol{q}(0)))}|\psi_n\rangle = |\psi_n\rangle$$

$$\therefore f(\boldsymbol{q}(T)) - f(\boldsymbol{q}(0)) = 2n\pi \tag{24}$$

Thus when the Berry phase evolves in a closed path, we cannot choose a gauge that cancels out the Berry phase, only change the gauge which invariantly adds multiples of 2π. Thus, in a closed path, the Berry phase is a gauge-invariant quantity that cannot be removed, as is thus observable, and is expressed as:

$$\gamma_n = \oint \boldsymbol{A}_n(\boldsymbol{q})\cdot d\boldsymbol{q}. \tag{25}$$

Thus, the Berry phase only depends on geometric aspect of the closed path in parameter space, independent of time.

B. Curvature & topological notions

The Berry phase depends on how the potential changes in a closed path. More intuitively, the Berry phase depends on how eigenstates change (project onto each other) on a closed path in parameter space. Inspired by the fact that the Berry phase depends on a geometrical notion of a closed path, the Berry curvature tensor is defined from the Berry vector potential:

$$\Omega^n_{\mu\nu}(\boldsymbol{q}) = \frac{\partial}{\partial q^\mu}A^n_\nu - \frac{\partial}{\partial q^\nu}A^n_\mu, \tag{26}$$

$$\Omega^n_{\mu\nu}(\boldsymbol{q}) = i[\langle\partial q^\mu\psi_n|\,\partial q^\nu\psi_n\rangle - \langle\partial q^\nu\psi_n|\,\partial q^\mu\psi_n\rangle] \tag{27}$$

where n identifies the n-th eigenstate in question, and the Greek indices are the different coordinates of the parameter space. It is important to highlight that the curvature tensor is gauge-invariant, and thus a physical observable. We have our first topological notion. We can deform the Berry potential by choosing different gauges, but the curvature will remain invariant. The Berry curvature is invariant to first-order deformations.

Using Stoke's theorem[2], we can get an expression for the Berry phase as an integral over a surface S enclosed by a curve C:

$$\gamma_n = \frac{1}{2}\int_S \Omega^n_{\mu\nu}(\boldsymbol{q})\, dq^\mu \wedge dq^\nu. \tag{28}$$

Thus the Berry curvature can define the Berry phase. When the parameter space is three dimensional, the Berry curvature becomes a 3-vector:

$$\boldsymbol{\Omega}_n(\boldsymbol{q}) = \nabla_{\boldsymbol{q}} \times \boldsymbol{A}_n(\boldsymbol{q}), \tag{29}$$

which then seems to act as a magnetic field in parameter space:

$$\gamma_n = \int_S \boldsymbol{\Omega}_n(\boldsymbol{q})\cdot d\boldsymbol{S} = \int_S \nabla_{\boldsymbol{q}} \times \boldsymbol{A}_n(\boldsymbol{q})\cdot d\boldsymbol{S} \tag{30}$$

$$\gamma_n = \oint_C \boldsymbol{A}_n(\boldsymbol{q})\cdot d\boldsymbol{q}.$$

A question arises: curvature of what? By analyzing the equations, one realizes that it is in a sense, the curvature of the space of Hamiltonians, connected by paths along parameters which serve as coordinates. The Berry vector potential is a measure of first-order change in eigenstates when moving along the parameters. The Berry curvature tensor is a measure of second-order change in eigenstates when moving along the parameters. Thus, the curvature remains invariant to gauge transformations, which are first-order changes. Gauge transformations are homeomorphic maps in our manifold of Hamiltonians.

It is instructive to show the definition of Berry curvature via perturbation theory:

$$\Omega^n_{\mu\nu}(\boldsymbol{q}) = i \sum_{n' \neq n} \frac{\langle \psi_n | \partial H/\partial q^\mu | \psi_{n'} \rangle \langle \psi_{n'} | \partial H/\partial q^\nu | \psi_n \rangle - (\mu \leftrightarrow \nu)}{(E_n - E_{n'})^2}. \tag{31}$$

We can then see that as the eigenenergies approach each other, the curvature explodes to infinity. Since the curvature is a physical observable, this means that we have a singularity. This in turn would mean that, if you change the Hamiltonian along a curve and it becomes degenerate, it is not simply connected to the "other side" of the singularity (through that path). The following figure might perhaps serve as intution:

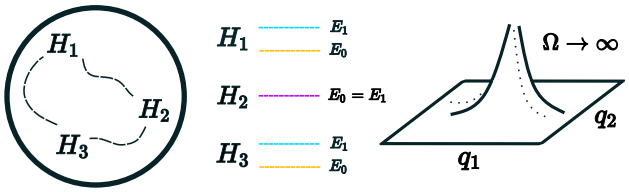

FIG. 1. Hamiltonian evolution along degenerate path, which gives rise to infinite curvature.

the space of Hamiltonians has paths connecting the Hamiltonians (via the parameters). When evolving one Hamiltonian to the other, it may happen that the eigenstates becomes degenerate. Should this be the case, you can not uniquely define a smooth map of one eigenstate to another eigenstate along that path. We can now partition our space of Hamiltonians into different classes, consisting of eigenstates that can be uniquely and smoothly mapped to each other i.e Hamiltonians whose eigenstates are homeomorphic.

