Quantum Mechanics

Perturbation Theory

Time-Independent Perturbation

- A Toy Model of Qubit
- General Ideas of Perturbation Theory

Perturbation theory: a set of approximation schemes that allows us to extend our knowledge about an exactly solvable quantum system to its vicinity (in the parameter space).

Why do we need perturbation theory?
- Exact solutions are rare. ⇒ We have to rely on perturbation theory to go beyond them and make the most of these exact solutions.
- Separation of scales: physics often takes place at different energy scales, e.g. ... → quarks (GeV) → nucleus (MeV) → atoms (eV) → molecules (100meV) → ... ⇒ We can refine our descriptions by adding perturbative corrections progressively.

What are the central problems in perturbation theory?
- Time-independent perturbation: given the spectrum (eigenstates and eigenenergies) of $H_0$, find the spectrum of $H = H_0 + \lambda V$, in power series of $\lambda$ (given that $\lambda$ is small).
- Time-dependent perturbation: given the (bare) propagator $U_0(t) = e^{-iH_0 t}$, find the propagator

$$U(t) = \mathcal{T} \exp \left( -i \int_0^t dt' H(t') \right),$$

$$H(t) = H_0 + \lambda V(t),$$

in power series of $\lambda$ (given that $\lambda$ is small). [We will explain the notations in Eq. (1) later.]

How is perturbation theory useful?
- Conceptually: to establish effective Hamiltonians, to analyze renormalization group flows ...
- Practically: to calculate scattering amplitudes, response functions, spectral weights ...

Qubit Model and its Exact Solution

Let us start with a toy model of a single qubit. Consider

$$H(\lambda) = H_0 + \lambda V,$$
where \( H_0 = \sigma^z \) and \( V = \sigma^x \), s.t. \( H(\lambda) \) can be more explicitly written as
\[
H(\lambda) = \sigma^z + \lambda \sigma^x
\]
\[
\approx \left( \begin{array}{cc} 1 \quad \lambda \\ \lambda \quad -1 \end{array} \right).
\]

What are the eigenenergies and eigenstates of \( H(\lambda) \)?
\[
H(\lambda) |\psi_\pm(\lambda)\rangle = E_\pm(\lambda) |\psi_\pm(\lambda)\rangle.
\]

- **Eigenenergies**
  \[
  E_\pm(\lambda) = \pm \sqrt{1 + \lambda^2}.
  \]

- **Eigenstates**
  \[
  |\psi_+(\lambda)\rangle = \frac{\left(1 + \sqrt{1 + \lambda^2}\right) |\uparrow\rangle + \lambda |\downarrow\rangle}{\sqrt{2 \left(1 + \lambda^2 + \sqrt{1 + \lambda^2}\right)}}.
  \]
  \[
  |\psi_-(\lambda)\rangle = \frac{\left(1 + \sqrt{1 + \lambda^2}\right) |\downarrow\rangle - \lambda |\uparrow\rangle}{\sqrt{2 \left(1 + \lambda^2 + \sqrt{1 + \lambda^2}\right)}}.
  \]

### Taylor Expansion

Assuming \( \lambda \) is small (i.e. \( \lambda \ll 1 \)), Eq. (5) and Eq. (6) can be expanded in power series of \( \lambda \).

- As a reminder, the **Taylor expansion** of a function \( f(\lambda) \) is given by
  \[
  f(\lambda) = \sum_{k=0}^{\infty} \frac{\partial f}{\partial \lambda^k} \frac{(\lambda - 0)^k}{k!} = f(0) + f'(0) \lambda + \frac{f''(0)}{2} \lambda^2 + \frac{f'''(0)}{6} \lambda^3 + ... .
  \]

- Applying Eq. (7) to Eq. (5) and Eq. (6), we get
  \[
  E_\pm = \pm \left( 1 + \frac{\lambda^2}{2} - \frac{\lambda^4}{8} + ... \right),
  \]
  \[
  |\psi_+(\lambda)\rangle = |\uparrow\rangle + \frac{\lambda}{2} |\downarrow\rangle - \frac{\lambda^2}{8} |\uparrow\rangle - \frac{3 \lambda^3}{16} |\downarrow\rangle + \frac{11 \lambda^4}{128} |\uparrow\rangle + ...,
  \]
  \[
  |\psi_-(\lambda)\rangle = |\downarrow\rangle - \frac{\lambda}{2} |\uparrow\rangle - \frac{\lambda^2}{8} |\downarrow\rangle + \frac{3 \lambda^3}{16} |\uparrow\rangle + \frac{11 \lambda^4}{128} |\downarrow\rangle + ... .
  \]

**Goal**: obtain these power series *without* first calculating the exact solution! - This is possible as long as we know how to evaluate the **derivatives** \( \partial f/\partial \lambda |E(0)\rangle \) and \( \partial f/\partial \lambda |\psi_\pm(0)\rangle \).

The **perturbation theory** is essentially an **iterative algorithm** to calculate these derivatives...
order by order, based on our knowledge about $H_0$ and $V$.

- **Non-Degenerate Perturbation Theory**

- **Problem Setup**

  The starting point is the following Hamiltonian (*linearly* parameterized by $\lambda$)

  $$H(\lambda) = H_0 + \lambda \ V.$$  \hspace{1cm} (10)

- This implies
  
  $$H(0) = H_0,$$
  $$\partial_\lambda H(0) = V,$$
  $$\partial_\lambda^2 H(0) = \partial_\lambda^3 H(0) = \ldots = 0.$$  \hspace{1cm} (11)

- To simplify the notation, we will suppress the argument $\lambda$ if it is evaluated at $\lambda = 0$.
  
  $$H = H_0,$$
  $$\partial_\lambda H = V,$$
  $$\partial_\lambda^2 H = \partial_\lambda^3 H = \ldots = 0.$$  \hspace{1cm} (12)

Rule: Everything is treated as a function of $\lambda$, like $f(\lambda)$. But if the dependence on $\lambda$ is not explicitly spelt out, we assume it to be the function evaluated at $\lambda = 0$, i.e. $f \equiv f |_{\lambda=0} = f(0)$.

Consider the **eigen equation**

$$H(\lambda) |n(\lambda)\rangle = E_n(\lambda) |n(\lambda)\rangle.$$  \hspace{1cm} (13)

For each given $\lambda$, there is a different $H(\lambda)$, and hence a different set of $E_n(\lambda)$ and $|n(\lambda)\rangle$, labeled by $n = 1, 2, 3, \ldots$.

- $E_n(\lambda)$ is the $n$th energy level. It is a real number depending on $\lambda$.

- $|n(\lambda)\rangle$ is the $n$th eigenstate (in correspondence to $E_n(\lambda)$). It is a state vector in the Hilbert space that can change with $\lambda$. Note: The notation $|n(\lambda)\rangle$ does *not* imply that the index $n$ is $\lambda$ dependent, it should be understood as

  $$|n(\lambda)\rangle = \sum_m \psi_{nm}(\lambda) |m\rangle.$$  \hspace{1cm} (14)

We assume a *discrete spectrum* without degeneracy, such that the “$n$th” level/state is uniquely defined. [The case with degeneracy will be discussed latter.]

