SKKU 2025 Quantum Challenge Problem: Measuring Berry phase in quantum computing

Designer: Yu-Ping Lin, IonQ, Inc. (yuping.lin@ionq.co)

Prelude

Understanding the time evolution of quantum states has been a central topic in quantum mechanics. This knowledge can help us evaluate the robustness of quantum states at hand, such as those observed in materials or prepared in experiments. The quantum states can also acquire new properties under time evolution, which may not be available in their stationary states. Time evolution of quantum states also plays an important role in quantum computing, since the quantum circuits can be thought of as unitary time evolutions of the qubits.

In this Challenge Problem, we will explore a particular type of time evolution, known as the adiabatic time evolution. In this formalism, the system that governs the quantum state changes very slowly in time. If a quantum state is an eigenstate of the initial system, it can remain an eigenstate of the time-dependent system throughout its evolution. A particularly interesting situation is when the system varies back to itself after a time period. Since the time evolution is adiabatic, the quantum state can evolve back to its initial state (sometimes it won't, but this is beyond the scope of our discussion!) with an additional dynamical phase related to its energy. Remarkably, it may also acquire another quantum phase, known as the Berry phase. In the following Parts, we will explore **how the Berry phase appears** under adiabatic time evolution. We will further investigate **how to measure it with quantum circuits** in quantum computing. Finally, we will apply our knowledge and skills to study the classification of **topological phases** in quantum many-body systems.

Part 1: What is Berry phase?

Our journey begins with understanding what the Berry phase is and how it appears under adiabatic time evolution. As a refreshment, let us review the time evolution of the quantum states $|\psi(t)\rangle$ under a time-independent Hamiltonian H. The time evolution is governed by the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

and takes the form

$$|\psi(t)\rangle = e^{-iHt}|\psi(t=0)\rangle.$$

Here we have taken the convenient notation of $\hbar = 1$. When the initial state is an eigenstate $|\psi(t=0)\rangle = |E\rangle$ of the Hamiltonian H with energy E, the quantum state remains stationary

$$|\psi(t)\rangle = e^{-iEt}|E\rangle.$$

The only change is a time-dependent dynamical phase related to its energy.

Now let us consider a time-dependent Hamiltonian $H(\lambda(t))$. Here the Hamiltonian is determined by a parameter $\lambda(t)$, which we allow to change with time. The time evolution of a quantum state $|\psi(t)\rangle$ is again governed by the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H(\lambda(t))|\psi(t)\rangle \tag{1}$$

and takes a refined form

$$|\psi(t)\rangle = \mathcal{T}e^{-iH(\lambda(t))t}|\psi(t=0)\rangle.$$

Since the Hamiltonians at different times may not commute with one another, a time-ordering operator $\mathcal{T}$ is introduced to guarantee the proper time order of exponential time-evolution operator.

The solution of time-dependent systems are generally nontrivial. However, when the variation of the Hamiltonian $H(\lambda(t))$ is sufficiently slow, the quantum state can remain adiabatic. That is, if it starts from an eigenstate $|\psi(t=0)\rangle = |E(\lambda(t=0))\rangle$ of the initial Hamiltonian $H(\lambda(t=0))$, it can remain its role as the eigenstate $|E(\lambda(t))\rangle$ of the Hamiltonian $H(\lambda(t))$ at the same level, except when level crossing occurs. This statement is known as the **adiabatic theorem**, and the time evolution is said to be adiabatic. Under adiabatic time evolution, the quantum state $|\psi(t)\rangle$ which begins with an initial eigenstate $|\psi(t=0)\rangle = |E(\lambda(t=0))\rangle$ will take a time-dependent form

$$|\psi(t)\rangle = u(t)|E(\lambda(t))\rangle. \tag{2}$$

Here $u(t)$ is a complex phase with $|u(t)| = 1$ and $|E(\lambda(t))\rangle$ is an eigenstate of the time-dependent Hamiltonian $H(\lambda(t))$.

