Adiabatic Approximation
Quantum Mechanics II

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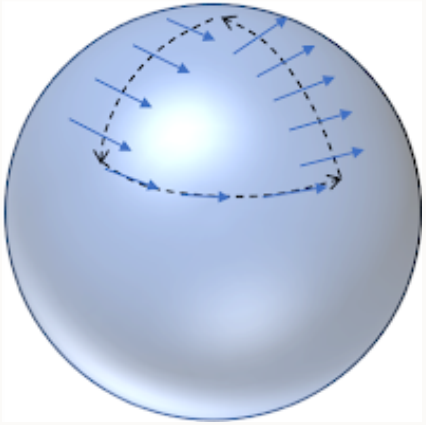

Contents

1 Adiabatic Changes and Adiabatic Invariants

- Adiabatic processes are ubiquitous in physics. They involve time-dependent changes in parameters that control the dynamics of a system, with these changes occurring slowly compared to the system's natural timescale.
- Consider parameters in the Hamiltonian that are typically constant but acquire time dependence. When the parameter changes slowly relative to the system's natural timescale τ, the process is adiabatic. For such systems:
  - Let τ denote the natural timescale of the system.
  - Let $\lambda(t)$ be a time-dependent parameter in the Hamiltonian (e.g., a mass or a magnetic field).
  - The adiabatic condition requires

$$\tau \left| \frac{d\lambda}{dt} \right| \ll |\lambda|$$

  - This condition implies that the change in λ over a time τ is small compared to λ itself.
- Even slowly varying parameters that vary over long times can end up changing by a

sizable factor. Let $\Delta\lambda$ denote a fixed, finite change of λ slowly accumulated over a long time T. Holding $\Delta\lambda$ fixed as we vary T means that the larger T is, the slower the change in λ.

- Let us summarize the various symbols introduced and the key constraint:

$$\begin{aligned} \tau &: \text{ natural timescale of the system} \\ \lambda(t) &: \text{ slowly varying parameter} \\ \Delta\lambda &: \text{ total change in } \lambda \\ T &: \text{ duration of the adiabatic process that is, } t \in [0, T] \\ \tau \left|\frac{d\lambda}{dt}\right| \ll |\lambda| &: \lambda \text{ changes adiabatically.} \end{aligned}$$

adiabatic invariant

- The concept of an **adiabatic invariant** naturally arises in such systems:
  - An adiabatic invariant I is a quantity constructed in terms of $\lambda(t)$ and other slowly varying quantities.
  - The invariant remains approximately constant throughout the time interval $[0, T]$ as λ changes by $\Delta\lambda$.
  - More precisely, the change ΔI approaches zero as $T \to \infty$. The definition is:

$$I \text{ is an adiabatic invariant if for any } t \in [0, T], \quad |I(t) - I(0)| \to 0 \text{ as } T \to \infty$$

2 From Classical to Quantum Adiabatic Invariants

- The simple harmonic oscillator provides a concrete setup to describe adiabatic changes and introduces an interesting example of an adiabatic invariant.
- In the simple harmonic oscillator:
  - The mass of the particle is denoted by m.
  - The frequency of oscillations is denoted by ω.
  - Assume ω becomes a function of time, $\omega(t)$.
- The classical Hamiltonian H of the oscillator is

$$H(x, p, \omega(t)) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2(t) x^2$$

  where x and p are the position and momentum canonical variables, respectively, and are functions of time.
- At any instant, the Hamiltonian's value corresponds to the energy of the system. The time-varying $\omega(t)$ plays the role of the time-dependent parameter $\lambda(t)$.

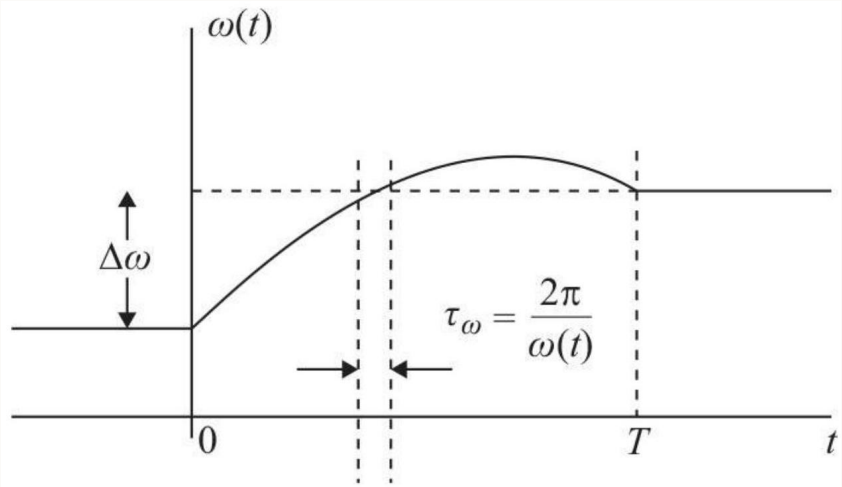

Figure 1: A process with a finite change $\Delta\omega$ of ω occurring in the interval $t \in [0, T]$. The natural timescale of the oscillator is $\tau_\omega = 2\pi/\omega(t)$. In an adiabatic process, $\tau_\omega \ll T$.

- Consider a finite change $\Delta\omega$ in ω over the interval $t \in [0, T]$ (see Figure 1). The natural timescale of the oscillator, τ_ω, is defined as:

$$\tau_\omega(t) \equiv \frac{2\pi}{\omega(t)}$$

- When ω is time-dependent, the motion is not necessarily periodic. Following the adiabatic condition:

$$\tau_\omega \left| \frac{d\omega}{dt} \right| \ll \omega$$

- Substituting $\tau_\omega = \frac{2\pi}{\omega}$, the condition becomes:

$$\frac{2\pi}{\omega^2}\left|\frac{d\omega}{dt}\right| \ll 1 \rightarrow \left|\frac{d}{dt}\frac{2\pi}{\omega}\right| \ll 1$$

  or equivalently:

$$\left|\frac{d\tau_\omega}{dt}\right| \ll 1$$

- This is the condition anticipated earlier. It can also be written as:

$$\left|\frac{\dot{\omega}}{\omega^2}\right| \ll 1$$

- Consider the total change in τ_ω during the time interval $[0, T]$:

$$|\Delta\tau_\omega| = \left|\int d\tau_\omega\right| \leq \int |d\tau_\omega| \ll \int_0^T dt = T$$

