Quantum Adiabatic Theorem and Geometric Phases

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Why is it important?

1. It makes our lives easier!
    - Allows us to treat slow and fast degrees of freedom separately i.e., disentangle slow and fast degrees of freedom.
    - It helps us to neglect fast varying terms in the equation.
2. It is interesting!!
    - Gives raise to new physics - Berry phases.
    - Connected to lot of other interesting(fancy) topics such as topology.

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Classical system

Let us consider a classical case of harmonic oscillator to get a notion of adiabaticity. The Hamiltonian of such a system is given by

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

Question: How does the Hamiltonian vary with time? Take the time derivative! We have

$$\begin{aligned} \frac{dH}{dt} &= \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial t} &(2)\\ &= \frac{\partial H}{\partial t} = m\omega\dot{\omega}q^2 &(3)\end{aligned}$$

If ω changes slowly, the Hamiltonian changes slowly! Does this statement sound convincing or dramatic?

How slow is slow?

Can we come up with a more precise argument to imply an adiabatic change? **There is hope!!**
Time scale for change $\gg$ Time scale of the oscillation

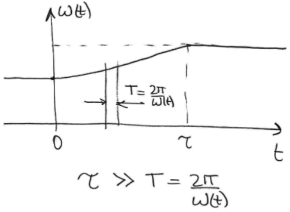

Figure: Adiabatic change[1]

More precise argument: **Change in $\omega(t)$ over a period is much smaller than $\omega(t)$.** Is there something which varies much slower than $\dot{\omega}/\omega^2$? In other words, its practically a constant. It is not trivial.

[1]Image credits: B.Zwiebach, Lecture notes, MIT OCW 8.06

Adiabatic Invariant

Claim

$I(t) \equiv \frac{H(t)}{\omega(t)}$ is almost constant in adiabatic change

Proof:

$$\frac{dI}{dt} = \frac{1}{\omega^2}\left(\omega\frac{dH}{dt} - H(t)\dot{\omega}\right) \tag{4}$$

$$= (\dot{\omega}/\omega^2)(PE(t) - KE(t)) \tag{5}$$

The first term is small whereas the second one is oscillatory. Let us investigate the change in $I(t)$ over a period.

$$I(t+T) - I(t) = \int_t^{t+T} \frac{\dot{\omega}}{\omega^2}(t')(PE(t') - KE(t'))dt' \tag{6}$$

$$\approx \frac{\dot{\omega}}{\omega^2}\int_t^{t+T}(PE(t') - KE(t'))dt' \approx 0 \tag{7}$$

Intuition to Quantum case

Can we guess what would be an Adiabatic invariant in Quantum case? Consider the quantum treatment of a harmonic oscillator. The eigenvalues of a single oscillator with frequency ω is given by,

Eigenvalues of a Quantum Harmonic Oscillator

$$E_n = \hbar\omega(n + 1/2) \tag{8}$$

Carrying the notion of adiabatic invariant, what do we expect?

$$\frac{E}{\omega} = n + 1/2 \tag{9}$$

The quantity E/ω is the quantum number of the oscillator. We thus note a key observation following the above semi-classical arguments:

Key Observation

The quantum numbers may not change under adiabatic changes.

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Quantum Adiabatic Theorem

Theorem (statement)

A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum.

Key terms

- instantaneous eigenstates
- perturbation
- slow
- gap

Assumptions

- perturbation acting on the system varies slowly
- energy gap should be present between eigenvalue and the rest of the Hamiltonian

Quantum Adiabatic Theorem

More precisely..

- Consider a set of instantaneous eigenstates:

$$H(t)\,|\psi_n(t)\rangle = E_n(t)\,|\psi_n(t)\rangle \tag{10}$$

  with $E_1(t) < E_2(t) < E_3(t) < ...$, so that there are no degeneracies.
- If at $t = 0$, $|\Psi(0)\rangle = |\psi_k(0)\rangle$, then if $H(t)$ is slowly varying for $0 \leq t \leq T$, then at time T we have $|\Psi(T)\rangle \approx |\psi_n(T)\rangle$ up to calculable phase.