Question 1.1

From the Schrödinger equation, show that the complex phase takes the form

$$u(t) = e^{-i\theta_{\text{total}}(t)}.$$

Here the time-dependent total phase

$$\theta_{\text{total}}(t) = \int_0^t dt' E(\lambda(t')) + \theta_{\text{Berry}}(t)$$

not only includes the dynamical phase related to energy $E(\lambda(t))$, but also an additional phase

$$\theta_{\text{Berry}}(t) = \int_{\lambda(t'=0)}^{\lambda(t'=t)} d\lambda A(\lambda).$$

This additional phase is known as the **Berry phase**, which is the main character of our Challenge Problem. The integrand is called the Berry connection

$$A(\lambda) = -i\langle E(\lambda)|\frac{d}{d\lambda}|E(\lambda)\rangle.$$

The Berry phase can have significant impact on the adiabatic time evolution of quantum states. A particular scenario is when the parameter travels through a closed loop in the parameter space under a time period T. Since the initial and final parameters are the same $\lambda(t=0) = \lambda(t=T)$, the initial and final Hamiltonians are also the same $H(\lambda(t=0)) = H(\lambda(t=T))$. If a quantum state starts from an eigenstate $|E(\lambda(t=0))\rangle$ of the initial Hamiltonian, it will return to this eigenstate at the end. While the initial and final states are the same, their quantum phases are different. We have learned that the quantum state can acquire a Berry phase in addition to the dynamical phase. Interestingly, the Berry phase depends significantly on the trajectory of the closed loop in the parameter space

$$\theta_{\text{Berry}} = \oint d\lambda A(\lambda).$$

As an important example for qubits, let us consider the time-dependent Bloch-sphere Hamiltonian

$$H(\vec{h}(t)) = \vec{h}(t) \cdot \vec{\sigma}.$$

Here the time-dependent parameter is the three-component real Bloch vector $\vec{h} = (h_x, h_y, h_z) \in \mathbb{R}^3$, and $\sigma = (X, Y, Z)$ are the Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Question 1.2

Show that the eigenstates $|E_0(\vec{h})\rangle$ and $|E_1(\vec{h})\rangle$ and their energies of the Hamiltonian $H(\vec{h})$ are

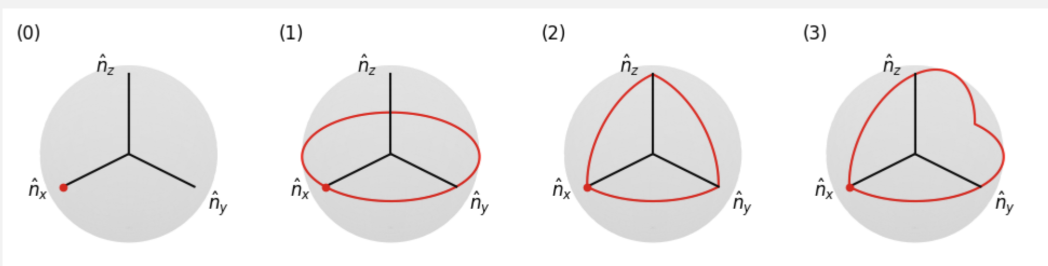
$$\begin{aligned} E_0(\vec{h}) &= -|\vec{h}|, \quad |E_0(\vec{h})\rangle = \frac{1}{\sqrt{2|\vec{h}|(h_z+|\vec{h}|)}}\begin{pmatrix} h_x - ih_y \\ -h_z - |\vec{h}| \end{pmatrix} \\ E_1(\vec{h}) &= |\vec{h}|, \qquad |E_1(\vec{h})\rangle = \frac{1}{\sqrt{2|\vec{h}|(-h_z+|\vec{h}|)}}\begin{pmatrix} h_x - ih_y \\ -h_z + |\vec{h}| \end{pmatrix}. \end{aligned}$$

You may find that the formula for the eigenstates are invalid for $\vec{h} = (0, 0, \pm 1)$. This invalidity is really there, and is actually why the Berry phase would occur! See, for example, Sec. 1.5 of this Lecture Note arXiv:1606.06687 for more explanation.

We now focus on the special case of $|\vec{h}| = 1$. That is, the Bloch vector $\vec{h}$ is a unit vector that traverses on the unit spherical shell around the origin. We will consider several trajectories for the time variation of the Bloch vector $\vec{h}(t)$ and examine the Berry phase acquired by the ground state. For later convenience, we parametrize the Bloch vector $\vec{h}(\lambda)$ with respect to a new time-dependent parameter $\lambda(t)$, such that $\lambda(t = 0) = 0$ and $\lambda(t = T) = 1$ are the initial and final parameters, respectively. This parametrization allows us to define a trajectory in the parameter space with respect to $\lambda \in [0, 1]$, while keeping the flexibility of tuning the time period T to test whether it is sufficiently long.