  Using the relation $|d\tau_\omega| \ll dt$, this implies:

$$|\Delta\tau_\omega| \ll T$$

- For finite changes in τ_ω, where $|\Delta\tau_\omega| \sim \tau_\omega$, the inequality implies:

$$\text{For finite changes in } \tau_\omega: \quad \tau_\omega \ll T$$

- Having established the condition of adiabaticity, let us calculate the change in energy of the oscillator as a function of time:
  - For a constant ω, the energy is constant.
  - For a time-dependent $\omega(t)$, the time derivative of H is given by:

$$\frac{dH}{dt} = \frac{\partial H}{\partial x}\dot{x} + \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial t}$$

  - Using Hamilton's equations:

$$\dot{x} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial x}$$

  - The first two terms vanish, leaving:

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = m\omega\dot{\omega}x^2$$

- **Claim**: The ratio $I(t)$ of the energy $H(t)$ and the frequency $\omega(t)$ is an adiabatic invariant:

$$I(t) \equiv \frac{H(t)}{\omega(t)}$$

Proof. To begin, we compute the time derivative of I:

$$\begin{aligned}\frac{dI}{dt} &= \frac{1}{\omega^2}\left(\omega\frac{dH}{dt} - H(t)\dot{\omega}\right)\\ &= \frac{1}{\omega^2}\left[\omega(m\omega\dot{\omega}x^2) - \left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2\right)\dot{\omega}\right]\\ &= \frac{\dot{\omega}}{\omega^2}\left(\frac{1}{2}m\omega^2x^2 - \frac{p^2}{2m}\right)\\ &= \frac{\dot{\omega}}{\omega^2}(V(t) - K(t)) \qquad (1)\end{aligned}$$

Here, V and K are the potential and kinetic energies of the oscillator, respectively.

We want to understand why this expression for $\dot{I}$ is small. We know that $\dot{\omega}/\omega^2$ is small in absolute value, but this alone is not sufficient. If the factor multiplying $\dot{\omega}/\omega^2$ were just a constant c, then the change in I over time T would not be small:

$$I(T) - I(0) = \int_0^T \frac{dI}{dt}dt \sim \int_0^T \frac{\dot{\omega}}{\omega^2}\cdot c\,dt = c\left(\frac{1}{\omega(0)} - \frac{1}{\omega(T)}\right). \qquad (2)$$

It also would not vanish for large T. As it turns out, the factor $V(t) - K(t)$ is neither small nor slowly varying, but it varies rapidly with zero average, which plays a crucial

role.

- Consider an oscillator with fixed ω. In that case, we can write:

$$x = A\sin(\omega t) \quad \text{and} \quad p = Am\omega\cos(\omega t), \tag{3}$$

where A is a constant amplitude. Then:

$$V - K = \frac{1}{2}m\omega^2 x^2 - \frac{p^2}{2m} = \frac{1}{2}m\omega^2 A^2(\sin^2\omega t - \cos^2\omega t) = -\frac{1}{2}m\omega^2 A^2\cos(2\omega t). \tag{4}$$

This quantity oscillates rapidly and has zero average over a long time interval.

- Consider again the change in I:

$$I(T) - I(0) = \int_0^T \frac{dI}{dt}dt = \int_0^T \frac{\dot{\omega}}{\omega^2}(t)(V(t) - K(t))dt. \tag{5}$$

If $\omega(t)$ is slowly varying, then $V(t) - K(t)$ can be approximated by the rapidly oscillating form above, with ω and A replaced by slowly varying functions $\omega(t)$ and $A(t)$. Thus:

$$V(t) - K(t) \simeq -\frac{1}{2}m\omega^2(t)A^2(t)\cos[2\omega(t)t]. \tag{6}$$

Substituting this:

$$I(T) - I(0) \simeq -\frac{1}{2}m\int_0^T \dot{\omega}(t)A^2(t)\cos[2\omega(t)t]dt. \tag{7}$$

- To build intuition, consider a linear variation of $\omega(t)$ over the time interval $[0, T]$:

$$\omega(t) = \omega(0) + \frac{t}{T}\Delta\omega \quad \Rightarrow \quad \dot{\omega} = \frac{\Delta\omega}{T}. \tag{8}$$

Then:

$$I(T) - I(0) \simeq -\frac{m\Delta\omega}{2T} \int_0^T A^2(t) \cos[2\omega(t)t] dt. \tag{9}$$

If $A(t)$ varies slowly, the integral of the rapidly oscillating cosine does not grow proportionally to T. Instead, due to the averaging effect, it remains bounded by some constant C:

$$\int_0^T A^2(t) \cos[2\omega(t)t] dt \simeq C, \tag{10}$$

where C does not scale with T. Hence:

$$I(T) - I(0) \simeq -\frac{m\Delta\omega}{2T} C. \tag{11}$$

As $T \to \infty$, this goes to zero. The adiabatic invariant I remains constant in the limit of infinitely slow variation of $\omega(t)$.

- The adiabatic invariant E/ω has a geometric interpretation in phase space. Consider the classical motion of an oscillator with constant ω in the (x, p) plane. The trajectory is an ellipse defined by:

$$\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = E. \tag{12}$$

- The ellipse intersects the x-axis at $\pm a$ and the p-axis at $\pm b$, where:

$$a = \sqrt{\frac{2E}{m\omega^2}} \quad \text{and} \quad b = \sqrt{2mE}. \tag{13}$$

- The area A of the ellipse is:

$$A = \pi ab = 2\pi \frac{E}{\omega} = 2\pi I. \tag{14}$$

  Thus, the adiabatic invariant I is directly related to the enclosed area in phase space.

- We can rewrite the area as a contour integral:

$$A = \oint p\, dx.$$

  For this example:

$$\oint p\, dx = 2\pi I. \tag{15}$$

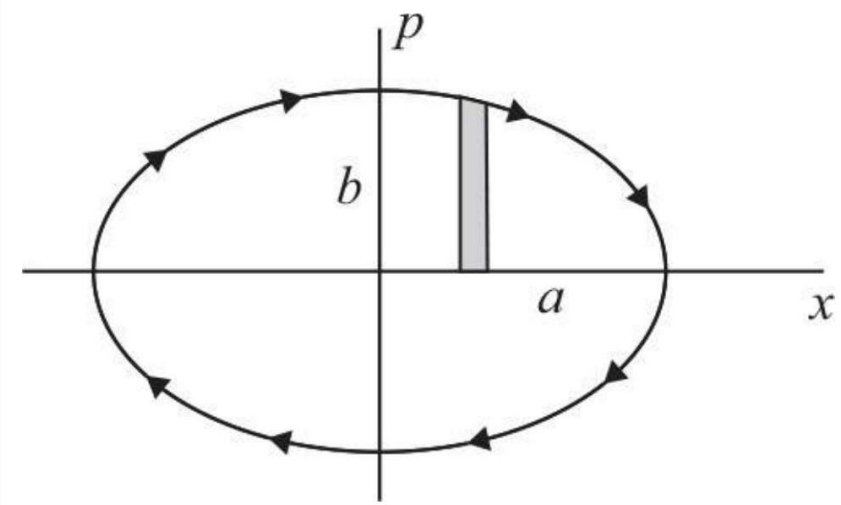

Figure 2: Phase-space trajectory of a harmonic oscillator. The ellipse corresponds to constant energy E.