Remembering that our paths must form closed curves, we can visualize nicely some topological notions in the following figure.

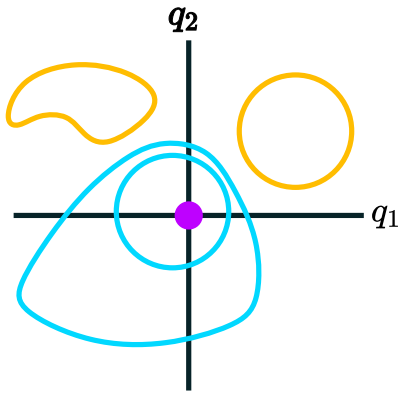

FIG. 2. Closed curves in parameter space. Middle purple dot indicates infinite curvature $\Omega = \infty$. One cannot continuously deform paths that enclose the singularity to paths that do not contain the singularity.

In Figure 2, it can be seen that if a path encloses a singularity, it cannot be smoothly mapped to a path without the singularity. Since these Hamiltonians do not have smooth maps to each other (due to the infinite curvature at the origin), we can partition our space of Hamiltonians to topologically distinct Hamiltonians. This is our first concrete sense of topological spaces. A more intuitive understanding, is that perturbations that do not close the energy band-gap conform topologically equivalent Hamiltonians, while those that collapse the band-gap are topologically inequivalent. Since we are working with topology, it means that we can characterize the different spaces using topological properties, called topological invariants in condensed matter physics.

C. Comparison to general relativity

Should any reader (such as myself) be already familiar with relativity, it can be instructive to make an analogy. In relativity, one considers the curvature of space-time, defined by the Riemann curvature tensor $R_{\alpha\beta\mu\nu}$. It is defined by second derivatives of the metric tensor along space-time coordinates:

$$R_{\alpha\beta\mu\nu} = \frac{1}{2}\left(\partial x^\mu \partial x^\beta g_{\alpha\nu} - \partial x^\nu \partial x^\beta g_{\alpha\mu} + \ldots\right). \tag{32}$$

It is a measure of how much a vector changes via parallel-transport in a closed loop[4]:

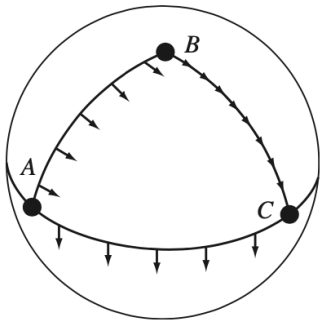

FIG. 3. Parallel transport in a closed loop on a sphere. Figure from Schutz[4].

Just like the curvature of space-time involves second derivatives, the Berry curvature involves second derivatives of the eigenstates in our Hamiltonian space. The space of eigenstates is the field we are concerned with, whose coordinates are the parameters. The curvature measures how much our eigenstates change when evolving them in a closed loop in parameter space.

III. THE HEISENBERG MODEL

The Heisenberg model, as stated in the introduction, describes interactions between spins on a lattice. It's most basic mathematical statement is[5]:

$$H = \frac{1}{2}\sum_{ij} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{33}$$

where J_{ij} is the link strength, and $\boldsymbol{S}_i$ are the typical spin vectors whose entries are the Pauli matrices:

$$\boldsymbol{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z). \tag{34}$$

A. Dimerized spin chain

The dimerized model is a 1D spin chain of nearest neighbor interactions:

$$H = \sum_i J_i \vec{S}_i \cdot \vec{S}_{i+1} = \sum_i H_i \tag{35}$$

which has a *dimer pattern*, which we define as

$$J_i = \begin{cases} J & i = 0\,(mod\,2) \\ \alpha = J/g & i = 1\,(mod\,2) \end{cases} \tag{36}$$

,

with g acting as a modulator. If the system is finite in size, then a periodic condition is assumed. The model can be seen in Figure 4.

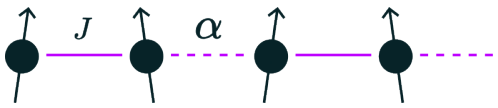

FIG. 4. Dimerized Heisenberg model

This model can be characterized by local topological order parameters on each link. The topological order parameter is the Berry phase as will be explained in the following subsections. One can calculate the Berry phase on each link, quantized, and takes on the same pattern as the dimer chain, being π for the strong links and 0 for the weak links.

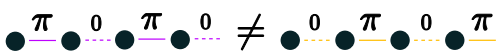

FIG. 5. Local Berry phase on links with different patterns.