**Statement of the problem**: suppose we know the eigenenergies and eigenstates *at and only at* $\lambda = 0$,

$$H |n\rangle = E_n |n\rangle,$$  \hspace{1cm} (15)

and we also know what the perturbation is: $V = \partial_\lambda H$,
\[ V_{mn} = \langle m | V | n \rangle = \langle m | \partial_\lambda H | n \rangle, \]  

(16)
calculate \( E_\lambda(\lambda) \) and \(|n(\lambda)\rangle\) in power series of \( \lambda \) (to any desired order) in terms of \( E_n, V_{mn} \) and \(|n\rangle\).

- **Hellmann-Feynman Theorems**

  - Applying \( \partial_\lambda \) to both sides of \( H |n\rangle = E_n |n\rangle \),
    \[ \partial_\lambda H |n\rangle + H |\partial_\lambda n\rangle = \partial_\lambda E_n |n\rangle + E_n |\partial_\lambda n\rangle. \]  
    (17)
    
  - Note: \(|\partial_\lambda n\rangle\) stands for the derivative of the state \(|n\rangle\) (not the index \( n \))
    \[ |\partial_\lambda n\rangle = \left( \sum_m \partial_\lambda \psi_{nm}(\lambda) |m\rangle \right)_{\lambda=0}. \]  
    (18)
    It does *not* imply that the integer index \( n \) can be differentiated.

  - Overlap with \( \langle m | \) from the left,
    \[ \langle m | \partial_\lambda H |n\rangle + \langle m | H |\partial_\lambda n\rangle = \partial_\lambda E_n \langle m | n \rangle + E_n \langle m | \partial_\lambda n\rangle. \]  
    (19)
    Using \( \langle m | H = \langle m | E_m \),
    \[ \langle m | \partial_\lambda H |n\rangle + E_m \langle m | \partial_\lambda n\rangle = \partial_\lambda E_n \langle m | n \rangle + E_n \langle m | \partial_\lambda n\rangle \]
    \[ \Rightarrow \langle m | \partial_\lambda H |n\rangle = \partial_\lambda E_n \langle m | n \rangle + (E_n - E_m) \langle m | \partial_\lambda n\rangle. \]  
    (20)

  - Note that \( \partial_\lambda H = V \) and \( \langle m | n \rangle = \delta_{mn} \).
    \[ V_{mn} = \langle m | V | n \rangle = \partial_\lambda E_n \delta_{mn} + (E_n - E_m) \langle m | \partial_\lambda n\rangle. \]  
    (21)

This establishes a relation between the matrix element \( V_{mn} \) (of the perturbation) and the derivatives \( \partial_\lambda E_n \) and \(|\partial_\lambda n\rangle\).

  - When \( m = n \), Eq. (21) implies
    \[ \partial_\lambda E_n = V_{nn}. \]  
    (22)

This is the **first Hellmann-Feynman** theorem.

  - When \( m \neq n \), Eq. (21) implies
    \[ \langle m | \partial_\lambda n\rangle = \frac{V_{mn}}{E_n - E_m}, \]
    \[ \langle \partial_\lambda m | n\rangle = \frac{V_{mn}}{E_m - E_n}. \]  
    (23)

This is the **second Hellmann-Feynman** theorem. Tip: the *energy denominator* is always given by the energy of the state that is being *differentiated* minus the energy of the other state.

The **Hellmann-Feynman theorems** tell us how the derivative of the energy \( \partial_\lambda E_n \) or the state \(|\partial_\lambda n\rangle\) and \( \langle \partial_\lambda m | \) on the left-hand-side is related to something on the right-hand-side which
does not contain $\partial_\lambda$. ⇒ This effectively reduces the order of $\partial_\lambda$ by one. ⇒ Applying them iteratively, we will be able to calculate the derivatives to any order for both energies and states, which are all we need to construct the power series of the perturbative expansion.

- **Energy Corrections**

According to the Taylor expansion,

$$E_n(\lambda) = \sum_{k=0}^{\infty} \frac{\partial^k E_n}{k!} \lambda^k = E_n + \partial_\lambda E_n \lambda + \frac{1}{2} \partial^2_\lambda E_n \lambda^2 + \ldots$$

(24)

- We already know from Eq. (22) that

$$\partial_\lambda E_n = V_{nn} = \langle n | \partial_\lambda H | n \rangle.$$  

(25)

- We continue to evaluate

$$\partial^2_\lambda E_n = \partial_\lambda \langle n | \partial_\lambda H | n \rangle$$

$$= \langle \partial_\lambda n | \partial_\lambda H | n \rangle + \langle n | \partial_\lambda^2 H | n \rangle + \langle n | \partial_\lambda H | \partial_\lambda n \rangle.$$  

(26)

Note that $\partial^2_\lambda H = 0$ according to the setup in Eq. (12).

$$\partial^2_\lambda E_n = \sum_m \left( \langle \partial_\lambda n | m \rangle \langle m | \partial_\lambda H | n \rangle + \langle n | \partial_\lambda H | m \rangle \langle m | \partial_\lambda n \rangle \right)$$

$$= \sum_m \left( \frac{V_{nm}}{E_n - E_m} V_{mn} + \frac{V_{nm}}{E_n - E_m} \right)$$

$$= 2 \sum_m \frac{V_{nm} V_{mn}}{E_n - E_m}.$$  

(27)

But, wait a moment ... The energy denominator diverges when $m = n$, what is wrong? - Note that Eq. (23) only holds for $m \neq n$, so we must be careful. Let us restart from the 2nd line of Eq. (27),

$$\partial^2_\lambda E_n = \sum_m \left( \langle \partial_\lambda n | m \rangle \langle m | \partial_\lambda H | n \rangle + \langle n | \partial_\lambda H | m \rangle \langle m | \partial_\lambda n \rangle \right)$$

$$= \sum_{m \neq n} \left( \langle \partial_\lambda n | m \rangle \langle m | \partial_\lambda H | n \rangle + \langle n | \partial_\lambda H | m \rangle \langle m | \partial_\lambda n \rangle \right) +$$

$$+ \langle \partial_\lambda n | n \rangle \langle n | \partial_\lambda H | n \rangle + \langle n | \partial_\lambda H | n \rangle \langle n | \partial_\lambda n \rangle$$

$$= 2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n - E_m} + V_{nn} \langle n | \partial_\lambda H | n \rangle + \langle n | \partial_\lambda H | n \rangle$$

$$= 2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n - E_m} + V_{nn} \partial_\lambda \langle n | n \rangle.$$  

(28)

Given that $\langle n | n \rangle = 1$, taking $\partial_\lambda$ on both sides, $\partial_\lambda \langle n | n \rangle = \partial_\lambda 1 = 0$. So

$$\partial^2_\lambda E_n = 2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n - E_m}.$$  