More generally, for any system with a closed phase-space trajectory, the enclosed area is an adiabatic invariant.

Insights into quantum systems

- Consider the classical harmonic oscillator adiabatic invariant E/ω, and evaluate it for eigenstates of the quantum harmonic oscillator:

$$\frac{E}{\omega} = \frac{1}{\omega}\hbar\omega\left(n+\frac{1}{2}\right) = \hbar\left(n+\frac{1}{2}\right)$$

  The adiabatic invariant is the quantum number of the energy eigenstate. This suggests that in quantum mechanics the quantum number does not easily change under adiabatic changes. This is reasonable because quantum numbers are integers, and changes from one integer to another are necessarily discontinuous.

- A similar intuition follows more generally from the WKB approximation. Consider a potential with two turning points a, b. In that case, the Bohr-Sommerfield quantization condition reads

$$\frac{1}{\hbar}\int_a^b p(x)\,dx = \left(n+\frac{1}{2}\right)\pi, \quad n = 0, 1, \ldots$$

  The classical motion here is that of a particle bouncing between the two turning points. In phase space, a closed trajectory is obtained when the particle begins at a, goes to b,

and then returns to a. For that trajectory, we see that

$$\oint p(x)\,dx = 2\pi\hbar\left(n+\frac{1}{2}\right), \quad n=0,1,\ldots$$

The left-hand side, as noted before, is an adiabatic invariant. Therefore, in the semi-classical approximation, the story for the harmonic oscillator holds now for arbitrary potential: the adiabatic invariant evaluates to the quantum number, suggesting again that transitions between energy eigenstates are suppressed under adiabatic changes. We will confirm that this is the case.

- The result for transition probabilities at first order in time-dependent perturbation theory gives complementary intuition:

$$P_{f\leftarrow i}(t) = \left|\int_0^t e^{i\omega_j t'}\frac{\delta H_{fi}(t')}{i\hbar}\,dt'\right|^2$$

We can mimic adiabatic changes with a constant perturbation in which δH_{fi} is time-independent:

$$P_{f\leftarrow i}(t) = \frac{|\delta H_{fi}|^2}{\hbar^2}\left|\int_0^t e^{i\omega_j t'}\,dt'\right|^2 = \frac{|\delta H_{fi}|^2}{\hbar^2}\frac{\left|e^{i\omega_f t}-1\right|^2}{\omega_{fi}^2}$$

If the spectrum is discrete, the transition probability is suppressed by the energy gap squared, as shown by the ω_{fi}^2 factor in the denominator. It is reasonable to expect that for slowly varying perturbations, this suppression will remain. Thus, it is generally difficult to change state with constant or slow perturbations, suggesting again that quantum numbers are adiabatic invariants. Efficient transitions between energy levels require oscillatory perturbations at resonance.

3 Instantaneous Energy Eigenstates

- In a system with a time-dependent Hamiltonian $\hat{H}(t)$, it is possible to find states $|\psi(t)\rangle$ that satisfy the curious equation

$$\hat{H}(t)|\psi(t)\rangle = E(t)|\psi(t)\rangle$$

We say this is a curious equation because the similar equation $\hat{H}|\psi\rangle = E|\psi\rangle$ was defined for time independent Hamiltonians and position-dependent but time independent $|\psi\rangle$. The states solving $\hat{H}|\psi\rangle = E|\psi\rangle$ can be promoted to solutions $|\Psi\rangle = e^{-iEt/\hbar}|\psi\rangle$ of the Schrödinger equation.

- In the above equation, the spatial dependence is present but implicit, for brevity. In contrast to energy eigenstates, however, both $|\psi(t)\rangle$ and the energy are time dependent. The solution $|\psi(t)\rangle$ is built by solving the equation

$$H(t_0)|\psi(t_0)\rangle = E(t_0)|\psi(t_0)\rangle$$

for every value of the time t_0 and putting together these solutions into a single solution $|\psi(t)\rangle$ with some $E(t)$.

- We'll call the state $|\psi(t)\rangle$ defined by the above equation an *instantaneous eigenstate*. The name is appropriate because it is, at any time, an eigenstate of the Hamiltonian at that time.
- It is important to emphasize that, in general, an instantaneous eigenstate is not a solution of the time-dependent Schrödinger equation. Not even in the time-independent case is $\psi(x)$ a solution of the Schrödinger equation; it must be supplemented by a time-dependent phase to be one. As it turns out, for $|\psi(t)\rangle$, a simple time-dependent phase will not suffice. In the adiabatic approximation, however, $|\psi(t)\rangle$ can be upgraded to an approximate solution to the Schrödinger equation.
- Instantaneous eigenstates are less exotic than they may seem at first sight. There is a natural way to generate them. Consider a time-independent Hamiltonian $\hat{H}\left(R_1, \ldots, R_k\right)$ that depends on some parameters $R_1, \ldots, R_k$. These parameters could be masses, frequencies, magnetic fields, sizes of wells, parameters in a potential, and so on. We then find the familiar eigenstates

$$\hat{H}\left(R_1, \ldots, R_k\right)\left|\psi\left(R_1, \ldots, R_k\right)\right\rangle = E\left(R_1, \ldots, R_k\right)\left|\psi\left(R_1, \ldots, R_k\right)\right\rangle$$

As expected, both the energy and the state depend on the values of the parameters. In fact, they are continuous functions of the parameters. We write this more briefly as

$$\hat{H}(\boldsymbol{R})|\psi(\boldsymbol{R})\rangle = E(\boldsymbol{R})|\psi(\boldsymbol{R})\rangle$$

- Now imagine the parameters become time dependent in some arbitrary way:

$$\boldsymbol{R} \to \boldsymbol{R}(t)$$

Since the above equation holds for arbitrary values of the parameters, for any value of time we find that

$$\hat{H}(\boldsymbol{R}(t))|\psi(\boldsymbol{R}(t))\rangle = E(\boldsymbol{R}(t))|\psi(\boldsymbol{R}(t))\rangle$$

The $|\psi(\boldsymbol{R}(t))\rangle$ are indeed instantaneous eigenstates of the time-dependent Hamiltonian $\hat{H}(\boldsymbol{R}(t))$. This procedure naturally implements the continuity requirement on the instantaneous eigenstates because the original eigenstates $|\psi(\boldsymbol{R})\rangle$ are continuous functions of the parameters.