B. Quantization of the Berry phase: Antiunitary symmetry

The following discussion is taken from Hatusgai's work[6][7] and modified with the present notation. Seeing as the Berry phase is a gauge-invariant quantity when evolving in a closed loop, only being able to modify it in multiples of 2π (Equation 25), it has an invariant meaning up to an integer multiple:

$$\gamma_n = \oint \boldsymbol{A}_n \cdot d\boldsymbol{q}, \mod 2\pi n. \tag{37}$$

Let us now consider an antiunitary operator $\Phi = KU$, where K denotes complex conjugation and U is some unitary operator. We define a statevector expanded on a parameter independent basis:

$$|\psi(\boldsymbol{q})\rangle = \sum_j C_j(\boldsymbol{q})\,|j\rangle\,. \tag{38}$$

The action of the antiunitary operator is then:

$$|\psi'(\boldsymbol{q})\rangle = \Phi\,|\psi(\boldsymbol{q})\rangle = \sum_j C_j^*(\boldsymbol{q})\,|j'\rangle\,, \tag{39}$$

where $|j'\rangle = \Phi\,|j\rangle$. It is assumed that both bases $|j\rangle$ and $|j'\rangle$ form complete orthonormal bases. How is the Berry phase modified? Let us first explicitly write out the Berry connection expanded in the basis $|j\rangle$:

$$\boldsymbol{A} = i\,\langle\psi|\,\nabla_{\boldsymbol{q}}\,|\psi\rangle \tag{40}$$

$$= i\sum_j C_j^*\,\langle j|\,\nabla_{\boldsymbol{q}} \sum_k C_k\,|k\rangle$$

$$= i\sum_j \sum_k C_j^* \nabla_{\boldsymbol{q}} C_k\,\langle j|k\rangle$$

$$= i\sum_j C_j^* \nabla_{\boldsymbol{q}} C_j$$

Similarly, for the Berry connection on a vector being modified by the antiunitary operator:

$$\boldsymbol{A}' = i\,\langle\psi'|\,\nabla_{\boldsymbol{q}}\,|\psi'\rangle \tag{41}$$

$$= i\sum_j C_j \nabla_{\boldsymbol{q}} C_j^*.$$

Let's expand the coefficients into their amplitude and phase:

$$\boldsymbol{A}' = i\sum_j r_j(\boldsymbol{q}) e^{i\varphi_j(\boldsymbol{q})} \nabla_{\boldsymbol{q}} r_j(\boldsymbol{q}) e^{-i\varphi_j(\boldsymbol{q})} \tag{42}$$

$$= i\sum_j r_j e^{i\varphi_j}\left(e^{-i\varphi_j}\nabla_{\boldsymbol{q}} r_j(\boldsymbol{q}) - i r_j e^{-i\varphi_j}\nabla_{\boldsymbol{q}}\varphi_j(\boldsymbol{q})\right)$$

$$= i\sum_j r_j \left(\nabla_{\boldsymbol{q}} r_j(\boldsymbol{q}) - i r_j \nabla_{\boldsymbol{q}} \varphi_j(\boldsymbol{q})\right)$$

It is important to note that the first term in parantheses must cancel out since we asumed a complete orthornormal basis $\sum_j |C_j|^2 = \sum_j r_j^2 = 1$, thus:

$$\nabla_{\boldsymbol{q}} \sum_j r_j^2 = \sum_j 2 r_j \nabla_{\boldsymbol{q}} r_j = 0, \tag{43}$$

$$\therefore \nabla_{\boldsymbol{q}} r_j = 0. \tag{44}$$

We then arrive at the conclusion that:

$$\boldsymbol{A}' = \sum_j r_j^2 \nabla_{\boldsymbol{q}} \varphi_j(\boldsymbol{q}). \tag{45}$$

Similarly for the unmodified Berry connection:

$$\boldsymbol{A} = -\sum_j r_j^2 \nabla_{\boldsymbol{q}} \varphi_j(\boldsymbol{q}). \tag{46}$$

Which then clearly means that the Berry connections and phases are related, after the antiunitary operation, by:

$$\boldsymbol{A} = -\boldsymbol{A}', \tag{47}$$

$$\gamma_n = -\gamma_n{}'. \tag{48}$$

The situation becomes more interesting if we have a Hamiltonian that is invariant under said antiunitary operation:

$$[H, \Phi] = 0, \tag{49}$$

since this means that if an eigenstate $|\psi_n\rangle$ is unique, then the antiunitary operator leaves the state the same up to some phase factor, meaning it simply changes the gauge:

$$|\psi_n'\rangle = \Phi |\psi_n\rangle = e^{f(\boldsymbol{q})} |\psi_n\rangle, \tag{50}$$

but we already saw that gauge changes are invariant up to multiples of 2π:

$$\gamma_n = \gamma_n{}' \,(\mathrm{mod}\, 2n\pi). \tag{51}$$

This actually results in the quantization of the Berry phase. Only $\gamma = \{0, \pi\}$ satisfy both Equation 48 and Equation 51. It only fails if the gauge becomes singular, meaning that the Hamiltonian is degenerate.

