In these notes, we summarize the derivation of adiabatic approximation and Berry's phase.

1. **Instantaneous eigenkets v.s. solutions to time-dependent Schrödinger's equation**

   Our goal is to obtain the solution to the time-dependent SE

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

   which is usually hard to obtain. But at every moment t, the Hilbert space can be thought of as spanned by the complete basis of *instantaneous* energy eigenstates satisfying

$$H(t)|n(t)\rangle=E_n(t)|n(t)\rangle \tag{2}$$

   Since $|n(t)\rangle$ is complete, we can write the solution $|\psi(t)\rangle$ as a linear combination of $|n(t)\rangle$'s. Instead of writing

$$|\psi(t)\rangle=\sum_n c_n(t)|n(t)\rangle$$

   we decorate $|n(t)\rangle$ with a to-be-determined phase factor $e^{i\beta_n(t)}$

$$|\psi(t)\rangle=\sum_n c_n(t)e^{i\beta_n(t)}|n(t)\rangle \tag{3}$$

   We hope by cleverly choosing $\beta_n(t)$, we have a simpler differential equation for $c_n(t)$.
   Taking the time derivative of (3), we have

$$\frac{\partial|\psi(t)\rangle}{\partial t}=\sum_n\left[\dot{c_n}(t)e^{i\beta_n(t)}|n(t)\rangle+c_n(t)\cdot i\beta_n'(t)\cdot e^{i\beta_n(t)}|n(t)\rangle+c_n(t)e^{i\beta_n(t)}\frac{\partial|n(t)\rangle}{\partial t}\right] \tag{4}$$

   On the other hand, from (1), we have

$$\frac{\partial|\psi(t)\rangle}{\partial t}=\frac{1}{i\hbar}H(t)\sum_n c_n(t)e^{i\beta_n(t)}|n(t)\rangle=\frac{1}{i\hbar}\sum_n c_n(t)e^{i\beta_n(t)}E_n(t)|n(t)\rangle \tag{5}$$

   Compare (4) and (5), we can see that if we make

$$i\beta_n'(t)=\frac{1}{i\hbar}E_n(t) \qquad \text{or} \qquad \beta_n(t)=\exp\left[-\frac{1}{\hbar}\int_{t_0}^t E_n(t')dt'\right] \tag{6}$$

   a particularly simple differential equation for $c_n(t)$ will emerge

$$\sum_n e^{i\beta_n(t)}\left[\dot{c_n}(t)|n(t)\rangle+c_n(t)\frac{\partial|n(t)\rangle}{\partial t}\right]=0 \tag{7}$$

   Once $c_n(t)$ is solved in (7), we can go back to (3) and have the solution to the SE as

$$|\psi(t)\rangle=\sum_n c_n(t)\exp\left[-\frac{i}{\hbar}\int_{t_0}^t E_n(t')dt'\right]|n(t)\rangle \tag{8}$$

2. **Solving for the expansion coefficients** $c_n(t)$

   Left-apply $\langle m(t)|$ to (7), we have

$$e^{i\beta_m(t)}\dot{c_m}(t)+\sum_n e^{i\beta_n(t)}c_n(t)\left\langle m(t)\left|\frac{\partial}{\partial t}\right|n(t)\right\rangle=0 \qquad \Longrightarrow$$
$$\dot{c_m}(t)=-c_m(t)\left\langle m(t)\left|\frac{\partial}{\partial t}\right|m(t)\right\rangle-\sum_{n\neq m}e^{i[\beta_n(t)-\beta_m(t)]}c_n(t)\left\langle m(t)\left|\frac{\partial}{\partial t}\right|n(t)\right\rangle \tag{9}$$

Now to see the sum in (9), let's take the time derivative of (2) followed by left applying $\langle m(t)|$ for all $n \neq m$:

$$\dot{H}(t)|n(t)\rangle + H(t)\frac{\partial |n(t)\rangle}{\partial t} = \dot{E_n}(t)|n(t)\rangle + E_n(t)\frac{\partial |n(t)\rangle}{\partial t} \qquad \Longrightarrow \tag{10}$$

$$\langle m(t)|\dot{H}(t)|n(t)\rangle = [E_n(t) - E_m(t)] \left\langle m(t) \middle| \frac{\partial}{\partial t} \middle| n(t) \right\rangle \tag{11}$$

Then (9) becomes

$$\dot{c_m}(t) = -c_m(t) \left\langle m(t) \middle| \frac{\partial}{\partial t} \middle| m(t) \right\rangle - \sum_{n\neq m} c_n(t) e^{i[\beta_n(t)-\beta_m(t)]} \frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{E_n(t) - E_m(t)} \tag{12}$$

which is the *coupled* differential equation, since the time derivative of the m-th eigenstate coefficient $\dot{c_m}(t)$ will depend on other $c_n(t)$'s.