- We must emphasize that instantaneous eigenstates have a rather important phase ambiguity. This ambiguity originates at the level of the parameter-dependent states. Consider

changing the states $|\psi(\boldsymbol{R})\rangle$ as follows:

$$|\psi(\boldsymbol{R})\rangle \to e^{i\gamma(\boldsymbol{R})}|\psi(\boldsymbol{R})\rangle$$

where $\gamma(\boldsymbol{R})$ is a real function of the parameters. The new states will still satisfy the equation $\hat{H}(\boldsymbol{R})|\psi(\boldsymbol{R})\rangle = E(\boldsymbol{R})|\psi(\boldsymbol{R})\rangle$, and their normalization has not been altered, so the states are as good as the originals.

- Similarly, for the time-dependent eigenstates, if we let

$$|\psi(\boldsymbol{R}(t))\rangle \to e^{i\gamma(t;\boldsymbol{R}(t))}|\psi(\boldsymbol{R}(t))\rangle$$

the equation $\hat{H}(\boldsymbol{R}(t))|\psi(\boldsymbol{R}(t))\rangle = E(\boldsymbol{R}(t))|\psi(\boldsymbol{R}(t))\rangle$ will still hold. This phase ambiguity of instantaneous eigenstates will be relevant to the definition of geometric phases.

Example. Instantaneous spin one-half states.

- A simple example of instantaneous eigenstates is provided by spin one-half eigenstates. The Hamiltonian for an electron in a magnetic field reads

$$\hat{H} = \mu_B \mathbf{B} \cdot \boldsymbol{\sigma}$$

For a uniform, time-independent magnetic field $\mathbf{B} = B_0 \mathbf{n}$, with $\mathbf{n}$ a unit vector,

$$\hat{H}\left(B_0, \mathbf{n}\right) = \mu_B B_0 \mathbf{n} \cdot \boldsymbol{\sigma}$$

Here we have made explicit that B_0 and $\mathbf{n}$ are parameters in the Hamiltonian. The eigenstates are $|\mathbf{n}; \pm\rangle$ satisfying $\mathbf{n} \cdot \boldsymbol{\sigma} |\mathbf{n}; \pm\rangle = \pm |\mathbf{n}; \pm\rangle$, and therefore,

$$\hat{H}\left(B_0, \mathbf{n}\right) |\mathbf{n}; \pm\rangle = \pm \mu_B B_0 |\mathbf{n}; \pm\rangle$$

- More explicitly, and with $\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the spin states are

$$|\mathbf{n}; +\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}, \quad |\mathbf{n}; -\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} e^{-i\phi} \\ \cos\frac{\theta}{2} \end{pmatrix}$$

- Now imagine that both the magnitude B_0 and the direction $\mathbf{n}$ of the magnetic field change in time so that $B_0 \to B_0(t)$, and $\mathbf{n} \to \mathbf{n}(t)$. The change of $\mathbf{n}$ can be described explicitly by giving the time dependence $\theta(t)$ and $\phi(t)$ of the spherical angles θ, ϕ that define the direction $\mathbf{n}(t)$. It follows that

$$\hat{H}\left(B_0(t), \mathbf{n}(t)\right) |\mathbf{n}(t); \pm\rangle = \pm\mu_B B_0(t) |\mathbf{n}(t); \pm\rangle$$

- The eigenvalues $\pm\mu_B B_0(t)$ are now time dependent, and so are the eigenstates, which become

$$|\mathbf{n}(t); +\rangle = \begin{pmatrix} \cos\frac{\theta(t)}{2} \\ \sin\frac{\theta(t)}{2} e^{i\phi(t)} \end{pmatrix}, \quad |\mathbf{n}(t); -\rangle = \begin{pmatrix} -\sin\frac{\theta(t)}{2} e^{-i\phi(t)} \\ \cos\frac{\theta(t)}{2} \end{pmatrix}$$

- The magnitude $B_0(t)$ of the magnetic field appears in the instantaneous eigenvalues but does not appear in the instantaneous eigenstates.

Building on the instantaneous eigenstates

- Let us try to understand the relation between the instantaneous eigenstate $|\psi(t)\rangle$ and a solution $|\Psi(t)\rangle$ of the Schrödinger equation

$$i\hbar\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle$$

- We try an ansatz for $|\Psi(t)\rangle$ in terms of the instantaneous eigenstate:

$$|\Psi(t)\rangle = c(t)\exp\left(\frac{1}{i\hbar}\int_0^t E\left(t'\right)dt'\right)|\psi(t)\rangle$$

- Here $c(t)$ is a function of time to be determined, and we have included a time-dependent phase that is a natural generalization of the phase $e^{-iEt/\hbar}$ appropriate for time-independent Hamiltonians.
- The left-hand side of the Schrödinger equation then becomes

$$\begin{aligned} i\hbar\partial_t|\Psi(t)\rangle =& \, i\hbar\dot{c}(t)\exp\left(\frac{1}{i\hbar}\int_0^t E\left(t'\right)dt'\right)|\psi(t)\rangle \\ &+ E(t)|\Psi(t)\rangle + i\hbar c(t)\exp\left(\frac{1}{i\hbar}\int_0^t E\left(t'\right)dt'\right)|\dot{\psi}(t)\rangle \end{aligned}$$

- For the right-hand side, using the instantaneous eigenstate equation, we have

$$\hat{H}(t)|\Psi(t)\rangle = c(t)\exp\left(\frac{1}{i\hbar}\int_0^t E\left(t'\right)dt'\right)\hat{H}(t)|\psi(t)\rangle = E(t)|\Psi(t)\rangle$$

- Equating the two sides gives

$$\dot{c}(t)\exp\left(\frac{1}{i\hbar}\int_0^t E\left(t'\right)dt'\right)|\psi(t)\rangle + c(t)\exp\left(\frac{1}{i\hbar}\int_0^t E\left(t'\right)dt'\right)|\dot{\psi}(t)\rangle = 0$$

- Canceling the exponentials, we find

$$\dot{c}(t)|\psi(t)\rangle = -c(t)|\dot{\psi}(t)\rangle$$

- Multiply by $\langle\psi(t)|$ to get a differential equation for $c(t)$:

$$\dot{c}(t) = -c(t)\langle\psi(t)\mid\dot{\psi}(t)\rangle$$

- Solving this, with $c(0) = 1$, we find

$$c(t) = \exp\left(-\int_0^t \left\langle\psi\left(t'\right)\mid\dot{\psi}\left(t'\right)\right\rangle dt'\right)$$