Hatsugai[6] shows that the quantization of the Berry phase serves as a local characterization of a quantum liquid, such as a spin chain. The Berry phase serves as a local topological order parameter, since it becomes robust against small perturbations[7].

C. Twisting the chain

How then are we to calculate the Berry phase and characterize the dimerized spin chain? We have to evolve some parameter of the Hamiltonian in Equation 35 which does not close the energy-gap (clearly if $J = \alpha$ the gap closes, the ground state is a degenerate ferromagnet[8]). Hatsugai[6] introduces a local twist on one link, which can be evolved in a closed loop without closing the energy gap. The adiabatic twist on the link T in the chain can be defined as:

$$H_T \to J_T \left(\frac{e^{-i\theta}}{2} S_T^+ S_{T+1}^- + \frac{e^{+i\theta}}{2} S_T^- S_{T+1}^+ + Z_T Z_{T+1} \right), \tag{52}$$

with the ladder operators

$$S_T^+ = X_T + iY_T \tag{53}$$

$$S_T^- = X_T - iY_T \tag{54}$$

and X, Y, Z are the Pauli matrices. Now we expand the ladder operators in terms of Pauli matrices only, and calling $T+1 = T'$.

$$e^{-i\theta} (X_T + iY_T)(X_{T'} - iY_{T'})/2 + e^{i\theta} (X_T - iY_T)(X_{T'} + iY_{T'})/2 \tag{55}$$

$$= e^{-i\theta} (X_T X_{T'} + Y_T Y_{T'} - iX_T Y_{T'} + iY_T X_{T'})/2 + e^{i\theta} (X_T X_{T'} + Y_T Y_{T'} + iX_T Y_{T'} - iY_T X_{T'})/2 \tag{56}$$

Re-grouping :

$$= \left(\frac{e^{i\theta} + e^{-i\theta}}{2} \right) (X_T X_{T'} + Y_T Y_{T'}) + \left(\frac{e^{i\theta} - e^{-i\theta}}{2} \right) (iX_T Y_{T'} - iY_T X_{T'}) \tag{57}$$

$$= \cos\theta (X_T X_{T'} + Y_T Y_{T'}) - \sin\theta (X_T Y_{T'} - Y_T X_{T'}). \tag{58}$$

So the twist then results in the local interaction:

$$H_t = J_T \cos\theta (X_T X_{T'} + Y_T Y_{T'}) - J_T \sin\theta (X_T Y_{T'} - Y_T X_{T'}) + Z_T Z_{T'} \tag{59}$$

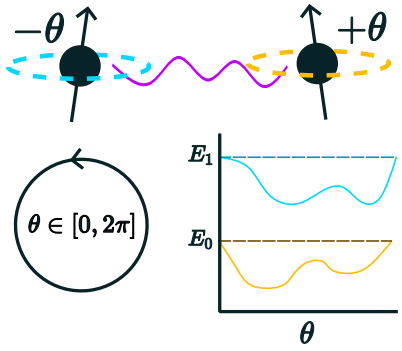

FIG. 6. Local twist

The Berry phase at a link (and other similar systems) can be calculated via numerical algorithms shown by Hatsugai's work[67], which involve diagonalizing twisted Hamiltonians and computing the integral for γ_n. The Berry phase ends up picking the dimer pattern as seen in Figure 7 taken from Hatsugai's paper.

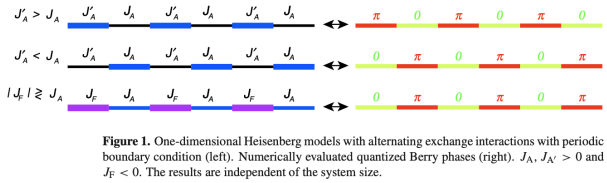

Figure 1. One-dimensional Heisenberg models with alternating exchange interactions with periodic boundary condition (left). Numerically evaluated quantized Berry phases (right). J_A, $J_{A'} > 0$ and $J_F < 0$. The results are independent of the system size.

FIG. 7. Local characterization of the dimerized spin chain by numerical algorithm[6].

We now turn to the question: how can we calculate the Berry phase using a quantum algorithm?

IV. QUANTUM ALGORITHM

A. Canceling the dynamical phase

As exposed in section II, when a quantum system is evolved adiabatically, the final state picks up two phases, the dynamical phase φ_D and the Berry phase φ_B. More specifically, in a closed loop, the initial state (prepared in the ground state) and final state are related[9]:

$$|\psi_0(T)\rangle = e^{-i\varphi_D} e^{i\varphi_B} |\psi_0(0)\rangle, \tag{60}$$

$$\varphi_D = \frac{1}{\hbar}\int_0^T E(\boldsymbol{q}(t))dt, \tag{61}$$

$$\varphi_B = i\oint_C \langle\psi_0(\boldsymbol{q})|\nabla_{\boldsymbol{q}}|\psi_0(\boldsymbol{q})\rangle\cdot d\boldsymbol{q}. \tag{62}$$