(29)
So to the 2nd order in \( \lambda \), the perturbative correction to the energy is given by

\[
E_n(\lambda) = E_n + V_{nn}\lambda + \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n - E_m} \lambda^2 + \ldots
\]  
(30)

- **Comment on Gauge Fixing**

In fact, \( \langle n \mid \partial_\lambda n \rangle \) is the *connection* of the vector bundle which can always be set to zero by *gauge fixing* along the path of \( \lambda \). To see this, we start with

\[
\langle n \mid n \rangle = 1
\]
\[
\Rightarrow \langle \partial_\lambda n \mid n \rangle + \langle n \mid \partial_\lambda n \rangle = \partial_\lambda \langle n \mid n \rangle = \partial_\lambda 1 = 0
\]
\[
\Rightarrow \Re \langle n \mid \partial_\lambda n \rangle = 0.
\]

So \( \langle n \mid \partial_\lambda n \rangle \) can only be purely imaginary. But we are free to perform the gauge transformation

\[
|n(\lambda)) \rightarrow e^{i \phi(\lambda)} |n(\lambda)),
\]

under which,

\[
\langle n \mid \partial_\lambda n \rangle \rightarrow \langle n \mid \partial_\lambda n \rangle + i \partial_\lambda \phi.
\]

We can always choose \( \partial_\lambda \phi \) to transform \( \langle n \mid \partial_\lambda n \rangle \) to zero. So in addition to Eq. (23), we can further require

\[
\langle n \mid \partial_\lambda n \rangle = \langle \partial_\lambda n \mid n \rangle = 0.
\]

- **State Corrections**

According to the Taylor expansion,

\[
|n(\lambda)) = \sum_{k=0}^{\infty} \frac{\partial^k n}{k!} \lambda^k = |n) + |\partial_\lambda n) \lambda + \frac{1}{2} |\partial^2_\lambda n) \lambda^2 + \ldots
\]

(35)

By Eq. (23), we know

\[
|\partial_\lambda n) = \sum_{m \neq n} |m \rangle \langle m \mid \partial_\lambda n \rangle = \sum_{m \neq n} |m \rangle \frac{V_{mn}}{E_n - E_m}.
\]

(36)

Let us continue to calculate the next order derivative [Please bear with me ...]

\[
|\partial^2_\lambda n) = \partial_\lambda \sum_{m \neq n} |m \rangle \langle m \mid \partial_\lambda H |n\rangle \frac{E_n - E_m}{E_n - E_m} = \sum_{m \neq n} \left( \partial_\lambda m \right) \frac{\langle m \mid \partial_\lambda H |n\rangle}{E_n - E_m} + \sum_{m \neq n} |m \rangle \langle m \mid \partial_\lambda H |n\rangle \frac{E_n - E_m}{E_n - E_m} + \sum_{m \neq n} \left( \partial_\lambda m \right) \frac{\langle m \mid \partial_\lambda H |n\rangle}{E_n - E_m} \frac{E_n - E_m}{E_n - E_m} \frac{E_n - E_m}{E_n - E_m} \right)
\]

\[
= \sum_{m \neq n} \left( \sum_{l \neq m} \frac{V_{lm}}{E_m - E_l} \frac{V_{mn}}{E_n - E_m} + \sum_{l \neq m} \frac{V_{ml}}{E_m - E_l} \frac{V_{ln}}{E_n - E_m} + \sum_{l \neq m} \frac{V_{ml}}{E_m - E_l} \frac{V_{ln}}{E_n - E_m} \right)
\]

(37)
\[
\sum_{l \neq n} |m\rangle \frac{V_{ml}}{E_n - E_m} \frac{V_{ln}}{E_n - E_l} |m\rangle - |m\rangle \frac{V_{mn}}{(E_n - E_m)^2} (V_{nn} - V_{mm})
\]

Push \(l = m\) or \(l = n\) terms out of the summation, so as to combine the first three summations under \(\sum_{n \neq m, n}\) (sum over \(l\) excluding both \(m\) and \(n\),

\[
|\partial^2 n\rangle = \sum_{n \neq m} \left( \sum_{l \neq m, n} |l\rangle \frac{V_{ml}}{E_m - E_l} \frac{V_{mn}}{E_n - E_m} + |m\rangle \frac{V_{ml}}{E_m - E_l} \frac{V_{ln}}{E_n - E_m} + |m\rangle \frac{V_{mn}}{(E_n - E_m)^2} (\frac{V_{nn}}{E_n - E_m} - \frac{V_{mm}}{E_m - E_m}) \right) +
\]

\[
|n\rangle \frac{V_{mn}}{(E_n - E_m)^2} + |m\rangle \frac{V_{mn}}{(E_n - E_m)^2} + |m\rangle \frac{V_{mn}}{(E_n - E_m)^2} \frac{V_{mn} V_{mm}}{(E_n - E_m)^2}
\]

\[(38)\]

The double summation \(\sum_{n \neq m} \sum_{l \neq m, n}\) means to sum over \(l\) and \(m\), under the constraint that \(l, m, n\) are mutually exclusive. The summation is symmetric under the exchange of \(l\) and \(m\). So for the first term in Eq. (38),

\[
\sum_{n \neq m} \sum_{l \neq m, n} |l\rangle \frac{V_{ml}}{E_m - E_l} \frac{V_{mn}}{E_n - E_m} = \sum_{n \neq m, n} \sum_{l \neq m} |m\rangle \frac{V_{ml}}{E_l - E_m} \frac{V_{ln}}{E_n - E_l},
\]

therefore

\[
|\partial^2 n\rangle = \sum_{n \neq m, n} \left( \sum_{l \neq m} |l\rangle \frac{V_{ml}}{E_l - E_m} \frac{V_{ln}}{E_n - E_l} \frac{1}{(E_n - E_m)(E_n - E_l) + \frac{1}{(E_m - E_l)(E_n - E_m)} + \frac{1}{(E_n - E_m)(E_n - E_l)}} \right)
\]

\[
\sum_{l \neq m} |l\rangle \frac{V_{mn}}{(E_n - E_m)^2} - 2 |m\rangle \frac{V_{mn} V_{nn}}{(E_n - E_m)^2} + 2 |m\rangle \frac{V_{mn} V_{mm}}{(E_n - E_m)^2}
\]

\[(40)\]

Finally we absorb the last term to the summation \(\sum_{m \neq n, n}\) to eliminate the constraint of \(l \neq m\),

\[
|\partial^2 n\rangle = \sum_{m \neq n} \left( \sum_{l \neq m} 2 |m\rangle \frac{V_{ml}}{E_n - E_m} \frac{V_{ln}}{E_n - E_l} - |n\rangle \frac{V_{mn} V_{nn}}{(E_n - E_m)^2} - 2 |m\rangle \frac{V_{mn} V_{nn}}{(E_n - E_m)^2} + 2 |m\rangle \frac{V_{mn} V_{mm}}{(E_n - E_m)^2} \right)
\]

\[(41)\]

Put together Eq. (36) and Eq. (41), to the 2nd order in \(\lambda\), the perturbative correction to the basis state is given by

\[
|n(\lambda)\rangle = |n\rangle + \sum_{m \neq n} \frac{V_{mn}}{E_n - E_m} \lambda +
\]

\[(42)\]
\[
\left( \sum_{m \neq n} \sum_{l \neq n} |m\rangle \langle n| \frac{V_{ml} V_{ln}}{(E_m - E_n)(E_l - E_n)} - \sum_{m \neq n} |m\rangle \langle n| \frac{V_{mn} V_{nn}}{(E_m - E_n)^2} - \frac{1}{2} \sum_{m \neq n} |n\rangle \langle m| \frac{V_{nm} V_{nn}}{(E_m - E_n)^2} \right) \lambda^2 + \ldots
\]

Following this procedure, one can calculate the perturbative correction order by order. Higher order results can be found on Wikipedia under Perturbation Theory (Quantum Mechanics).