3. **Adiabatic approximation and the γ phase**

   (12) is an exact equation without any approximation. Now the adiabatic condition says if the rate of change of the Hamiltonian $\dot{H}(t)$ is slow in the sense that the second term in (12) is much smaller than the first term, we can solve for the approximate equation

$$\dot{c_m}(t) = -c_m(t) \left\langle m(t) \middle| \frac{\partial}{\partial t} \middle| m(t) \right\rangle \tag{13}$$

   which gives the solution

$$c_m(t) = e^{i\gamma_m(t)} \qquad \text{where} \qquad \gamma_m(t) = i \int_{t_0}^{t} \left\langle m(t') \middle| \frac{\partial}{\partial t'} \middle| m(t') \right\rangle dt' \tag{14}$$

   A few points are worth noting

   - $\gamma_m(t)$ is real, since

$$\langle m(t)|m(t)\rangle = 1 \qquad \Longrightarrow \qquad \frac{\partial}{\partial t}\langle m(t)|m(t)\rangle = 0$$

     which, by the chain rule, indicates that the integrand in (14) plus its own complex conjugate is zero, which means it's purely imaginary, hence $\gamma_m(t)$ real.
   - Under adiabatic approximation, if the initial state is $|n(t_0)\rangle$, then (13) ensures that the solution of the time-dependent SE will remain on the $|n(t)\rangle$ trajectory, i.e.,

$$|\psi(t)\rangle = c_n(t)e^{i\beta_n(t)}|n(t)\rangle = e^{i\gamma_n(t)}e^{i\beta_n(t)}|n(t)\rangle \tag{15}$$

     In other words, the system's state will follow the instantaneous energy eigenstate all the time.
   - When there is actually no time dependency, $\gamma_n(t)$ vanishes by (14), and $\beta_n(t)$ becomes $e^{-iE_n(t-t_0)/\hbar}$, and (15) goes back to the time evolution of the stationary state.

4. **Geometric phase, a.k.a., Berry's phase**

   We consider the case where H is parameterized by a vector $\boldsymbol{R}$ of parameters. With each instance of $\boldsymbol{R}$, we assume the energy eigenstates are known, i.e.,

$$H(\boldsymbol{R})|n(\boldsymbol{R})\rangle = E_n(\boldsymbol{R})|n(\boldsymbol{R})\rangle \tag{16}$$

   Also assume that the time-dependent $H(t)$ is realized by making $\boldsymbol{R}$ trace out a trajectory $\boldsymbol{R}(t)$ in the configuration space. More verbosely, the i-th component R_i of $\boldsymbol{R}$ changes according to a function $R_i(t)$, and so on.

   Now the $\gamma_m(t)$ phase in (14) becomes

$$\begin{aligned}\gamma_m(t) &= i \int_{t_0}^{t} \left\langle m(\boldsymbol{R}(t')) \middle| \frac{d}{dt'} \middle| m(\boldsymbol{R}(t')) \right\rangle dt' \\ &= i \int_{t_0}^{t} \left\langle m(\boldsymbol{R}(t')) \middle| \boldsymbol{\nabla}_{\boldsymbol{R}} \middle| m(\boldsymbol{R}(t')) \right\rangle \cdot \frac{d\boldsymbol{R}}{dt'} dt' \end{aligned} \tag{17}$$

where the dot product in the integral is just a compact way of expressing the chain rule

$$\left\langle m(\boldsymbol{R}(t'))\left|\frac{d}{dt'}\right|m(\boldsymbol{R}(t'))\right\rangle=\sum_i\left\langle m(\boldsymbol{R}(t'))\left|\frac{\partial}{\partial R_i}\right|m(\boldsymbol{R}(t'))\right\rangle\frac{dR_i(t)}{dt}$$

If we define the Berry's connection (or, Berry's potential)

$$\boldsymbol{A}_m(\boldsymbol{R})\equiv i\,\langle m(\boldsymbol{R})|\boldsymbol{\nabla_R}|\,m(\boldsymbol{R})\rangle \tag{18}$$

which is a real vector of $\boldsymbol{R}$'s dimension, then (17) can be written as

$$\gamma_m(\Gamma)=\int_\Gamma \boldsymbol{A}_m(\boldsymbol{R'})\cdot d\boldsymbol{R'} \tag{19}$$

which is a path integral along the trajectory $\Gamma:\boldsymbol{R}(t_0)\to\boldsymbol{R}(t)$. In particular, when going from (17) to (19), the differential time dt' drops out, and (19) is a quantity only dependent on the geometry of path Γ in the configuration space.