Question 1.3

Let us set the initial Hamiltonian at the Bloch vector $\vec{h}(\lambda = 0) = (1, 0, 0)$. In this case, the initial state is the corresponding ground state $|\psi(t = 0)\rangle = |E_0(\vec{h}(\lambda = 0))\rangle = (1, -1)/\sqrt{2}$. We consider four different trajectories as illustrated in the following figures:



For each of the four trajectories, compute the time evolution numerically and draw two figures that show the variation of the overlap with the initial state $O(t) = \langle\psi(t = 0)|\psi(t)\rangle$:

- Amplitude: $|O(t)|$.
- Complex phase: $\theta_{\text{total}}(t) = -\arg(O(t))$. In this figure, draw the total phase and the one with the dynamical phase subtracted. Note that the second one is the Berry phase for a particular choice of ground states $|E_0(\lambda)\rangle$, whose overlap with the initial ground state is positive $\langle E_0(\lambda = 0)|E_0(\lambda)\rangle > 0$.

To study the time evolution numerically, we need to choose the time period T and the number of discrete time steps N_t. Since the ground state has a constant energy $E_0 = -1$ throughout the time evolution, we can choose the time period as a multiple of 2π to remove the dynamical phase $E_0 T = -T \equiv 0 \pmod{2\pi}$ from the final state. Then the remaining complex phase is the Berry phase we want. You may push the computation to the asymptotic limit of large T and N_t to get the fully adiabatic result. However, be sure to also do some test with moderate numbers, as we will use them for the quantum-circuit implementation in Part 2.
Look at your computational results: Can you see a relation between the Berry phase and the closed-loop trajectory?

Part 2: How to measure Berry phase with quantum computers?

Quantum computers have been proposed as a promising platform for efficient simulations of various quantum systems. A question we might want to ask is: Can we use them to simulate the time evolution of quantum states and measure their Berry phases? This Part of the Challenge Problem aims at exploring this possibility, particularly how the measurement can be achieved with quantum circuits.

In quantum computing, our measurement does not reveal the overall phase of the whole qubit system. Therefore, we can not measure the overall phase if we use all qubits to simulate the quantum state. Due to this fact, you may wonder how it is possible for us to measure the Berry phase? In fact, the measurement can be achieved by utilizing the **interference** between qubit states! Before diving directly into the simulation of Bloch-sphere Hamiltonian and the measurement of Berry phase, let us first explore how the interference is used to measure the quantum phases in quantum computing.

For the computations and illustrations of quantum circuits, you can choose whatever library you like. If you do not know which one to use, you may try IBM's `qiskit`, the most widely used open-source library for quantum computing. The official website includes many helpful resources for implementation and learning.

> **Question 2.1**
>
> Consider a single-qubit system with the quantum state
>
> $$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\theta}|1\rangle).$$
>
> If we measure this single-qubit state $|\psi\rangle$ in the computational basis $\{|0\rangle, |1\rangle\}$, the probabilities of getting the two basis states $|0\rangle$ and $|1\rangle$ will be the same $P(0) = P(1) = 1/2$. In this case, we can not extract any information of the relative phase θ. Nevertheless, interference can help us resolve this problem. Find out a quantum circuit that can determine the relative phase θ from the measured probabilities $P(0)$ and $P(1)$ in the computational basis.

We have learned how to measure the relative phase of basis states $|0\rangle$ and $|1\rangle$ in a single-qubit quantum register. The next step is to think about how this could help us measure the Berry phase. A natural proposal is to use a quantum register to simulate the target quantum state $|\psi\rangle$, then attach an ancilla qubit and encode the quantum phase $\theta_{\text{total}}(t)$ to its basis state $|1\rangle$. If we can achieve this quantum circuit, then the Berry phase can be extracted by measuring the ancilla qubit.