### Optional problem

Using the techniques above to show that the 3rd order correction to energy is given by

\[
E_n = \ldots + \left( \sum_{m \neq n} \sum_{l \neq n} \frac{V_{mn} V_{nl}}{(E_m - E_n)(E_l - E_n)} - V_{nn} \sum_{m \neq n} \frac{V_{nm} V_{mn}}{(E_m - E_n)^2} \right) \lambda^3 + \ldots
\]

### Summary of Results

Sometimes, it is simpler to redefine \( \lambda V \) as \( V \)

\[
H(\lambda) = H_0 + \lambda V \rightarrow H_0 + V.
\]

**Rule:** whenever we encounter \( \lambda V_{mn} \) we rewrite it as \( V_{mn} \).

Instead of thinking that the parameter \( \lambda \) is small, we can think that the operator \( V \) is small (i.e. all matrix elements \( V_{mn} \rightarrow 0 \) uniformly). The perturbative corrections are actually in power series of \( V \),

\[
E_n(\lambda V) = E_n + V_{nn} + \sum_{m \neq n} \frac{V_{mn} V_{nn}}{E_n - E_m} + \ldots,
\]

\[
|n(\lambda V)\rangle = |n\rangle + \sum_{m \neq n} |m\rangle \frac{V_{mn} V_{nn}}{E_n - E_m} + \ldots
\]

To summarize, given the unperturbed Hamiltonian \( H_0 \) and the perturbation \( V \) (represented in the eigenbasis of \( H_0 \)),

\[
H_0 = \sum_n |n\rangle \langle n|, \quad V = \sum_{m,n} |m\rangle \langle n| V_{mn} |n\rangle \langle m|,
\]

the **perturbation theory** allows us to construct the **spectral decomposition** of the perturbed Hamiltonian \( H_0 + V \) (i.e. its corrected eigenenergies and eigenstates)

\[
H_0 + V = \sum_n |n(\lambda V)\rangle E_n(\lambda V) \langle n(\lambda V)|.
\]

### Physical Intuitions

In matrix form, \( H_0 \) is diagonal in its eigenbasis, but \( V \) is not.

\[
H_0 + V \approx \begin{pmatrix}
\vdots & \vdots & \vdots \\
\vdots & E_n + V_{nn} & \vdots & V_{nm} & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
V_{mn} & \vdots & E_m + V_{mm} & \vdots & \vdots
\end{pmatrix}.
\]
we will need to **re-diagonalize** the new Hamiltonian $H_0 + V$. But if the off-diagonal elements are weak ($V \to 0$), $H_0 + V$ is *approximately* diagonal, that is why the new eigenenergies and eigenstates can be obtained from the old ones by **perturbative corrections**.

- To the 1st order, $E_n(V)$ simply takes out the *diagonal* matrix element of $H_0 + V$, which amounts to re-evaluating the **energy expectation value** on the old eigenstate $|n\rangle$:

$$E_n + V_{nn} = \langle n | H_0 + V | n \rangle.$$  \hspace{1cm} (48)

- **State hybridization**: the 1st order correction of $|n(V)\rangle$ *hybridizes* (mixes) the original state $|n\rangle$ with all the other $|m\rangle$ states that are *connected* to $|n\rangle$ by non-vanishing $V_{mn}$.

$$|n(V)\rangle = |n\rangle + \sum_{m \neq n} |m\rangle \frac{V_{mn}}{E_n - E_m}$$  \hspace{1cm} (49)

The **hybridization coefficient** is

- proportionally to the **transition rate** $V_{mn}$,
- inversely proportional to the energy **level spacing** $(E_n - E_m)$.

- When $E_n - E_m \to 0$ (energy levels become degenerated) $\Rightarrow$ the hybridization coefficient diverges $\Rightarrow$ signifies the breakdown of the non-degenerate perturbation theory. This scenario is called a **level resonance**.

- **Level repulsion**: the 2nd order energy correction always repel the levels apart (by making the higher level higher and the lower level lower).

$$E_n + \sum_m |V_{nm}|^2 \left\{ \begin{array}{ll} \frac{E_n - E_m}{E_n - E_m} < E_n & \text{if } E_n < E_m, \\ > E_n & \text{if } E_n > E_m. \end{array} \right.$$  \hspace{1cm} (50)

- **Application: the Qubit Model**

$$H_0 + V \simeq \begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix}.$$  \hspace{1cm} (51)

- Unperturbed spectrum. $|\uparrow\rangle$: $E_\uparrow = +1$, $|\downarrow\rangle$: $E_\downarrow = -1$.

- State hybridization:
\[
|\uparrow\rangle' = |\uparrow\rangle + \frac{V_{\uparrow\downarrow}}{E_{\uparrow} - E_{\downarrow}} |\downarrow\rangle + \ldots = |\uparrow\rangle + \frac{\lambda}{2} |\downarrow\rangle + \ldots,
\]
\[
|\downarrow\rangle' = |\downarrow\rangle + \frac{V_{\downarrow\uparrow}}{E_{\downarrow} - E_{\uparrow}} |\uparrow\rangle + \ldots = |\downarrow\rangle - \frac{\lambda}{2} |\uparrow\rangle + \ldots.
\]

- Level repulsion:

\[
E_{\uparrow}' = E_{\uparrow} + \frac{V_{\uparrow\downarrow} V_{\downarrow\uparrow}}{E_{\uparrow} - E_{\downarrow}} + \ldots = +1 + \frac{\lambda^2}{2} + \ldots,
\]
\[
E_{\downarrow}' = E_{\downarrow} + \frac{V_{\downarrow\uparrow} V_{\uparrow\downarrow}}{E_{\downarrow} - E_{\uparrow}} + \ldots = -1 - \frac{\lambda^2}{2} + \ldots.
\]

Here we use a ′ to denote the corrected states \(|n\rangle' \equiv |n(V)\rangle\) and energies \(E_n' \equiv E_n(V)\).

**A Numerical Interlude: Jacobi Algorithm**

**Algorithm**

The Jacobi Algorithm is an *iterative* approach to diagonalize a Hamiltonian.