Key facts

- perturbation acting on the system varies slowly
- energy gap should be present between eigenvalue and the rest of the Hamiltonian

Proof

We start off with (10) and taking an ansatz for the wave function at time 't' as

$$|\Psi(t)\rangle = \sum_n c_n(t) |\psi_n(t)\rangle \tag{11}$$

We turn to the TDSE and plug the ansatz:

$$i\hbar \sum_n \left(\dot{c}_n(t) |\psi_n(t)\rangle + c_n |\dot{\psi_n}(t)\rangle \right) = \sum_n c_n(t) E_n(t) |\psi_n(t)\rangle \tag{12}$$

project it onto $\langle \psi_k(t)|$

$$i\hbar \dot{c}_k = E_k c_k - i\hbar \sum_n \left\langle \psi_k \middle| \dot{\psi}_n \right\rangle c_n \tag{13}$$

$$i\hbar \dot{c}_k = \left(E_k c_k - i\hbar \left\langle \psi_k \middle| \dot{\psi}_k \right\rangle c_k \right) - i\hbar \sum_{n \neq k} \left\langle \psi_k \middle| \dot{\psi}_n \right\rangle c_n \tag{14}$$

Proof(Continued)

We will express $\left\langle \psi_k \middle| \dot{\psi}_n \right\rangle$ in terms of Hamiltonian matrix elements. Take a time derivative in (10). We get

$$\dot{H}(t) \left| \psi_n \right\rangle + H(t) \left| \dot{\psi}_n \right\rangle = \dot{E}_n(t) \left| \psi_n \right\rangle + E_n(t) \left| \dot{\psi}_n \right\rangle \tag{15}$$

project it onto $\langle \psi_k(t)|$ with $k \neq n$

$$\langle \psi_k(t)| \dot{H}(t) \left| \psi_n \right\rangle + E_k(t) \left\langle \psi_k(t) \middle| \dot{\psi}_n \right\rangle = E_n(t) \left\langle \psi_k(t) \middle| \dot{\psi}_n \right\rangle \tag{16}$$

$$\implies \left\langle \psi_k \middle| \dot{\psi}_n \right\rangle = \frac{\langle \psi_k(t)| \dot{H}(t) \left| \psi_n \right\rangle}{E_n(t) - E_k(t)} \equiv \frac{(\dot{H})_{nk}}{E_n - E_k} \tag{17}$$

Plugging back in (13)

$$i\hbar \dot{c}_k = \left(E_k - i\hbar \left\langle \psi_k \middle| \dot{\psi}_k \right\rangle c_k \right) - i\hbar \sum_{n \neq k} \frac{(\dot{H})_{nk}}{E_n - E_k} c_n \tag{18}$$

Proof(Continued)

If we ignore the second term and integrate

$$c_k(t) = c_k(0)e^{i\theta_k(t)}e^{i\gamma_k(t)} \tag{19}$$

where

Dynamical phase

$$\theta_k(t) = -\frac{1}{\hbar}\int_0^t E_k(t')dt' \tag{20}$$

Geometric phase

$$\gamma_k(t) = \int_0^t i\left\langle \psi_k(t') \middle| \dot{\psi}_k(t') \right\rangle dt' \tag{21}$$

- Example: Born-Oppenheimer approximation

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Berry Phase

Let us begin with our old friend Hamiltonian and assume it depends on a set of coordinates $\mathbf{R}(t) = (R_1(t), R_2(t), ..., R_N(t))$. Also, assume some of them are tunable.

Simple yet important idea

Suppose we solve the TISE for all possible set of parameters given above. Essentially, we have solved the instantaneous eigenvalue equation at all times.