> **Question 2.2**
>
> We now explore how to measure the Berry phase with quantum circuits. Before discussing the time-dependent Hamiltonian, we first consider the measurement of time-evolved quantum phase under a time-independent Hamiltonian. Expressing the unitary time-evolution operator as $U = \exp(-iHT)$, find out the quantum circuit that measures the total phase of a quantum state $|\psi(t)\rangle$ which evolves from an eigenstate $|\psi(t=0)\rangle = |E\rangle$ of H (I know the notation is misleading since there is also Hadamard gate.... so we will only use the unitary time-evolution operator U in the quantum circuit).

Having understood how to measure the time-evolved quantum phase under a time-independent Hamiltonian, we now proceed to explore how to measure the Berry phase of an eigenstate under an adiabatic time evolution. For a general parameter trajectory, the previous measurement scenario would not work. The reason is that the time evolution not only changes the quantum phase, but also the quantum state itself. In this case, the basis states $|0\rangle$ and $|1\rangle$ of the ancilla qubit will be paired to different states $|\psi(t=0)\rangle$ and $|\psi(t)\rangle$, and the interference will involve the additional ingredients from the state mismatch. Nevertheless, if the parameter trajectory is a closed loop in the parameter space $\lambda(t=0) = \lambda(t=T)$, the initial and final states are the same under the adiabatic theorem $|\psi(t=0)\rangle = |\psi(t=T)\rangle$. In this case, the basis states $|0\rangle$ and $|1\rangle$ of the ancilla qubit are paired to the same quantum state with different quantum phases. The previous measurement can then be applied to extract the Berry phase.

> **Question 2.3**
>
> Apply the measurement quantum circuit in Question 2.2 to the four different trajectories of Bloch-sphere Hamiltonian in Part 1. Compute the measurement outcomes by sampling with `StatevectorSampler` in `qiskit` or its equivalence. You can use any function in `qiskit` or the other libraries you prefer for quantum-circuit computations. For the numerical setup, you can use the same time period T and number of discrete time steps N_t as in Part 1. Check out whether the measurement outcomes are consistent with the overlap computations in Part 1!

Part 3: How does Berry phase appear in topological phases?

We have studied the Berry phase in adiabatic time evolution of quantum states and its measurement with quantum circuits. In fact, the Berry phase is not limited to time evolution. It applies generally to any adiabatic evolution under sufficiently slow parameter variation. Among its broad applications, a particularly important one is the **topological classification of quantum phases of matter**. In this Part of the Challenge Problem, we will explore a paradigmatic example of topological fermionic phase, the **Su-Schriffer-Heeger (SSH) model**. We will see how the Berry phase distinguishes different quantum phases of matter in this model. Furthermore, we will transform this fermionic model to a qubit model and measure the Berry phase with quantum circuits.

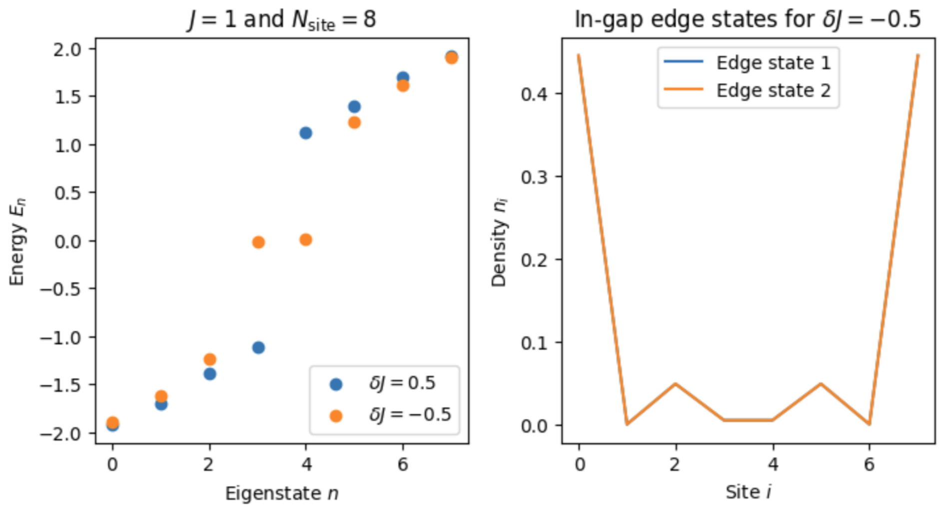
The SSH model describes noninteracting spinless fermions on a one-dimensional lattice

$$H_{\mathrm{SSH}} = -\left[(J+\delta J)\sum_{j\equiv 0 \pmod 2} -(J-\delta J)\sum_{j\equiv 1 \pmod 2}\right] c_{j+1}^{\dagger} c_j + \text{h.c.}.$$

Here $c_j^{(\dagger)}$ is the annihilation (creation) operator for the fermion at the lattice site j. $J \pm \delta J$ are nearest-neighbor hoppings, with two different strengths assigned alternately to the bonds.

