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

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

   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 $\mathbf{R}$ of parameters. With each instance of $\mathbf{R}$, we assume the energy eigenstates are known, i.e.,

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

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

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

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

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

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

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

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

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

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

which is a path integral along the trajectory $\Gamma : \mathbf{R}(t_0) \to \mathbf{R}(t)$. 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 $|m(\mathbf{R})\rangle$ can have a freedom to multiply any phase factor $e^{i\delta(\mathbf{R})}$. Then under this transform

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

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

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

which will in general produce a different $\gamma_m(\mathbf{R})$ 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,

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

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

5. **Three dimensional configuration space**

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

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

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

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

Note we can apply the formula

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

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

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

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

Now from (2), we have

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

Finally with this, (25) becomes

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