Instantaneous states are given by:

$$H(\mathbf{R}) |\psi_n(\mathbf{R})\rangle = E_n(\mathbf{R}) |\psi_n(\mathbf{R})\rangle \tag{22}$$

Let us evaluate the geometric phase. We start by defining

$$\nu_n(t) \equiv i \langle\psi_n(\mathbf{R})| \frac{d}{dt} |\psi_n(\mathbf{R})\rangle \tag{23}$$

We require the term $\frac{d}{dt} |\psi_n(\mathbf{R})\rangle$

Berry phase

$$\frac{d}{dt}|\psi_n(\mathbf{R}(t))\rangle = \sum_{i=1}^{N}\frac{d}{dR_i}|\psi_n(\mathbf{R}(t))\rangle\frac{dR_i}{dt} = \nabla_{\mathbf{R}}|\psi_n(\mathbf{R}(t))\rangle\cdot\frac{d\mathbf{R}(t)}{dt} \quad (24)$$

$$\nu_n(t) = i\langle\psi_n(\mathbf{R}(t))|\nabla_{\mathbf{R}}|\psi_n(\mathbf{R}(t))\rangle\cdot\frac{d\mathbf{R}(t)}{dt} \quad (25)$$

and

$$\gamma_n(\tau) = \int_0^{\tau}\nu_n(t)dt = \int_0^{\tau} i\langle\psi_n(\mathbf{R}(t))|\nabla_{\mathbf{R}}|\psi_n(\mathbf{R}(t))\rangle\cdot\frac{d\mathbf{R}(t)}{dt}dt \quad (26)$$

Berry phase

$$\gamma_n(t_f) = \int_{\mathbf{R}_i}^{\mathbf{R}_f} i\langle\psi_n(\mathbf{R})|\nabla_{\mathbf{R}}|\psi_n(\mathbf{R})\rangle\cdot d\mathbf{R} \quad (27)$$

Properties of the Berry phase

Berry connection

$$\mathbf{A}_n(\mathbf{R}) = i \langle \psi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \psi_n(\mathbf{R}) \rangle \tag{28}$$

We can rewrite the Berry phase

Berry phase

$$\gamma_n(t_f) = \int_{\mathbf{R}_i}^{\mathbf{R}_f} \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R} \tag{29}$$

If we redefine the instantaneous eigenstates by an overall phase

$$|\psi_n(\mathbf{R})\rangle \rightarrow \left|\tilde{\psi}_n(\mathbf{R})\right\rangle = e^{-i\beta(\mathbf{R})} |\psi_n(\mathbf{R})\rangle \tag{30}$$

where $\beta(\mathbf{R})$ is an arbitrary real function, what happens to $\mathbf{A}_n(\mathbf{R})$?

Properties of Berry phase

$$\tilde{\mathbf{A}}_n(\mathbf{R}) = i \left\langle \tilde{\psi}_n(\mathbf{R}) \middle| \nabla_{\mathbf{R}} \middle| \tilde{\psi}_n(\mathbf{R}) \right\rangle \tag{31}$$

$$= i \left\langle \psi_n(\mathbf{R}) \right| e^{i\beta(\mathbf{R})} \nabla_{\mathbf{R}} e^{-i\beta(\mathbf{R})} \left| \psi_n(\mathbf{R}) \right\rangle \tag{32}$$

$$= i(-i\nabla_{\mathbf{R}}\beta(\mathbf{R})) + \mathbf{A}_n(\mathbf{R}) \tag{33}$$

$$\tilde{\mathbf{A}}_n(\mathbf{R}) = \mathbf{A}_n(\mathbf{R}) + \nabla_{\mathbf{R}}\beta(\mathbf{R}) \tag{34}$$

What about the Berry Phase?

$$\tilde{\gamma}_n(t_f) = \int_{\mathbf{R}_i}^{\mathbf{R}_f} \tilde{\mathbf{A}}_n(\mathbf{R}) \cdot d\mathbf{R} = \gamma_n(t_f) + \int_{\mathbf{R}_i}^{\mathbf{R}_f} \nabla_{\mathbf{R}}\beta(\mathbf{R}) \cdot d\mathbf{R} \tag{35}$$

$$= \gamma_n(t_f) + \beta(\mathbf{R}_f) - \beta(\mathbf{R}_i) \tag{36}$$

Properties of Berry phase

- Berry Phase is Gauge invariant for closed path in configuration/parameter space.
- If the $\psi_n(t)$ are real, then the Berry phase vanishes.
- If the configuration space is one dimensional, Berry phase vanishes.

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