Since the bonds are alternate, as indicated by the red and blue ones in the figure, the periodicity of this model is 2 lattice sites. We usually think of the lattice as being composed of two sublattices, indicated by the black and white ones in the figure. Each unit cell contains two sublattice sites with one from each sublattice.

A remarkable property of the SSH model is that it hosts different phases at $\delta J > 0$ and $\delta J < 0$ under open boundary condition (OBC). Particularly, the later phase hosts in-gap edge states at zero energy, while the former phase does not.



The existence of in-gap edge states is related to the electronic polarization. In the modern theory of polarization, the electronic polarization can be written as a momentum-space integral

$$P = -\frac{e}{2\pi}\phi_{\rm Zak} \pmod e.$$

Here $\phi_{\rm Zak}$ is usually called the Zak phase and defined as

$$\phi_{\rm Zak} = \oint dk A_k, \quad A_k = i\langle E_k|\frac{d}{dk}|E_k\rangle,$$

where E_k is the eigenstate of the Fourier-transformed Bloch Hamiltonian $\mathcal{H}_k$ at momentum k. In the SSH model at half filling, due to inversion symmetry, the Zak phase can take two different quantized values $\phi_{\rm Zak} = 0, \pi$, leading to two different values of polarization $P = 0, -e/2$. When $P = 0$, the fermionic density centers in each unit cell sit at the unit-cell centers, that is, the 4 red-bond centers. In this case, the 4 occupied states at half filling can be uniformly distributed at these centers under the inversion symmetry, and the system is a trivial insulator. However, when $P = -e/2$, the fermionic density centers are shifted to the unit-cell edges, that is, the 3 blue-bond centers. After occupying these 3 positions, there remains 1 occupation that has to be distributed under the inversion symmetry. The only way is to separate it half-half to the two edges, leading to an in-gap edge state with fractional edge charges. This type of topological insulators with fractional boundary charges are called the obstructed atomic insulators with filling anomaly.

The discussion here aims for a quick introduction to the novel in-gap edge states in the SSH model, which is a bit sloppy and incomplete. If you are interested in more rigorous details on this topic, please refer to the nice paper Phys. Rev. B 99, 245151 (2019).

The most imporant message for us is that the Zak phase $\phi_{\rm Zak}$ is a Berry phase, where the Berry connection A_k accumulates as the momentum k varies adiabatically over the momentum space. We can see that the Berry phase indeed plays an important role in the classification of topological phases!

We have discussed the existence of in-gap edge states in the SSH model and its relation to the Berry phase. Now it is time for us to work out the computations and confirm its quantization.

Question 3.1

Given the the SSH model, apply the Fourier transform

$$\begin{pmatrix} c_{2j} \\ c_{2j+1} \end{pmatrix} = \frac{1}{\sqrt{N_{\rm uc}}} \sum_k \begin{pmatrix} c_{k0} \\ c_{k1} \end{pmatrix} e^{ik\cdot r_{2j}}$$

with unit Braivais lattice constant $r_{2j+2} - r_{2j} = 1$ for the $N_{\rm uc}$ unit cells. Here we have $N_{\rm uc}$ inequivalent momenta $k = 2\pi n/N_{\rm uc}$ with $n = -N_{\rm uc}/2 - 1, \ldots, N_{\rm uc}/2$, which form the Brillouin zone $[-\pi, \pi]$ in momentum space. Confirm that in the momentum-space representation

$$H = \sum_k c_k^\dagger \mathcal{H}_k c_k, \quad c_k = \begin{pmatrix} c_{k0} \\ c_{k1} \end{pmatrix},$$

the momentum-space Bloch Hamiltonian takes the form

$$\mathcal{H}_k = \vec{h}_k \cdot \vec{\sigma}, \quad \vec{h}_k = (-(J + \delta J) - (J - \delta J)\cos k, -(J - \delta J)\sin k, 0).$$

Plot its spectrum with respect to the momentum k in the Brillouin zone $[-\pi, \pi]$, known as the band structure, for $J = 1$ and $\delta J = -0.5, 0, 0.5$. Can you see the relation between the band structure and the Bloch-vector trajectory?