- Given a Hamiltonian \(H\) (as a matrix).
- Pick an *off-diagonal* element \(H_{mn}\) (labeled by two indices \(m\) and \(n\)), called a pivot. In practice, the *largest* \(H_{mn}\) is taken as the pivot, but that is not necessary in general.

\[
\begin{pmatrix}
\vdots & \vdots & \vdots \\
\cdots & H_{mn} & \cdots \\
\vdots & \vdots & \vdots \\
\cdots & H_{mn} & \cdots \\
\vdots & \vdots & \vdots \\
\end{pmatrix}
\]

\((54)\)

The goal is to suppress \(H_{mn}\).

- First introduce two angles \(\theta\) and \(\phi\) to parameterize the following ratio

\[
\frac{H_{mn}}{H_{nn} - H_{mm}} = \frac{1}{2} e^{i\phi} \tan 2\theta.
\]

\((55)\)

- Then construct a *unitary* matrix \(G\) (called the *Givens matrix*)

\[
G = \begin{pmatrix}
1 & \cos \theta & -e^{-i\phi} \sin \theta \\
\cos \theta & 1 & e^{i\phi} \sin \theta \\
e^{i\phi} \sin \theta & e^{-i\phi} \sin \theta & 1
\end{pmatrix}.
\]

\((56)\)

Consider a quantum pendulum described by the Hamiltonian \(H = -\frac{1}{2} \partial^2 \theta - g \cos \theta\).
Assume \(g \ll 1\), calculate (i) the eigenenergies to the 2nd order in \(g\), and (ii) the eigenstates to the 1st order in \(g\).
• The following transformation will eliminate $H_{mn}$ and brings $H$ closer to diagonal

$$H \rightarrow H' = G^\dagger \ H \ G.$$  

(57)

• Take the new Hamiltonian $H'$ and start over again (until it is sufficiently diagonalized).

**Demonstration**

Here is a demonstration of how the Hamiltonian matrix looks like in each step (lighter color: smaller magnitude, color: phase), and a list of diagonal elements in the initial and final Hamiltonian (compared to the exact eigenvalues).

The algorithm can be used to **block-diagonalize** a Hamiltonian as well. We just need to restrict the choice of the pivot *outside* the diagonal blocks.

**Perturbative Limit**

Denote the diagonal and off-diagonal elements as
\[ E_n = H_{nn}, \]
\[ V_{mn} = H_{nn} \text{ (for } m \neq n). \tag{58} \]

In the limit \( V_{mn} \to 0 \), the angle \( \theta \to 0 \) according to Eq. (55),

\[ e^{i \phi} \theta \approx \frac{V_{mn}}{E_n - E_m}. \tag{59} \]

The Givens matrix becomes

\[
G \approx \begin{pmatrix}
1 & \frac{V_{mn}}{E_n - E_m} \\
\frac{V_{mn}}{E_m - E_n} & 1
\end{pmatrix}.	ag{60}
\]

This corresponds to the following basis transform

\[
\begin{pmatrix} |n\rangle' \\ |m\rangle' \end{pmatrix} = \begin{pmatrix} |n\rangle \\ |m\rangle \end{pmatrix} G \approx \begin{pmatrix} |n\rangle \\ |m\rangle \end{pmatrix} \begin{pmatrix}
1 & \frac{V_{mn}}{E_n - E_m} \\
\frac{V_{mn}}{E_m - E_n} & 1
\end{pmatrix},
\tag{61}
\]

which is consistent with the perturbation theory

\[
|n\rangle' \approx |n\rangle + |m\rangle \frac{V_{mn}}{E_n - E_m},
\]

\[
|m\rangle' \approx |m\rangle + |n\rangle \frac{V_{nm}}{E_m - E_n}. \tag{62}
\]

**Conclusion:** for small \( V \), one can use the non-degenerate perturbation theory to implement the Givens rotation (approximately) and to bring the Hamiltonian to diagonal or block-diagonal.

- **Degenerate Perturbation Theory**

- **General Ideas**

  How do we deal with degeneracies in \( H_0 \) spectrum?

  **Strategy:** divide and conquer.

  ![Diagram](image)

  The degenerated states span a Hilbert *subspace*, called the **degenerate subspace**.
• First apply non-degenerate perturbation theory to bring the Hamiltonian to diagonal blocks in the degenerate subspaces.
• Each diagonal block represents an effective Hamiltonian within the degenerated subspace.

previously: perturbative correction to each energy level \(\rightarrow\) now: perturbative correction to each effective Hamiltonian.

• Then go on with each effective Hamiltonian:
  • If the degeneracy has been lifted (typically), we proceed with non-degenerate perturbation in each block.
  • If the diagonal elements are still fully degenerated, we proceed with exact diagonalization (no perturbative approach available in this case).

The degenerate perturbation theory: applying non-degenerate perturbation theory in hierarchies. It progressively focus on lower and lower energy scales ⇒ A key idea of the renormalization group approach in quantum field theory.

■ Generalized Hellmann-Feynman Theorems

We can generalize the Hellmann-Feynman theorems to generic spectrum with degeneracies. When the unperturbed Hamiltonian \(H_0\) has degenerate levels, we use two indices to label the basis state

\[
|n\rangle_{\text{generalize}} \rightarrow |na\rangle
\]

• \(n\): principal quantum number, labels degenerate subspaces.
• \(\alpha\): secondary quantum number, labels orthogonal degenerate state within each subspace.

The states with the same index \(n\) are degenerated:

\[
H_0 |na\rangle = E_n |na\rangle,
\]

such that the eigenenergy \(E_n\) only depends on \(n\).

• \(|na\rangle\) form a set of orthonormal basis: \(\langle ma | n\beta\rangle = \delta_{mn} \delta_{\alpha\beta}\).

• The perturbation operator \(V\) can be represented in this basis:

\[
V = \sum_{ma,n\beta} |ma\rangle V_{ma,n\beta} \langle n\beta|.
\]

However, once the perturbation \(V\) is included,

\[
H(\lambda) = H_0 + \lambda V,
\]

the degeneracy in each subspace can no longer be maintained in general. Instead, we will only require the perturbed Hamiltonian \(H(\lambda)\) to be block-diagonalized in the \(|na(\lambda)\rangle\) basis, meaning that
\[ H(\lambda) | n\beta(\lambda) \rangle = \sum_{a} |na(\lambda)\rangle E_{n,a\beta}(\lambda). \] (67)

- \(E_{n,a\beta}(\lambda)\) is the matrix element of the effective Hamiltonian in the \(n\)th degenerate subspace.
- \(E_{n,a\beta}(\lambda)\) should take the form of
  \[ E_{n,a\beta}(\lambda) \equiv E_{n,a\beta}(0) = E_n \delta_{a\beta}, \] (68)
to restore Eq. (64) in the \(\lambda = 0\) unperturbed limit.
- The Hermitian conjugate version of Eq. (67) reads
  \[ \langle my(\lambda) | H(\lambda) = \sum_{\delta} \langle m\delta(\lambda) | E_{n,\delta\gamma}(\lambda) = \sum_{\delta} E_{m,\gamma\delta}(\lambda) \langle m\delta(\lambda) |, \] (69)
where we have assumed that the effective Hamiltonian is Hermitian: \(E_{m,\delta\gamma}(\lambda) = E_{m,\gamma\delta}(\lambda)\).