It is important to note that the Berry phase φ_B is independent of time, it only depends on the closed curved itself, not on how it is travelled on. On the other hand, the dynamical phase φ_D is time dependent. If we evolve the system backwards time, the dynamical phase changes sign:

$$\varphi_D' = \frac{1}{\hbar}\int_T^0 E(\boldsymbol{q}(t))dt \tag{63}$$

$$= \frac{1}{\hbar}\int_0^T E(\boldsymbol{q}(t))(-dt) = -\varphi_D$$

So consider first evolving forward in time, where the parameters form a closed loop, for a period T and then backwards in time for another closed loop period T:

$$|\psi_0\rangle \to e^{-i\varphi_D} e^{i\varphi_B} |\psi_0\rangle \to e^{2i\varphi_B} |\psi_0\rangle. \tag{64}$$

The forward propagation picks up both phases normally. Backwards propagation removes the dynamical phase, as the new contribution has a sign flip. Since the Berry phase does not depend on time, it is again picked up. We now need to remove the factor 2 from the Berry phase, since it renders the quantization of 0 and π meaningless, they become equal. Instead of fully evolving during a period T, we evolve it during a period $T/2$. Calling $U(t_0,t_f)$ a unitary operator which evolves a system adiabatically from an initial time t_0 to a final time t_f, the evolution of the state can be represented as:

$$U(T/2,0)U(0,T/2)|\psi_0(0)\rangle = e^{i\varphi_B}|\psi_0(0)\rangle. \tag{65}$$

The evolution would follow the paths:

$$\begin{cases} t & 0 \to T/2 \to 0 \\ \theta & 0 \to \pi \to 2\pi \end{cases} \tag{66}$$

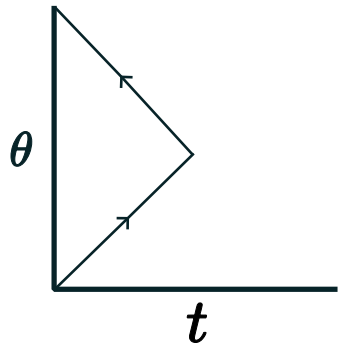

FIG. 8. Path evolution of parameters

The scheme for evolving for half-periods does not work generally, only if the energy spectrum is symmetric in the parameter space. Evolving for half a period forward and then backwards only applies when we have a symmetric energy spectrum along the parameter curve, which is the case for the

local twist in the dimerized spin chain (whose energy spectrum does not vary with the twist, it remains constant). The concept can be visualized in the following figure.

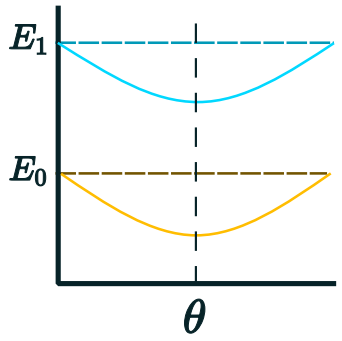

FIG. 9. Symmetric energy spectrum with respect to parameter.

B. Hadamard test

Supposing we have a quantum circuit that can prepare qubits in an initial ground state of the dimerized chain and then evolve it in time via a unitary operator, we can then measure the Berry phase. The idea is to do a simple Hadamard test, with the aid of an auxiliary qubit[10]. This is possible by initializing the auxiliary qubit in the $|+\rangle$ superposition state. Then by conditioning the unitary evolution of the spin-chain on the qubit, the Berry phase will be kicked into the auxiliary qubit as a relative phase:

$$|\psi_{\text{aux}}\rangle = \begin{cases} \text{Initial state} & |0\rangle \\ \text{Hadamard} & |+\rangle \\ \text{Controlled unitary} & \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\varphi_B}|1\rangle\right) \end{cases} \tag{67}$$

Due to the quantization of the berry phase $\varphi = \{0, \pi\}$, the state after the controlled unitary should be one of the two X-basis states (superposition states) $|+\rangle$ or $|-\rangle$. We then apply another Hadamard gate, the auxiliary qubit can only be in two different states:

$$|\psi_{\text{aux}}\rangle = \begin{cases} |0\rangle & \varphi_B = 0 \\ |1\rangle & \varphi_B = \pi \end{cases} \tag{68}$$

which means that if 100% of measurements are 0, then the Berry phase is 0, and if 100% are 1, then the Berry phase is π. We can visualize the circuit in the following diagram:

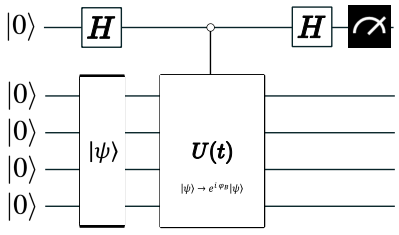

FIG. 10. Circuit visualizations

Of course the correct thing to do is to not assume quantization and explicitly calculate the phase. Thus, having prepared the algorithm, we can run it many times and collect statistics, from which we extract the Berry phase.