Recall that the energy eigenstate $|m(\boldsymbol{R})\rangle$ can have a freedom to multiply any phase factor $e^{i\delta(\boldsymbol{R})}$. Then under this transform

$$|m(\boldsymbol{R})\rangle\to e^{i\delta(\boldsymbol{R})}|m(\boldsymbol{R})\rangle \tag{20}$$

the Berry's connection $\boldsymbol{A}_m(\boldsymbol{R})$ will undergo a transform

$$\begin{aligned}\boldsymbol{A}_m(\boldsymbol{R})&=i\,\langle m(\boldsymbol{R})|\boldsymbol{\nabla_R}|\,m(\boldsymbol{R})\rangle\\&\to\\ i\left[\left\langle m(\boldsymbol{R})\right|e^{-i\delta(\boldsymbol{R})}\right]\boldsymbol{\nabla_R}\left[e^{i\delta(\boldsymbol{R})}\left|m(\boldsymbol{R})\right\rangle\right]&=\boldsymbol{A}_m(\boldsymbol{R})-\boldsymbol{\nabla_R}\delta(\boldsymbol{R})\end{aligned} \tag{21}$$

which will in general produce a different $\gamma_m(\boldsymbol{R})$ for a given path Γ according to (19), except for the case where Γ represents a loop in the configuration space (which means a periodic change of configurations).

(20) reminds us of the gauge transformation of vector magnetic potential.

In summary, for a closed loop C in the configuration space,

$$\gamma_m(C)=\oint_C \boldsymbol{A}_m(\boldsymbol{R})\cdot d\boldsymbol{R} \tag{22}$$

is completely independent of the pace to travel the loop, neither does it depend on the arbitrary phase of the state $|m(\boldsymbol{R})\rangle$.

5. **Three dimensional configuration space**

If $\boldsymbol{R}$ is 3-dimensional, by Stoke's theorem, (22) is equal to

$$\gamma_m(C)=\oint_C \boldsymbol{A}_m(\boldsymbol{R})\cdot d\boldsymbol{R}=\int_S\overbrace{[\boldsymbol{\nabla_R}\times\boldsymbol{A}_m(\boldsymbol{R})]}^{\equiv\boldsymbol{B}_m(\boldsymbol{R})}\cdot d\boldsymbol{a} \tag{23}$$

then we can calculate $\boldsymbol{B}_m(\boldsymbol{R})$ by (18)

$$\boldsymbol{B}_m(\boldsymbol{R})=i\boldsymbol{\nabla_R}\times\langle m(\boldsymbol{R})|\boldsymbol{\nabla_R}|\,m(\boldsymbol{R})\rangle \tag{24}$$

Note we can apply the formula

$$\boldsymbol{\nabla}\times(\phi\boldsymbol{a})=\boldsymbol{\nabla}\phi\times\boldsymbol{a}+\phi\boldsymbol{\nabla}\times\boldsymbol{a}$$

to (24) and notice the fact that curl of a gradient will vanish, then we obtain

$$\begin{aligned}\boldsymbol{B}_m(\boldsymbol{R})&=i\,[\boldsymbol{\nabla_R}\langle m(\boldsymbol{R})|]\times[\boldsymbol{\nabla_R}|m(\boldsymbol{R})\rangle]\\&=i\sum_{n\neq m}[\boldsymbol{\nabla_R}\langle m(\boldsymbol{R})|]\,|n(\boldsymbol{R})\rangle\times\langle n(\boldsymbol{R})|\,[\boldsymbol{\nabla_R}|m(\boldsymbol{R})\rangle]\end{aligned} \tag{25}$$

where the $n=m$ case drops out because $(\boldsymbol{\nabla}\langle m|)|m\rangle=-|m\rangle(\boldsymbol{\nabla}|m\rangle)$, hence their cross product vanishes.

Now from (2), we have

$$\begin{aligned}\boldsymbol{\nabla_R}[H(\boldsymbol{R})|m(\boldsymbol{R})\rangle]&=\boldsymbol{\nabla_R}[E_m(\boldsymbol{R})|m(\boldsymbol{R})\rangle] &&\Longrightarrow\\ [\boldsymbol{\nabla_R}H]\,|m(\boldsymbol{R})\rangle+H\,[\boldsymbol{\nabla_R}|m(\boldsymbol{R})\rangle]&=[\boldsymbol{\nabla_R}E_m]\,|m(\boldsymbol{R})\rangle+E_m\,[\boldsymbol{\nabla_R}|m(\boldsymbol{R})\rangle] &&\Longrightarrow\\ \langle n(\boldsymbol{R})|\,[\boldsymbol{\nabla_R}H]\,|m(\boldsymbol{R})\rangle&=(E_m-E_n)\langle n(\boldsymbol{R})|\,[\boldsymbol{\nabla_R}|m(\boldsymbol{R})\rangle]\end{aligned} \tag{26}$$

Finally with this, (25) becomes

$$\boldsymbol{B}_m(\boldsymbol{R})=i\sum_{n\neq m}\frac{\langle m(\boldsymbol{R})|\,[\boldsymbol{\nabla_R}H]\,|n(\boldsymbol{R})\rangle\times\langle n(\boldsymbol{R})|\,[\boldsymbol{\nabla_R}H]\,|m(\boldsymbol{R})\rangle}{(E_m-E_n)^2} \tag{27}$$