P.S. You might wonder why we choose the same coordinate for both sublattice sites in the Fourier transform. Actually, this choice is the proper one to obtain the correct polarization that is consistent with OBC phase classification. In general, you can use their real and different coordinates, and the resulting band structure will be the same. However, there are some tricky results in the computation of Berry phase and polarization, which we will not discuss here. Whichever choice is more appropriate is actually unresolved in the research community. If you are interested in the related discussions, please refer to, for example, this paper Phys. Rev. B 104, 235428 (2021).

Since the Bloch Hamiltonian takes the Bloch-sphere form, the tools we develop in the previous Parts can be used to study the Berry phase. We will consider the ground state of the SSH model at half filling, where the fermions fully occupy the ground states $|E_{0k}\rangle$ of the Bloch Hamiltonians $\mathcal{H}_k$ at all momenta k. We can take the momentum $k(t)$ as the time-dependent parameter from $k(t = 0) = -\pi$ to $k(T) = \pi$ and study the adiabatic evolution of the ground state $|E_{0k}\rangle$. However, since the Bloch vector is no longer a unit vector, the ground-state energy E_{0k} varies with momentum k. In this case, the choice of time period as a multiple of 2π does not remove the dynamical phase from the total phase. Fortunately, there is a simple trick of "half time reversal" which we can use for the SSH model. Due to the inversion symmetry, the band structures at k and $-k$ are symmetric. This symmetry means that the accumulated dynamical phases are the same in the two regions. The trick we can use is to evolve forward in time for the first half $[-\pi, 0]$, then backward in time for the second half $[0, \pi]$

$$|\psi_{\rm initial}\rangle = |\psi(t = 0)\rangle \to |\psi_{\rm final}\rangle = \mathcal{T}\left[e^{-i\int_0^{T/2} dt \mathcal{H}_{k(t)}}\right] \mathcal{T}^{-1}\left[e^{-i\int_{T/2}^{0} dt \mathcal{H}_{k(t)}}\right] |\psi(t = 0)\rangle.$$

Here $\mathcal{T}^{-1}$ means we are taking the time ordering reversely. The momentum as a function of time in the two periods are

$$k(t) = \begin{cases} -\pi\left(1 - \frac{t}{T/2}\right), & \text{first half} \\ \pi\left(1 - \frac{t}{T/2}\right), & \text{second half.} \end{cases}$$

In this case, the dynamical phases $\exp[-i\int_0^{T/2} dt E_{k(t)}]$ and $\exp[-i\int_{T/2}^{0} dt E_{k(t)}]$ will cancel with each other, but the Berry phases $\exp(i\int_{-\pi}^{0} dk A_k)$ and $\exp(i\int_0^{\pi} dk A_k)$ will sum up to the result we want. Therefore, the final total phase will be the Berry phase from the adiabatic evolution in the momentum space. The Berry phase can be computed from the overlap between the initial and final states

$$\theta_{\rm Berry} = \arg(O_{\rm if}), \quad O_{\rm if} = \langle\psi_{\rm initial}|\psi_{\rm final}\rangle.$$

Note that there is no minus sign in the Berry phase, since the definition of Berry connection has an opposite sign from the one in time evolution.

Question 3.2

Applying the half-time-reversal trick, obtain the Berry phase of the ground state in the half-filled SSH model. Plot the results for the parameters $J = 1$ and $\delta J \in [-1, 1]$. The Berry phase should be obtained by both the overlap computation in Part 1, together with the overlap magnitude, and the quantum-circuit measurement in Part 2. You can use any function in `qiskit` or the other libraries you prefer for quantum circuit computations. For the numerical setup, you can use the same time period T and number of discrete time steps N_t as in Part 1 and Part 2. Confirm the (nearly) quantized values of Berry phase at $\delta J > 0$ and $\delta J < 0$, and think about the behavrior close to the phase transition $\delta J = 0$!