$$P(|0\rangle) = \cos^2\theta_B/2 \tag{69}$$

C. Time-stepping: Trotterization

The time-evolution of a time-dependent Hamiltonian is a time-ordered exponential of the form[11]:

$$U(t_0, t_f) = T\left[\exp\left(-i\int_{t_0}^{t_f} H(t)dt\right)\right]. \tag{70}$$

We can split our Hamiltonian into even indices and odd indices, the usefulness will become apparent later.

$$H(t) = H_{even}(t) + H_{odd}(t) = A(t) + B(t). \tag{71}$$

When a Hamiltonian has the form $H(t) = A(t) + B(t)$, an infinitesimal evolution from a time t to $t + \Delta t$ can be approximated to second order by[11]

$$G(t, t+\Delta t) = e^{-\frac{i}{2}\Delta t A(t+\frac{\Delta t}{2})} e^{-i\Delta t B(t+\frac{\Delta t}{2})} e^{-\frac{i}{2}\Delta t A(t+\frac{\Delta t}{2})}. \tag{72}$$

The Hamiltonian we are considering only has time-dependence in the twisted link, which belongs either to the even subset of interactions or odd. We will define $B(t)$ as the subset with the twist. Thus $H(t) = A + B(t)$ and

$$G(t, t+\Delta t) = e^{-\frac{i}{2}\Delta t A} e^{-i\Delta t B(t+\frac{\Delta t}{2})} e^{-\frac{i}{2}\Delta t A}. \tag{73}$$

The even index interactions commute amongst themselves, and odd interactions communte amongst themselves, but in general even interactions do not commute with odd. In other words, pairs of interactions separated by one link commute, i.e

$$\left[\sigma_i^{(\alpha)}\sigma_j^{(\alpha+1)}, \sigma_k^{(\alpha+2)}\sigma_l^{(\alpha+3)}\right] = 0, \tag{74}$$

with upper indices referring to the spin "position" in the chain and σ_i being a Pauli matrix. It is also important to note that "normal" spin interactions (XX, YY, ZZ) on the same link commute, i.e

$$\left[\sigma_i^{(\alpha)}\sigma_i^{(\beta)}, \sigma_j^{(\alpha)}\sigma_j^{(\beta)}\right] = \sigma_i\sigma_j^{(\alpha)}\sigma_i\sigma_j^{(\beta)} - \sigma_j\sigma_i^{(\alpha)}\sigma_j\sigma_i^{(\beta)}. \tag{75}$$

Clearly if $i = j$, the commutator is 0. If they are not equal, using $[\sigma_i, \sigma_j] = i\varepsilon_{ijk}\sigma_k$ we find that

$$\left[\sigma_i^{(\alpha)}\sigma_i^{(\beta)},\sigma_j^{(\alpha)}\sigma_j^{(\beta)}\right]=-\sigma_k^{(\alpha)}\sigma_k^{(\beta)}+\sigma_k^{(\alpha)}\sigma_k^{(\beta)}=0. \quad (76)$$

Thus each part of the evolution (even and odd) can be decomposed into it's constituent interactions via the known multiplication of exponents:

$$e^{-i\Delta t H_{\mathrm{A}/B}}=e^{-i\Delta t X_iX_{i+1}}e^{-i\Delta t Y_iY_{i+1}}e^{-i\Delta t Z_iZ_{i+1}}e^{-i\Delta t X_{i+2}X_{i+3}}... \quad (77)$$

A problem arises when considering the twist in $B(t)$, it contains non-commutative terms within the link, specifically

$$\left[X^{(\alpha)}Y^{(\alpha+1)},Y^{(\alpha)}X^{(\alpha+1)}\right]\neq 0, \quad (78)$$

We must again split this part of Hamiltonian with the twist into commuting parts and non-commuting parts, i.e

$$B\left(t+\frac{\Delta t}{2}\right)=B_1\left(t+\frac{\Delta t}{2}\right)+B_2\left(t+\frac{\Delta t}{2}\right), \quad (79)$$

for convenience giving B_2 the XY and YX interactions, which do not commute with the rest of B. We then approximate this using using a Suzuki decomposition to second order[11]:

$$e^{-i\Delta t B(t+\frac{\Delta t}{2})}\approx e^{\frac{-i\Delta t}{2}B_1(t+\Delta t/2)}e^{-i\Delta t B_2(t+\Delta t/2)}e^{\frac{-i\Delta t}{2}B_1(t+\Delta t/2)}. \quad (80)$$

We now arrive to an approximation of discrete time-evolution to second order:

$$G(t,t+\Delta t)=e^{-i\Delta t A/2}e^{\frac{-i\Delta t}{2}B_1(t+\frac{\Delta t}{2})}e^{-i\Delta t B_2(t+\frac{\Delta t}{2})} e^{\frac{-i\Delta t}{2}B_1(t+\frac{\Delta t}{2})}e^{-i\Delta t A/2}, \quad (81)$$

where

$$A=J_a\sum_{i\in A}\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}, \quad (82)$$

$$B_1(t)=J_b\sum_{i\neq T\in B}\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1} +J_b\cos\left(\theta(t)\right)\left(X_TX_{T+1}+Y_TY_{T+1}\right)+J_bZ_TZ_{T+1}, \quad (83)$$

$$B_2(t)=-J_b\sin\left(\theta(t)\right)\left(X_TY_{T+1}-Y_TX_{T+1}\right). \quad (84)$$