- The above exponential is a phase because the bracket in the integrand is actually purely imaginary. Indeed, taking a time derivative of $\langle \psi(t) \mid \psi(t) \rangle = 1$, we have

$$\langle \dot{\psi}(t) \mid \psi(t) \rangle + \langle \psi(t) \mid \dot{\psi}(t) \rangle = 0 \quad \Rightarrow \quad \langle \psi(t) \mid \dot{\psi}(t) \rangle^* + \langle \psi(t) \mid \dot{\psi}(t) \rangle = 0,$$

- To emphasize this fact, we write

$$c(t) = \exp\left(i \int_0^t i \left\langle \psi\left(t'\right) \mid \dot{\psi}\left(t'\right) \right\rangle dt' \right)$$

- Returning to our ansatz, we get

$$|\Psi(t)\rangle \simeq c(0) \exp\left(i \int_0^t i \left\langle \psi\left(t'\right) \mid \dot{\psi}\left(t'\right) \right\rangle dt' \right) \exp\left(\frac{1}{i\hbar} \int_0^t E\left(t'\right) dt' \right) |\psi(t)\rangle$$

- However, this is only an approximate solution because the Schrödinger equation is not fully solved by this ansatz. The approximate solution is valid if the Hamiltonian varies slowly.

- Defining

$$\theta(t) \equiv -\frac{1}{\hbar}\int_0^t E\left(t'\right)dt', \quad v(t) \equiv i\langle\psi(t) \mid \dot{\psi}(t)\rangle, \quad \gamma(t) \equiv \int_0^t v\left(t'\right)dt'.$$

  Here, $\theta(t), \nu(t)$, and $\gamma(t)$ are all real. The state can be written as

$$|\Psi(t)\rangle \simeq c(0)e^{i\gamma(t)}e^{i\theta(t)}|\psi(t)\rangle$$

- We call $\theta(t)$ the *dynamical phase* and $\gamma(t)$ the *geometric phase*.

4 Quantum Adiabatic Theorem

- Let us begin by stating precisely the content of the adiabatic theorem in quantum mechanics. For this, consider a family of instantaneous eigenstates:

$$\hat{H}(t)\,|\psi_n(t)\rangle = E_n(t)\,|\psi_n(t)\rangle$$

with $E_1(t) < E_2(t) < \ldots$ so that there are no degeneracies in this spectrum at any time. We will also assume, for simplicity, that the spectrum of $\hat{H}$ is only discrete and that the number of energy eigenstates is finite.

- **Adiabatic theorem**: *Let $\hat{H}(t)$ be a continuously varying Hamiltonian for $0 \leq t \leq T$. Let the state of the system at $t = 0$ be one of the instantaneous eigenstates: $|\Psi(0)\rangle = |\psi_m(0)\rangle$ for some m. Then at any time $t \in [0, T]$ we have $|\Psi(t)\rangle \simeq |\psi_m(t)\rangle$ up to a calculable phase. The amplitude to transition to any other instantaneous eigenstate is of order $1/T$. This implies that the probability of remaining in the instantaneous eigenstate is one up to corrections of order $1/T^2$.*

- To prove the adiabatic theorem, we begin by setting an expansion for our normalized, time-dependent state $|\Psi(t)\rangle$:

$$|\Psi(t)\rangle = \sum_n c_n(t)\,|\psi_n(t)\rangle$$

Since the instantaneous eigenstates are normalized, all c_n satisfy $|c_n(t)| \leq 1$. The Schrödinger equation then gives

$$i\hbar \sum_n \left(\dot{c}_n\,|\psi_n(t)\rangle + c_n|\dot{\psi}_n(t)\rangle\right) = \sum_n c_n(t)E_n(t)\,|\psi_n(t)\rangle$$

- Acting with $\langle\psi_k(t)|$ from the left gives

$$i\hbar\dot{c}_k = E_k c_k - i\hbar \sum_n \langle\psi_k \mid \dot{\psi}_n\rangle c_n$$

- From the sum, we separate out the term $n = k$:

$$i\hbar\dot{c}_k = \left(E_k - i\hbar\langle\psi_k \mid \dot{\psi}_k\rangle\right) c_k - i\hbar \sum_{n\neq k} \langle\psi_k \mid \dot{\psi}_n\rangle c_n$$

- It is clear that the terms in the sum are those that couple the $n \neq k$ eigenstates to the k eigenstate. This is the term that produces transitions. Absent that term, if at $t = 0$ we have $c_k(0) = 0$, then $c_k(t) = 0$ for all times, and no transition to the state $|\psi_k(t)\rangle$ happens.

- To relate $\langle \psi_k \mid \dot{\psi}_n \rangle$ to a matrix element of the time derivative of $\hat{H}(t)$, we start with the defining equation:

$$\hat{H}(t)\,|\psi_n(t)\rangle = E_n(t)\,|\psi_n(t)\rangle$$

  Taking a time derivative gives

$$\frac{d\hat{H}(t)}{dt}\,|\psi_n(t)\rangle + \hat{H}(t)\left|\dot{\psi}_n(t)\right\rangle = \frac{dE_n(t)}{dt}\,|\psi_n(t)\rangle + E_n(t)\left|\dot{\psi}_n(t)\right\rangle$$

- Multiplying by $\langle \psi_k(t)|$ from the left, with $k \neq n$, gives

$$\langle \psi_k(t)|\,\frac{d\hat{H}}{dt}\,|\psi_n(t)\rangle + E_k(t)\left\langle \psi_k(t) \mid \dot{\psi}_n(t)\right\rangle = E_n(t)\left\langle \psi_k(t) \mid \dot{\psi}_n(t)\right\rangle$$

- Solving for $\left\langle \psi_k(t) \mid \dot{\psi}_n(t)\right\rangle$, we find

$$\left\langle \psi_k(t) \mid \dot{\psi}_n(t)\right\rangle = \frac{\langle \psi_k(t)|\,\frac{d\hat{H}}{dt}\,|\psi_n(t)\rangle}{E_n(t) - E_k(t)} \equiv \frac{\left[\frac{d\hat{H}}{dt}\right]_{kn}}{E_n - E_k}, \qquad k \neq n$$

- Plugging this back into the Schrödinger equation gives

$$i\hbar\dot{c}_k = \left(E_k - i\hbar\left\langle \psi_k \mid \dot{\psi}_k\right\rangle\right)c_k - i\hbar\sum_{n\neq k}\frac{\left[\frac{d\hat{H}}{dt}\right]_{kn}}{E_n - E_k}c_n$$