Applying \(\partial_{\lambda}\) on both sides of Eq. (67) and overlapping with \(\langle my|\), we obtain
\[
\langle my | \partial_{\lambda} H | n\beta \rangle = \sum_{a} \partial_{\lambda} E_{n,a\beta} \langle my | na \rangle + \sum_{a} \langle my | \partial_{\lambda} na \rangle E_{n,a\beta} - \sum_{\delta} E_{m,\gamma\delta} \langle m\delta | \partial_{\lambda} n\beta \rangle = \partial_{\lambda} E_{n,a\beta} \delta_{mn} + (E_n - E_m) \langle m\gamma | \partial_{\lambda} n\beta \rangle
\] (70)

- When \(m = n\), the first Hellmann-Feynman theorem:
\[
\partial_{\lambda} E_{n,a\beta} = \langle na | \partial_{\lambda} H | n\beta \rangle = V_{na,n\beta}.
\] (71)

- When \(m \neq n\), the second Hellmann-Feynman theorem:
\[
\langle ma | \partial_{\lambda} n\beta \rangle = \frac{\langle ma | \partial_{\lambda} H | n\beta \rangle}{E_n - E_m} = \frac{V_{ma,n\beta}}{E_n - E_m},
\]
\[
\langle \partial_{\lambda} ma | n\beta \rangle = \frac{\langle ma | \partial_{\lambda} H | n\beta \rangle}{E_m - E_n} = \frac{V_{ma,n\beta}}{E_m - E_n}.
\] (72)

We also assume (by gauge fixing) that
\[
\langle na | \partial_{\lambda} n\beta \rangle = \langle \partial_{\lambda} na | n\beta \rangle = 0.
\] (73)

**Comment:** \(\langle na | \partial_{\lambda} n\beta \rangle\) is a non-Abelian connection that can be gauge fixed by unitary transformations within the \(n\)th degenerate subspace. [But we will not go into more details about this.]

**Effective Hamiltonian**

Using Eq. (71), Eq. (72), Eq. (73) and the techniques we have developed previously, the following derivatives can be calculated
\[
\partial_{\lambda} E_{n,a\beta} = V_{na,n\beta},
\]
\[
\partial^2_{\lambda} E_{n,a\beta} = 2 \sum_{m \neq n} \sum_{\gamma} V_{na,\gamma\beta} V_{\gamma\beta,m\beta} / (E_n - E_m),
\] (74)
\[ |\vartheta_n\alpha\rangle = \sum_{m \neq n} \sum_{\beta} |m\beta\rangle \frac{V_{n\beta,\alpha}}{E_n - E_m}. \]

With these, we can obtain:

- (the matrix element of) the effective Hamiltonian to the 2nd order in \( \lambda \)

\[
E_{n,\alpha\beta}(\lambda) = E_n \delta_{\alpha\beta} + V_{n\alpha,n\beta}\lambda + \sum_{m \neq n} \sum_{\gamma} \frac{V_{n\alpha,n\gamma} V_{m\gamma,n\beta}}{E_n - E_m} \lambda^2 + \ldots, \quad (75)
\]

- the corrected basis state to the 1st order in \( \lambda \)

\[
|n\alpha(\lambda)\rangle = |n\alpha\rangle + \sum_{m \neq n} \sum_{\beta} |m\beta\rangle \frac{V_{n\beta,\alpha}}{E_n - E_m} \lambda + \ldots. \quad (76)
\]

Note that the summation range of the secondary index will depend on the choice of the primary index, which can be inferred easily.

Eq. (75) and Eq. (76) allow us to construct the effective Hamiltonian in operator form

\[
H_n^{\text{eff}}(\lambda) = \sum_{\alpha,\beta} |n\alpha(\lambda)\rangle E_{n,\alpha\beta}(\lambda) \langle n\beta(\lambda)|. \quad (77)
\]

The full Hamiltonian: summation of effective Hamiltonians over degenerate subspaces

\[ H(\lambda) = \bigoplus_n H_n^{\text{eff}}(\lambda). \]

### Application: A Spin-1 Model

Consider a spin-1 system (3-dimensional Hilbert space).

- Basis: \(|+1\rangle, |0\rangle, |−1\rangle\).
- The matrix representations for spin operators \( S^x \) and \( S^z \)

\[
S^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (78)
\]

Hamiltonian

\[ H(\lambda) = H_0 + \lambda V, \]

\[ H_0 = (S^z)^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \]

\[ V = S^x + S^z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -1 \end{pmatrix}. \quad (79)\]
Degenerate subspaces

\begin{align}
\begin{array}{c|cc}
  n & \text{states} & \text{energy} \\
  \hline
  1 & |\pm 1\rangle, |\mp 1\rangle & E_1 = 1 \\
  0 & |0\rangle & E_0 = 0 \\
\end{array}
\end{align}

(80)

- Corrected basis (use \( \prime \) to denote the perturbed result)

\begin{align}
|\pm 1\rangle' &= |\pm 1\rangle + |0\rangle \frac{V_{0,\pm 1}}{E_1 - E_0} \lambda + \ldots = |\pm 1\rangle + \frac{\lambda}{\sqrt{2}} |0\rangle + \ldots,

|0\rangle' &= |0\rangle + |+1\rangle \frac{V_{+1,0}}{E_0 - E_1} \lambda + |\mp 1\rangle \frac{V_{-1,0}}{E_0 - E_1} \lambda + \ldots
\end{align}

(81)

\begin{align}
|0\rangle' &= |0\rangle - \frac{\lambda}{\sqrt{2}} (|+1\rangle + |\mp 1\rangle) + \ldots.
\end{align}

- Effective Hamiltonian

- \( n = 1 \) subspace

\begin{align}
H_1^{\text{eff}} &= |+1\rangle' \left( E_1 + V_{+1,+1} \lambda + \frac{V_{+1,0} V_{0,+1}}{E_1 - E_0} \lambda^2 \right) |+1\rangle' + |-1\rangle' \left( E_1 + V_{-1,-1} \lambda + \frac{V_{-1,0} V_{0,-1}}{E_1 - E_0} \lambda^2 \right) |-1\rangle' + \\
|+ 1\rangle' \left( V_{+1,-1} \lambda + \frac{V_{+1,0} V_{0,-1}}{E_1 - E_0} \lambda^2 \right) |+1\rangle' + |-1\rangle' \left( V_{-1,+1} \lambda + \frac{V_{-1,0} V_{0,+1}}{E_1 - E_0} \lambda^2 \right) |+1\rangle' + \ldots
\end{align}

(82)

\begin{align}
|+1\rangle' \left( 1 + \lambda + \frac{\lambda^2}{2} \right) |+1\rangle' + |-1\rangle' \left( 1 - \lambda + \frac{\lambda^2}{2} \right) |-1\rangle' + |+1\rangle' \frac{\lambda^2}{2} |-1\rangle' + |+1\rangle' \frac{\lambda^2}{2} |+1\rangle' + \ldots
\end{align}

On the corrected basis \(|+1\rangle', |-1\rangle'\), \( H_1^{\text{eff}} \) can be represented as a \( 2 \times 2 \) matrix

\begin{align}
H_1^{\text{eff}} &= \begin{bmatrix}
1 + \lambda + \frac{\lambda^2}{2} & \frac{\lambda^2}{2} \\
\frac{\lambda^2}{2} & 1 - \lambda + \frac{\lambda^2}{2}
\end{bmatrix}.
\end{align}

(83)

The degeneracy is lifted \( \Rightarrow \) we can proceed with non-degenerate perturbation in the next iteration.