We have studied the topological phase transition in the SSH model of noninteracting fermions. By Fourier transforming to momentum space and getting the Bloch Hamiltonian of Bloch-sphere type, the measurement of Berry phase clearly distinguishes the topological and trivial phases. In fact, the Berry phase also applies to the topological classification of interaction-driven phases! Here we extend our study of SSH model beyond the noninteracting case by introducing the nearest-neighbor repulsion $V \geq 0$

$$H_{\mathrm{SSH}} = \left(-(J+\delta J) \sum_{j \equiv 0 \pmod 2} -(J-\delta J) \sum_{j \equiv 1 \pmod 2} \right) c_{j+1}^\dagger c_j + \text{h.c.} + V \sum_j n_j n_{j+1},$$

where $n_j = c_j^\dagger c_j$ is the density operator. Due to the presence of interactions, the Fourier transform does not give us a simple Bloch Hamiltonian as in the noninteracting case. Therefore, we will work in the real space and study the lattice model directly.

The interacting-fermion models are generally hard to solve directly, since the treatment of fermionic exchange is nontrivial. Nevertheless, there exists a powerful tool that converts the one-dimensional fermionic models to qubit models without nontrivial exchange properties, known as the **Jordan-Wigner transformation**

$$c_j^\dagger = \prod_{k<j} Z_k \left(\frac{X_j - iY_j}{2} \right), \quad c_j = \prod_{k<j} Z_k \left(\frac{X_j + iY_j}{2} \right).$$

Question 3.3

Show that the fermionic occupation $\{0, 1\}$ is directly mapped to the qubit basis states $\{|0\rangle, |1\rangle\}$

$$n_j = \frac{I_j - Z_j}{2}.$$

Furthermore, verify that the fermionic exchange is encoded correctly in the Pauli strings $\prod_k Z_k$ with correct anticommutators

$$\{c_j, c_k^\dagger\} = \delta_{jk}, \quad \{c_j, c_k\} = \{c_j^\dagger, c_k^\dagger\}^\dagger = 0.$$

Since the qubit models do not have nontrivial exchange properties, they can be diagonalized directly, leading to straightforward studies of the ground states. This approach has been adopted widely in the numerical computations of interacting-fermion systems, including exact diagonalization and tensor-network methods like density-matrix renormalization group.

With this powerful tool, we can study the topological phase transitions in the repulsive SSH model. Here we will consider the finite lattices with periodic boundary condition (PBC), which are more convenient for our later study.

> **Question 3.4**
>
> Using the Jordan-Wigner transformation, derive the qubit model for the repulsive SSH model under PBC.

Since we are interested in the half filling, the repulsive SSH model needs to be projected to the subspace where the fermion number is half of the site numbers. Correspondingly, the qubit model needs to be projected to a subspace, where the bits of the computational basis states sum up to half of the site numbers. If we diagonalize the qubit Hamiltonian without this projection, the resulting ground state might be away from half filling and not what we want.

Having obtained the qubit model of the repulsive SSH model, we can now study the possible topological phase transitions. In the previous study of noninteracting model, we can obtain the Berry phase from the adiabatic evolution with momentum k. Since we are now working in the real-space lattice model, we need to find another way. There is actually an interesting trick that can achieve our goal. In the previous Fourier transform, we know that a nearest-neighbor hopping $c^\dagger_{j+1}c_j$ can generate a phase e^{-ik}. This mapping motivates us to consider adding a phase $e^{-i\phi}$ to the nearest-neighbor bonds and use ϕ as the parameter for adiabatic evolution. However, the $\delta J > 0$ and $\delta J < 0$ PBC models are related simply by a 1-site shift, so they are essentially the same. If we add the complex phase $e^{-i\phi}$ to all bonds, the resulting adiabatic evolution can not distinguish the trivial and topological phases we saw under OBC. Note that the OBC is related to PBC by cutting the PBC bond. According to Question 3.1, we know that cutting a strong bond leads to the topological phase with edge states, while cutting a weak bond gives the trivial phase. Based on this fact, we will add the complex phase $e^{-i\phi}$ to the PBC bond