- Ignoring the transition-causing terms, we would have

$$i\hbar\dot{c}_k = \left(E_k - i\hbar\left\langle \psi_k \mid \dot{\psi}_k \right\rangle\right) c_k$$

- This integrates to

$$c_k(t) = c_k(0)\exp\left[-\frac{i}{\hbar}\int_0^t E_k\left(t'\right)dt'\right]\exp\left[i\int_0^t i\left\langle \psi_k \mid \dot{\psi}_k \right\rangle dt'\right]$$

- Defining

$$\theta_k(t) = -\frac{1}{\hbar}\int_0^t E_k\left(t'\right)dt', \quad \gamma_k(t) = \int_0^t v_k\left(t'\right)dt', \quad v_k(t) = i\left\langle \psi_k(t) \mid \dot{\psi}_k(t) \right\rangle,$$

the result becomes

$$c_k(t) = c_k(0)e^{i\theta_k(t)}e^{i\gamma_k(t)}$$

- If $|\Psi(0)\rangle = |\psi_m(0)\rangle$, we have

$$|\Psi(t)\rangle \simeq e^{i\theta_m(t)}e^{i\gamma_m(t)}\,|\psi_m(t)\rangle$$

5 Berry Phase

- In our statement of the adiabatic theorem, we emphasized that for Hamiltonians varying continuously in the time interval $t \in [0, T]$ and for a state in an instantaneous eigenstate $|\psi_n(t)\rangle$ at $t = 0$, the state at any time $t \in [0, T]$ is rather accurately equal to $|\psi_n(t)\rangle$ up to a calculable phase. The probability that the system transitions to another energy eigenstate is suppressed by a factor of order $1/T^2$.
- Now we want to focus on the calculable phase, which we already determined as follows:

$$|\Psi(t)\rangle \simeq e^{i\theta_n(t)} e^{i\gamma_n(t)} |\psi_n(t)\rangle$$

- The dynamical phase $\theta_n(t)$ exists even if the Hamiltonian and the eigenstates are time independent. The geometric phase $\gamma_n(t)$, however, vanishes in this case. This phase is given by

$$\gamma_n(t) = \int_0^t v_n(t')dt', \quad v_n(t) = i\langle\psi_n(t)|\dot{\psi}_n(t)\rangle$$

- Let the time dependence of $\hat{H}$ be expressed in terms of a set of N parameters that are time dependent. We will refer to these parameters as coordinates in some configuration space:

$$\boldsymbol{R} = (R_1, \ldots, R_N)$$

- Assume that we have eigenstates for all values of the coordinates:

$$\hat{H}(\boldsymbol{R})|\psi_n(\boldsymbol{R})\rangle = E(\boldsymbol{R})|\psi_n(\boldsymbol{R})\rangle$$

- For time-dependent coordinates:

$$\boldsymbol{R}(t) = (R_1(t), \ldots, R_N(t))$$

- The instantaneous eigenstates satisfy:

$$\hat{H}(\boldsymbol{R}(t))|\psi_n(\boldsymbol{R}(t))\rangle = E(\boldsymbol{R}(t))|\psi_n(\boldsymbol{R}(t))\rangle$$

- At each instant of time, a point in configuration space determines the values of all parameters. The time evolution of the Hamiltonian can be thought of as a path in the configuration space, parameterized by time.

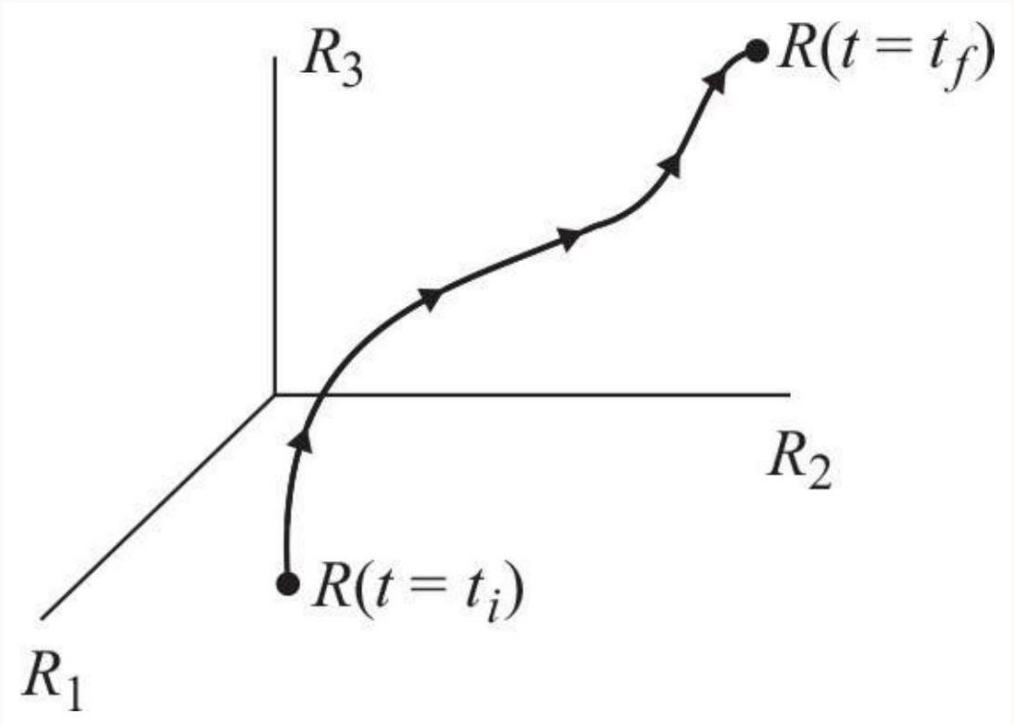

Figure 3: A time-dependent adiabatic process visualized as motion along a curve in the configuration space for the Hamiltonian.