- \( n = 0 \) subspace

\begin{align}
H_0^{\text{eff}} &= |0\rangle' \left( E_0 + V_{0,0} \lambda + \frac{V_{0,+1} V_{+1,0} + V_{0,-1} V_{-1,0}}{E_0 - E_1} \lambda^2 \right) |0\rangle' + \ldots
\end{align}

(84)

\begin{align}
|0\rangle' \left( -\lambda^2 \right) |0\rangle' + \ldots
\end{align}

We can use another round of the non-degenerate perturbation theory to further diagonalize \( H_1^{\text{eff}} \).

We start with

\begin{align}
H_1^{\text{eff}} &= |+1\rangle' E_{\pm 1} \langle +1\rangle' + |-1\rangle' E_{\mp 1} \langle -1\rangle' + |+1\rangle' V_{+1,-1} \langle -1\rangle' + |-1\rangle' V_{-1,+1} \langle +1\rangle',

E_{\pm 1} &= 1 \pm \lambda + \frac{\lambda^2}{2},

V_{\pm 1} &= \frac{\lambda^2}{2}, \quad V_{\mp 1} = 0.
\end{align}

(85)
In conclusion, in for the perturbative spin-1 model following we Eq. given found expansions we diagonalize exactly $H$ If

\[
+1)'' = |+1) + |-1) \frac{V_{2,1}}{E_{2} - E_{1}} + \ldots = |+1) + \frac{\lambda}{4} |-1) + \ldots
\]

\[
-1)'' = |-1) + |+1) \frac{V_{2,-1}}{E_{-2} - E_{1}} + \ldots = |-1) - \frac{\lambda}{4} |+1) + \ldots
\]

Plugging in Eq. (81),

\[
+1)'' = |+1) + \frac{\lambda}{\sqrt{2}} |0) + \frac{\lambda}{4} |-1) + \frac{\lambda^2}{4 \sqrt{2}} |0) + \ldots
\]

\[
-1)'' = |-1) + \frac{\lambda}{\sqrt{2}} |0) - \frac{\lambda}{4} |+1) - \frac{\lambda^2}{4 \sqrt{2}} |0) + \ldots
\]

The $\lambda^2$ terms should not be included, because the expansion is only reliable to the 1st order in $\lambda$.

- Corrected states

\[
+1)'' = |+1) + |-1) \frac{V_{2,1}}{E_{2} - E_{1}} + \ldots = |+1) + \frac{\lambda}{4} |-1) + \ldots
\]

\[
-1)'' = |-1) + |+1) \frac{V_{2,-1}}{E_{-2} - E_{1}} + \ldots = |-1) - \frac{\lambda}{4} |+1) + \ldots
\]

Plugging in Eq. (81),

\[
+1)'' = |+1) + \frac{\lambda}{\sqrt{2}} |0) + \frac{\lambda}{4} |-1) + \frac{\lambda^2}{4 \sqrt{2}} |0) + \ldots
\]

\[
-1)'' = |-1) + \frac{\lambda}{\sqrt{2}} |0) - \frac{\lambda}{4} |+1) - \frac{\lambda^2}{4 \sqrt{2}} |0) + \ldots
\]

The $\lambda^2$ terms should not be included, because the expansion is only reliable to the 1st order in $\lambda$.

In conclusion, we found following perturbative expansions for the spin-1 model given in Eq. (79)

\[
E''_+ = 1 + \lambda + \frac{\lambda^2}{2} + O(\lambda^3) \quad |+1)'' = |+1) + \frac{\lambda}{\sqrt{2}} |0) + \frac{\lambda}{4} |-1) + O(\lambda^2)
\]

\[
E'_0 = -\lambda^2 + O(\lambda^3) \quad |0)'' = |0) - \frac{\lambda}{\sqrt{2}} (+1) + |-1)) + O(\lambda^2)
\]

\[
E''_1 = -\lambda + \frac{\lambda^2}{2} + O(\lambda^3) \quad |-1)'' = |-1) + \frac{\lambda}{\sqrt{2}} |0) - \frac{\lambda}{4} |+1) + O(\lambda^2)
\]

If we exactly diagonalize $H(\lambda)$ and perform the Taylor expansion, the above results can be verified.

\[
-\lambda^2 + O(\lambda)^3 - |0) + \left( \frac{-1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right) \lambda + O(\lambda)^2
\]

\[
1 - \lambda + \frac{\lambda^2}{2} + O(\lambda)^3 - |1) + \left( \frac{0}{\sqrt{2}} - \frac{1}{4} \right) \lambda + O(\lambda)^2
\]

\[
1 + \lambda + \frac{\lambda^2}{2} + O(\lambda)^3 - |+1) + \left( \frac{0}{\sqrt{2}} + \frac{1}{4} \right) \lambda + O(\lambda)^2
\]
Time-Dependent Perturbation

- **Time-Dependent Perturbation Theory**

- **Problem Setup**

  Two schemes of the perturbation theory:

  - **Time-independent perturbation**: corrections to energy levels, states, effective Hamiltonians.
  - **Time-dependent perturbation**: corrections to time-evolution operators (propagators, Green’s functions).

  The time-dependent perturbation theory is more general (because we can always set the perturbation to be time-independent afterwards).

  Consider the Hamiltonian

  \[
  H(t) = H_0 + V(t).
  \] (90)

  - The spectrum of \(H_0\) is known

  \[
  H_0 |n\rangle = E_n |n\rangle. \tag{91}
  \]

  The basis states \(|n\rangle\) are fixed (time-independent), because \(H_0\) is time-independent.

  - All the time dependence is ascribed to the operator \(V(t)\), which can be represented in the eigenbasis of \(H_0\)

  \[
  V(t) = \sum_{m,n} |m\rangle V_{mn}(t) \langle n|. \tag{92}
  \]

  \(V_{mn}(t)\) is expected to be small (compared to the energy scale of \(H_0\)) through out the time \(t\).