The full time evolution is the approxiated as:

$$U(t_0,t_f)=\prod_{j=1}^{N}G(t_j,t_j+\Delta t) \quad (85)$$

$$=G((N-1)\Delta t,t_f)...G(t_0+\Delta t,t_0+2\Delta t)G(t_0,t_0+\Delta t).$$

D. Algorithm outline

We define an initial time t_0 and final time t_f. The twist will evolve in a loop, as time goes forward and then backwards. The period of the evolution is then $T=t_f-t_0$. We will evolve our system in small steps. So we discretize the evolution into N steps indexed by j:

$$\Delta t=T/N, \quad (86)$$

$$t_j=j\Delta t. \quad (87)$$

During the evolution, θ must be evolved to 2π, so then

$$\theta(t)=\frac{2\pi}{T}t \quad (88)$$

$$\theta_j=\frac{2\pi}{T}j\Delta t=\frac{2\pi j}{N}=j\Delta\theta. \quad (89)$$

Since the time propagation actually looks different, it is important to show

$$\theta(t_j+\Delta t/2)=\frac{2\pi}{T}(t_j+\Delta t) \quad (90)$$

$$=\frac{2\pi}{T}(j\Delta t+\Delta t/2)$$

$$=\frac{2\pi}{T}(j+\frac{1}{2})\frac{T}{N}$$

$$=(j+\frac{1}{2})\Delta\theta.$$

Thus we propagate forward in time for $N/2$ steps, then we propagate backwards in time by flipping the sign of time $(-\Delta t)$ for another $N/2$ steps, while twisting the link until it reaches 2π as in figure Figure 8.

E. Qiskit Gates

The exponentials of A and B_1 can easily be implemented in Qiskit.

$$e^{-iJ_a\Delta tA/2}=\prod_{i\in A}e^{-iJ_a\Delta tX_iX_{i+1}/2}e^{-iJ_a\Delta tY_iY_{i+1}/2}e^{-iJ_a\Delta tZ_iZ_{i+1}/2} \quad (91)$$

Qiskit has implementations for each of those unitary two qubit operators, RXXGate, RYYGate, RZZGate, respectively. These interactions can then be implemented in Qiskit:

$$e^{-iJ_a\Delta tA/2} = \prod_{i\in A} RXX_{i,i+1}(\varphi_a)RYY_{i,i+1}(\varphi_a)RZZ_{i,i+1}(\varphi_a), \tag{92}$$

with $\varphi_a = \Delta t J_a$. Similarly with the B_1 exponential, which has twist terms that commute:

$$\begin{aligned} &e^{-iJ_b\Delta tB_1/2} \\ &= RXX_{T,T+1}(\varphi_b\cos\theta)RYY_{T,T+1}(\varphi_b\cos\theta)RZZ_{T,T+1}(\varphi_b) \\ &\quad \prod_{i\neq T\in B} RXX_{i,i+1}(\varphi_b)RYY_{i,i+1}(\varphi_b)RZZ_{i,i+1}(\varphi_b), \end{aligned} \tag{93}$$

with $\varphi_b = \Delta t J_b$ and subindex T referring to the link with the twist. The interesting term is the exponent of B_2. It can be implemented with the RXXPlusYY gate, by setting it's second parameter $\beta = -\pi/2$. Qiskit defines the RXXPlusYYGate as:

$$R_{\frac{XX+YY}{2}}(\theta,\beta)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta/2 & -ie^{-i\beta}\sin\theta/2 & 0 \\ 0 & -ie^{i\beta}\sin\theta/2 & \cos\theta/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{94}$$

Setting $\beta = -\pi/2$, we call the resulting matrix an $RXY(\theta)$ gate:

$$R_{\frac{XX+YY}{2}}(\theta,-\pi/2) = RXY(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta/2 & \sin\theta/2 & 0 \\ 0 & -\sin\theta/2 & \cos\theta/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{95}$$

Also, it can be shown (quite quickly in Mathematica) that

$$\exp\left[-i\varphi\left(X\otimes Y - Y\otimes X\right)\right] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\varphi & \sin 2\varphi & 0 \\ 0 & -\sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{96}$$

x Clearly

$$\exp\left[-i\varphi\left(X\otimes Y - Y\otimes X\right)\right] = RXY(4\varphi). \tag{97}$$

Thus the B_2 exponent is explicitly:

$$\begin{aligned} e^{-iJ_b\Delta tB_2} &= e^{-iJ_b\Delta t(-\sin\theta(X_TY_{T+1}-Y_TX_{T+1}))} \\ &= RXY_{T,T+1}(-4\varphi_b\sin\theta) \end{aligned} \tag{98}$$

V. RESULTS

The algorithm exposed in the previous section was implemented in Qiskit using Python. The code can be found on my Github. A parameter sweep was performed for different dimer strengths α, setting $J = 1$, with $T = 20$ and $N = 200$. Square errors were calculated for the Berry phase in a bond, and different system sizes were tested. Results are plotted in Figure 11.