- To evaluate the geometric phase, we start by computing its integrand $v_n(t)$:

$$v_n(t) = i\langle\psi_n(\boldsymbol{R}(t))|\frac{d}{dt}|\psi_n(\boldsymbol{R}(t))\rangle$$

- Using the chain rule:

$$\frac{d}{dt}|\psi_n(\boldsymbol{R}(t))\rangle = \sum_{i=1}^{N}\frac{\partial}{\partial R_i}|\psi_n(\boldsymbol{R}(t))\rangle\frac{dR_i}{dt} = \nabla_{\boldsymbol{R}}|\psi_n(\boldsymbol{R}(t))\rangle\cdot\frac{d\boldsymbol{R}(t)}{dt}$$

- Substituting back, we find:

$$v_n(t) = i\langle\psi_n(\boldsymbol{R}(t))|\nabla_{\boldsymbol{R}}|\psi_n(\boldsymbol{R}(t))\rangle\cdot\frac{d\boldsymbol{R}(t)}{dt}$$

- The geometric phase $\gamma_n(t_i, t_f)$ is then:

$$\gamma_n(t_i,t_f) \equiv \int_{t_i}^{t_f} v_n(t)dt = \int_{t_i}^{t_f} i\langle\psi_n(\boldsymbol{R}(t))|\nabla_{\boldsymbol{R}}|\psi_n(\boldsymbol{R}(t))\rangle\cdot\frac{d\boldsymbol{R}(t)}{dt}dt$$

- Replacing dt with $d\boldsymbol{R}$, we get:

$$\gamma_n(\Gamma_{if}) = \int_{\boldsymbol{R}_i}^{\boldsymbol{R}_f} i\langle\psi_n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}|\psi_n(\boldsymbol{R})\rangle\cdot d\boldsymbol{R}$$

- The integral depends on the path Γ_{if} in configuration space but does not depend on time! The phase is thus geometric: it does not depend on the parameterization of the path by the time parameter. Whether the transition from $\boldsymbol{R}_i$ to $\boldsymbol{R}_f$ along Γ_{if} takes a nanosecond or an hour, the phase $\gamma_n(\Gamma_{if})$ accumulated is the same. The geometric phase is known as **Berry's phase**. Recalling that for a function $f(\mathbf{u})$ of several variables u_i one has $df = \sum_i \frac{\partial f}{\partial_i} du_i$, we recognize that

$$\nabla_{\boldsymbol{R}} |\psi_n(\boldsymbol{R})\rangle \cdot d\boldsymbol{R} = d\,|\psi_n(\boldsymbol{R})\rangle$$

- Compactly written:

$$\gamma_n(\Gamma_{if}) = \int_{\Gamma_{if}} i\langle\psi_n(\boldsymbol{R})|d|\psi_n(\boldsymbol{R})\rangle$$

- Defining the **Berry connection**:

$$\mathbf{A}_n(\boldsymbol{R}) \equiv i\langle\psi_n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}|\psi_n(\boldsymbol{R})\rangle$$

- Berry's phase becomes:

$$\gamma_n(\Gamma_{if}) = \int_{\Gamma_{if}} \mathbf{A}_n(\boldsymbol{R}) \cdot d\boldsymbol{R}$$

- This integral is similar to those in electrodynamics involving the integral of the vector potential along a path. Like any connection, $\mathbf{A}_n(\boldsymbol{R})$ has gauge transformations. The gauge transformations arise from redefinitions of the instantaneous eigenstates by phases reflecting the ambiguity of these states. Let us consider such a redefinition into "tilde" states:

$$|\psi_n(\boldsymbol{R})\rangle \to |\tilde{\psi}_n(\boldsymbol{R})\rangle \equiv e^{-i\beta(\boldsymbol{R})}|\psi_n(\boldsymbol{R})\rangle$$

- Under this redefinition, let us compute the new Berry connection:

$$\begin{aligned}\tilde{\mathbf{A}}_n(\boldsymbol{R}) &= i\langle\tilde{\psi}_n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}|\tilde{\psi}_n(\boldsymbol{R})\rangle \\ &= i\langle\psi_n(\boldsymbol{R})|e^{i\beta(\boldsymbol{R})}\nabla_{\boldsymbol{R}}e^{-i\beta(\boldsymbol{R})}|\psi_n(\boldsymbol{R})\rangle \\ &= i\left(-i\nabla_{\boldsymbol{R}}\beta(\boldsymbol{R})\right)\langle\psi_n(\boldsymbol{R})|\psi_n(\boldsymbol{R})\rangle + \mathbf{A}_n(\boldsymbol{R})\end{aligned}$$

- Since the eigenstates are normalized, we conclude that:

$$\widetilde{\mathbf{A}}_n(\boldsymbol{R}) = \mathbf{A}_n(\boldsymbol{R}) + \nabla_{\boldsymbol{R}}\beta(\boldsymbol{R})$$

- This result is analogous to the gauge transformations of the vector potential in electrodynamics $\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\Lambda$. Next, let us compute what happens to Berry's phase under

these gauge transformations:

$$\begin{aligned}\widetilde{\gamma}_n(\Gamma_{if}) &= \int_{\Gamma_{if}} \widetilde{\mathbf{A}}_n(\boldsymbol{R}) \cdot d\boldsymbol{R} \\ &= \int_{\Gamma_{if}} \mathbf{A}_n(\boldsymbol{R}) \cdot d\boldsymbol{R} + \int_{\Gamma_{if}} \nabla_{\boldsymbol{R}} \beta(\boldsymbol{R}) \cdot d\boldsymbol{R}\end{aligned}$$

- The second term is an integral of a total derivative, so it picks up the values of the integrand at the endpoints of the path:

$$\tilde{\gamma}_n(\Gamma_{if}) = \gamma_n(\Gamma_{if}) + \beta(\boldsymbol{R}_f) - \beta(\boldsymbol{R}_i)$$

- This result demonstrates that the geometric phase associated with an open path in configuration space (a path that begins and ends at different points) is ambiguous. The phase can be modified by redefinitions of the instantaneous eigenstates. By choosing the function $\beta(\boldsymbol{R})$ suitably, one could even make the geometric phase vanish along the open path.
- However, if the path is closed, $\boldsymbol{R}_f = \boldsymbol{R}_i$, and therefore $\beta(\boldsymbol{R}_f) = \beta(\boldsymbol{R}_i)$. In this case, the geometric phase becomes:

$$\tilde{\gamma}_n(\Gamma) = \gamma_n(\Gamma)$$

- This shows that the geometric phase for a closed path Γ in parameter space is gauge invariant. Such a phase is an observable quantity.
- While the phase of a single state is not observable, Berry's phase is observable in a setting with more than one state. Consider a Hamiltonian and build a state that at $t = 0$ is in a superposition of two instantaneous eigenstates.
- Suppose the Hamiltonian is time dependent and traces a loop in configuration space. Each of the two eigenstates will evolve, and each will acquire a Berry phase. At the end of the evolution, the difference between the phases of the two states, as usual, can be observed.
- Berry's phase has turned out to be a rather useful concept and features in various physical phenomena, such as:
  - Quantum magnetism,
  - Spin one-half chains,
  - Topological insulators.

Example: Berry phase for an electron in a slowly varying magnetic field.