$$H_{\mathrm{SSH}}(\phi) = \left\{ \left[-(J+\delta J) \sum_{i\equiv 0 \pmod 2} -(J-\delta J) \sum_{i\equiv 1 \pmod 2} \right] c^\dagger_{i+1}c_i - (J-\delta J)e^{i\phi}c^\dagger_{N_{\mathrm{site}}-1}c_0 \right\} + \mathrm{h.c.} + V\sum_{\langle ij\rangle} n_i n_j,$$

sometimes called the "twisted boundary condition". With this phase twisting, we can now measure the so called "local Berry phase" under the adiabatic evolution from $\phi = 0$ to $\phi = 2\pi$. This local topological indicator tells us whether cutting this bond gives us a trivial or topological phase. For more information about local topological indicators, please refer to this original paper arXiv:cond-mat/0603230.

> **Question 3.5**
>
> Perform the Jordan-Wigner transformation and obtain the qubit model for the phase-twisted repulsive SSH model $H_{\mathrm{SSH}}(\theta)$.

We now use the phase-twisted qubit model to measure the Berry phase and detect the topological phase transitions.

> **Question 3.6**
>
> Before jumping into the interacting case, let us re-examine the noninteracting case with $V = 0$ in a 8-site lattice model. Obtain the Berry phase across $\delta J \in [-1, 1]$ and confirm the detection of local topological transition. You can use any function in `qiskit` or the other libraries you prefer for quantum circuit computations. For the numerical setup, you can use the same time period T and

number of discrete time steps N_t as in Question 3.2. Note that you need to project the Hamiltonian to the half filling to get the initial ground state. Meanwhile, the projection is not necessary in the time evolution, since the fermion number is a good quantum number of the Hamiltonian.

Topological phase transitions can happen not only in the noninteracting case, but also under increasing interactions. It is known that the quantum phases of matter at strong coupling can be significantly different from those in the noninteracting case. The most well-known example is the metal-insulator transition in the repulsive Hubbard model. When the systems contain certain structures, such interaction-driven phase transitions can involve the changes of topological properties. The repulsive SSH model serves as a great example of interaction-driven topological phase transition.

Question 3.7

Apply the tools you developed in Question 3.6 to study the repulsion-driven topological phase transition in the SSH model. Perform the computation for $J = 1$, $\delta J = -0.5$, and $V \in [0, 20]$ on a 8-site lattice.

We have studied the topological phase transitions of SSH model in the noninteracting case and under increasing repulsion. An interesting question is whether the trivial phases in the two cases are the same. More generally, you may wonder what does the whole phase diagram look like if we tune the alternate hopping strength δJ and the nearest-neighbor repulsion V.

Question 3.8

Map out the δJ-V phase diagram of the repulsive SSH model at half filling with $J = 1$, $\delta J \in [-1, 1]$, and $V \in [0, 20]$ by computing the energy gap $\Delta E = E_1 - E_0$ between the two lowest-energy states. Here we consider a 8-site lattice with PBC. Remember to project the Hamiltonian to half filling! Looking at the phase diagram, do you think the trivial phases in the two cases are the same?

Final Remarks

We have investigated how the Berry phase appears under adiabatic time evolution, how to measure it with quantum circuits, and how it serves as an indicator to the topological phases of matter. The practical measurements with quantum circuits is particularly exciting. The development of quantum computers is advancing rapidly and may soon support the simulation of complex quantum states. When the simulation of novel topological phases becomes achievable, the measurement of Berry phase will be an important tool for our understanding of these phases. One important point to note is the gate count for this measurement. With the Z-Y-Z and ABC decompositions (see, for example, Sec. 2.2 of this book arXiv:1508.02595), the controlled unitary gate in our 2-qubit quantum circuit for Bloch-sphere Hamiltonians may be decomposed into 2 CNOT gates and 5 single-qubit gates. Multiplied by the number of time steps, we will be looking at over 1000 gates. This number is already very large for the near-term quantum computers due to the noise errors. For the finite-lattice interacting models, the gate counts are even more significant. Nevertheless, the fault-tolerant quantum computers (FTQCs) seem to be achievable in the near future. With the error corrections on FTQCs, quantum algorithms with very deep circuits can be implemented with confidence, and the measurement of Berry phase we study in this Challenge Problem will be valuable.