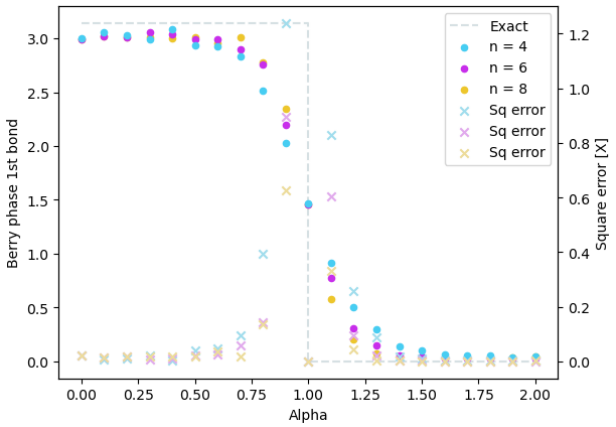

FIG. 11. Algorithm results running algorithm in Aer-Simulator with 100,000 shots.

A phase transition can be seen at a link, where the topological order changes from π to 0. We can see that the algorithm works relatively well. Errors increase when the alternating link strengths approach. Finite size effects are observable. Although it shows promise, the final gate depths varied between 70,000 gates and 140,000 gates. This algorithm is not runnable on hardware available to-day. To test this idea, a basic single qubit-error noise model was used as shown on Qiskit tutorials. To get sensible results, one would need a computer with less than 0.0001% errors. This can be seen in the following figure.

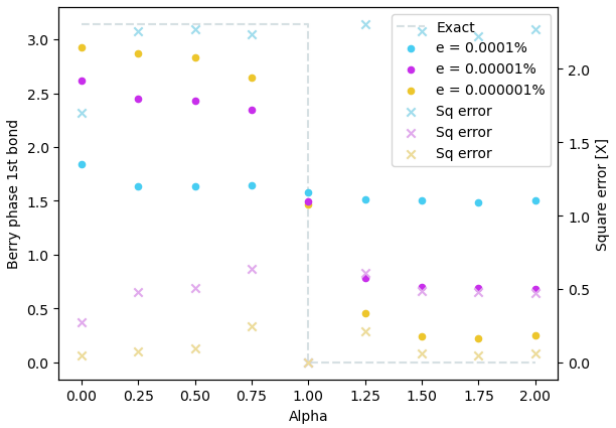

FIG. 12. Algorithm results for different noise levels, using 4 qubits.

The (uncontrolled) circuit can be visualizes in the following figure.

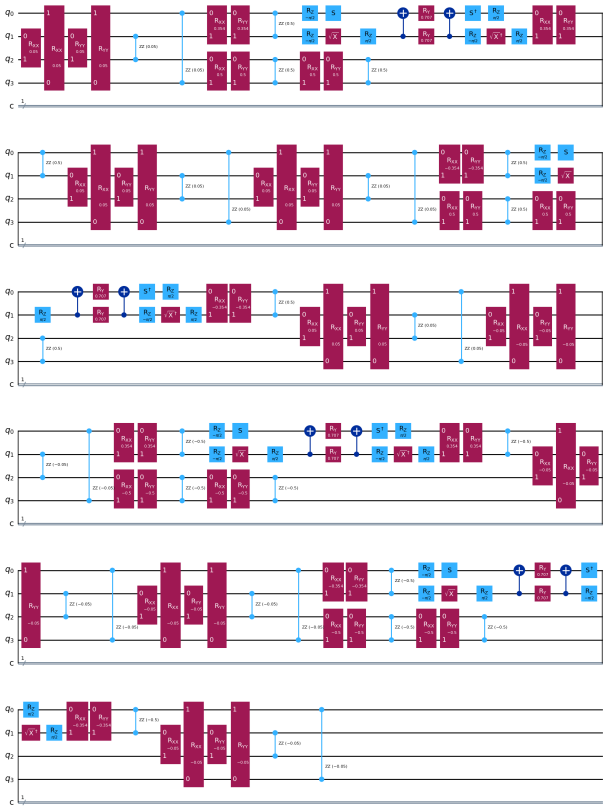

FIG. 13. Circuit diagram for 4 time steps.

VI. CONCLUSION

This work shows a quantum algorithm which can distinguish different states in dimerized spin chains and can characterize phase transitions, highlighting the use of quantum computers to understand quantum matter. It is important to note that although the algorithm works pretty well, there are too many gates in the circuit, so it is no realizable in real quantum computers available today.

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