- We have considered an electron in a uniform magnetic field $\mathbf{B} = B_0\mathbf{n}$. The Hamiltonian is

$$\hat{H} = \mu_B B_0 \mathbf{n} \cdot \boldsymbol{\sigma}.$$

  We now let the magnitude B_0 and the direction $\mathbf{n}$ of the magnetic field change in time so that $B_0 \to B_0(t)$ and $\mathbf{n} \to \mathbf{n}(t)$.

- The configuration space is described with three parameters:

$$(R_1, R_2, R_3) = (B_0, \theta, \phi).$$

- Assuming that the magnetic field traces a closed loop Γ in configuration space, the tip of $\mathbf{n}$ traces a path on the unit sphere, and B_0 returns to its initial value. We compute Berry's phase for this loop.

- For the eigenstate $|\mathbf{n}\rangle \equiv |\mathbf{n}; +\rangle$, we have:

$$|\mathbf{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}.$$

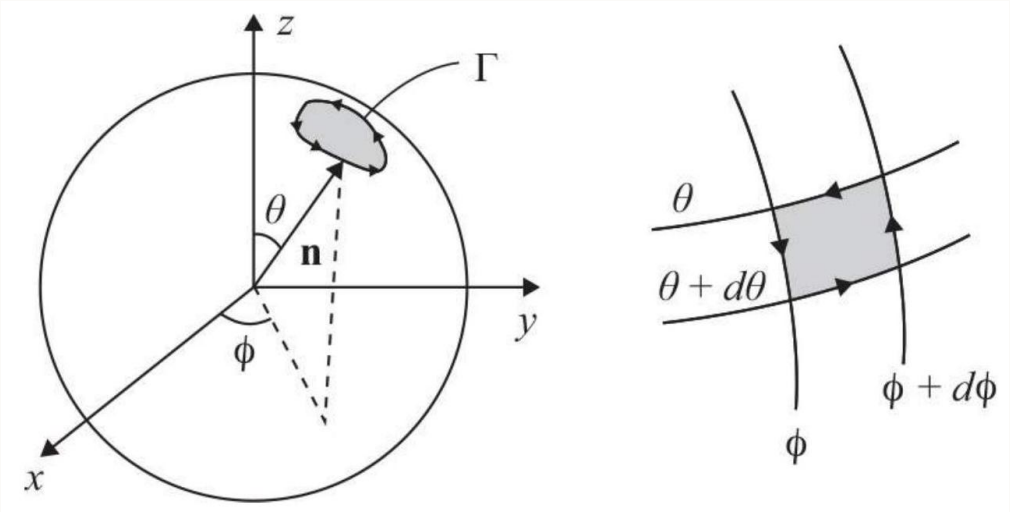

Figure 4: Left: The direction of a magnetic field is determined by the unit vector $\mathbf{n}$, specified by spherical angles (θ, ϕ). The tip of $\mathbf{n}$ traces a closed loop Γ on the unit sphere. Right: An infinitesimal rectangle in (θ, ϕ)-space.

- Using equations for Berry's phase and Berry connection, the phase is given by:

$$\gamma_+(\Gamma) = \int_\Gamma \mathbf{A}_+(\boldsymbol{R}) \cdot d\boldsymbol{R}, \quad \mathbf{A}_+(\boldsymbol{R}) \cdot d\boldsymbol{R} = i\langle \mathbf{n}|\nabla_{\boldsymbol{R}}|\mathbf{n}\rangle \cdot d\boldsymbol{R}.$$

- Expanding the derivative:

$$\mathbf{A}_+(\boldsymbol{R}) \cdot d\boldsymbol{R} = i\langle \mathbf{n}| \left(\frac{\partial}{\partial B_0}|\mathbf{n}\rangle dB_0 + \frac{\partial}{\partial \theta}|\mathbf{n}\rangle d\theta + \frac{\partial}{\partial \phi}|\mathbf{n}\rangle d\phi \right).$$

Since $|\mathbf{n}\rangle$ does not depend on B_0, this simplifies to:

$$\mathbf{A}_+(\boldsymbol{R}) \cdot d\boldsymbol{R} = i\langle \mathbf{n}|\frac{\partial}{\partial\theta}|\mathbf{n}\rangle d\theta + i\langle \mathbf{n}|\frac{\partial}{\partial\phi}|\mathbf{n}\rangle d\phi.$$

- Evaluating the components:

$$\langle \mathbf{n}|\frac{\partial}{\partial\theta}|\mathbf{n}\rangle = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{-i\phi}\right)\begin{pmatrix} -\frac{1}{2}\sin\frac{\theta}{2} \\ \frac{1}{2}\cos\frac{\theta}{2}e^{i\phi}\end{pmatrix} = 0$$

$$\langle \mathbf{n}|\frac{\partial}{\partial\phi}|\mathbf{n}\rangle = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{-i\phi}\right)\begin{pmatrix} 0 \\ i\sin\frac{\theta}{2}e^{i\phi}\end{pmatrix} = i\sin^2\frac{\theta}{2}$$

- Substituting back, we get:

$$\mathbf{A}_+(\boldsymbol{R}) \cdot d\boldsymbol{R} = -\sin^2\frac{\theta}{2}d\phi = -\frac{1}{2}(1-\cos\theta)d\phi.$$

- Therefore, Berry's phase becomes:

$$\gamma_+(\Gamma) = -\frac{1}{2}\int_\Gamma (1-\cos\theta)d\phi.$$

- Let S_Γ denote the surface on the unit sphere with boundary Γ. The solid angle spanned by S_Γ is $\Omega(S_\Gamma)$, and we have:

$$\gamma_+(\Gamma) = -\frac{1}{2}\Omega(S_\Gamma).$$

A simple test case is that of a closed curve of constant $\theta = \theta_0$, with $\phi \in [0, 2\pi]$. The associated solid angle is $\Omega(\theta_0) = 2\pi(1 - \cos\theta_0)$. On the other hand, the integral gives $\gamma_+ = -\frac{1}{2}(2\pi)(1 - \cos\theta_0) = -\frac{1}{2}\Omega(\theta_0)$, providing evidence for the claim

- To verify, we compute for a tiny rectangular patch:

$$\oint_{d\Gamma} (1 - \cos\theta) d\phi = (1 - \cos(\theta + d\theta)) d\phi - (1 - \cos\theta) d\phi$$
$$= \sin\theta \, d\theta \, d\phi = dA = d\Omega.$$

- Integrating over the surface S_Γ, we confirm:

$$\int_\Gamma (1 - \cos\theta) d\phi = \Omega(S_\Gamma).$$