  Time-evolution of quantum states in the Schrödinger picture is governed by the Schrödinger equation (set \(\hbar = 1\) for simplicity):

  \[
  i \partial_t |\psi(t)\rangle_S = H(t) |\psi(t)\rangle_S = (H_0 + V(t)) |\psi(t)\rangle_S. \tag{93}
  \]

  Time-evolution is **unitary**: the solution of \(|\psi(t)\rangle_S\) must take the form of

  \[
  |\psi(t)\rangle_S = U(t) |\psi(0)\rangle_S. \tag{94}
  \]

  - This defines the **unitary** operator \(U(t)\), called the time-evolution operator. Once we know \(U(t)\), we can apply it to any initial state \(|\psi(0)\rangle_S\) to obtain the final state \(|\psi(t)\rangle_S\) (we don’t need to solve the Schrödinger equation over and over again).

  Plug Eq. (94) to Eq. (93) leads to an equation for \(U(t)\),

  \[
  i \partial_t U(t) = H(t) U(t), \tag{95}
  \]
subject to the initial condition: \( U(0) = 1 \). Note: this is matrix (or operator) equation, which has many more variables to solve than the Schrödinger equation.

This is a hard problem in general. But we know the solution for a special case: the unperturbed case when \( V(t) = 0 \), where

\[
i \partial_t U_0(t) = H_0 \ U_0(t). \tag{96}
\]

The solution is given by

\[
U_0(t) = e^{-i H_0 t} = \sum_n |n\rangle \ e^{-i E_n t} \langle n|. \tag{97}
\]

Now suppose \( V(t) \) is small (as a perturbation), \( H(t) \) is only slightly modified from \( H_0 \), thus we expect that \( U(t) \) is also close to \( U_0(t) \) up to perturbative corrections. The goal of the time-dependent perturbation theory is to calculate these corrections in power series of \( V(t) \).

\[
\begin{align*}
H_0 & \xrightarrow{+V(t)} H(t) \\
\downarrow & \downarrow \\
U_0(t) & \xrightarrow{+???} U(t)
\end{align*}
\]

**Interaction Picture**

Strategy: changing the frame of reference. Switch to the comoving frame with the state (following the unperturbed evolution), so as to focus on the effect of the \( V(t) \) perturbation.

Use \( U_0(t) \) to transform everything to the Interaction picture.

- **State-based** formalism.

\[
|\psi(t)\rangle_I = U_0^\dagger(t) \ |\psi(t)\rangle_S = e^{i H_0 t} \ |\psi(t)\rangle_S, \tag{98}
\]

One can show that

\[
i \partial_t |\psi(t)\rangle_I = i \partial_t (e^{i H_0 t} \ |\psi(t)\rangle_S) \\
= i \partial_t (e^{i H_0 t} \ |\psi(t)\rangle_S + e^{i H_0 t} \ i \partial_t |\psi(t)\rangle_S) \\
= e^{i H_0 t} (E_0) \ |\psi(t)\rangle_S + e^{i H_0 t} (H_0 + V(t)) \ |\psi(t)\rangle_S \\
= U_0^\dagger(t) \ V(t) \ |\psi(t)\rangle_S \\
= U_0^\dagger(t) \ V(t) \ U_0(t) \ U_0^\dagger(t) \ |\psi(t)\rangle_S.
\]

Define the perturbation in the interaction picture:

\[
V_I(t) = U_0^\dagger(t) \ V(t) \ U_0(t) = \sum_{m,n} |m\rangle \ V_{mn}(t) \ e^{i(E_m-E_n) t} \langle n|. \tag{100}
\]

The time-evolution of \( |\psi(t)\rangle_I \) is described by

\[
i \partial_t |\psi(t)\rangle_I = V_I(t) \ |\psi(t)\rangle_I. \tag{101}
\]
• **Operator-based** formalism.

\[
U_T(t) = U_0^0(t) U(t).
\]  

(102)

\[i \partial_t U_T(t) = V_T(t) U_T(t),\]  

subject to the initial condition: \(U_T(0) = 1\). The solution of \(U_T(t)\) can be used

• to provide the universal solution for \(|\psi(t)\rangle_T = U_T(t) |\psi(0)\rangle_T\),

• and to construct \(U(t) = U_0(t) U_T(t)\).

There is no explicit dependence on \(H_0\) in either Eq. (101) or Eq. (103), which allows us to focus on the perturbation \(V_T(t)\).

### Dyson Series

Integrating both sides of Eq. (103) in time

\[i \ U_T(t) - i \ U_T(0) = i \ \int_0^t dt' \ \partial_{t'} U_T(t') = \int_0^t dt' \ V_T(t') U_T(t'),\]  

(104)

plugging in the initial condition \(U_T(0) = 1\), we obtain an integral equation, equivalent to the differential equation Eq. (103).

\[U_T(t) = 1 - i \ \int_0^t dt' \ V_T(t') U_T(t').\]  

(105)

This provides a self-consistent equation for \(U_T(t)\). If we take this expression and substitute \(U_T(t')\) under the integrand, we obtain

\[U_T(t) = 1 - i \ \int_0^t dt' \ V_T(t') + (-i)^2 \ \int_0^t dt' \ V_T(t') \ \int_0^{t'} dt'' \ V_T(t'') U_T(t').\]  

(106)

Iterating this procedure, we obtain a formal solution in power series of \(V_T\), known as the **Dyson series**:

\[U_T(t) = \sum_{k=0}^{\infty} (-i)^k \ \int_0^t dt_k \ \int_0^{t_k} dt_{k-1} \ldots \int_0^{t_2} dt_1 \ V_T(t_k) V_T(t_{k-1}) \ldots V_T(t_1).\]  

(107)

where the \(k = 0\) term corresponds to \(1\). The operators \(V_T(t)\) are organized in a time-ordered sequence with \(0 \leq t_1 \leq \ldots \leq t_{k-1} \leq t_k \leq t\). Rule: *earlier* operator on the *right*, *later* operator on the *left.*
**Green’s Function**

Let us take a closer look at the product of $V_I$ in the Dyson series. By definition

$$V_I(t) = U_0^r(t) V(t) U_0(t),$$

$$V_I(t_0) V_I(t_{k-1}) ... V_I(t_1)$$

$$= U_0^r(t_0) V(t_0) U_0^r(t_{k-1}) V(t_{k-1}) U_0(t_{k-1}) ... U_0^r(t_1) V(t_1) U_0(t_1).$$

This motivates us to introduce the unitary operator $G_0(t, t')$, known as the **bare Green’s function** or the **bare propagator**,

$$G_0(t, t') = U_0(t) U_0^r(t') = \sum_n |n\rangle e^{-i E_n (t-t')} \langle n|,$$ 

which propagates the state from time $t'$ to $t$. In terms of the bare Green’s function,

$$V_I(t_0) V_I(t_{k-1}) ... V_I(t_1)$$

$$= U_0^r(t_0) G_0(t, t_0) V(t_0) G_0(t_k, t_{k-1}) V(t_{k-1}) ... G_0(t_2, t_1) V(t_1) G_0(t_1, 0).$$

The left most $U_0^r(t_0)$ can be canceled out if we consider the **time-evolution operator** in the Schrödinger picture, i.e. $U(t) = U_0(t) U_I(t)$. According to Eq. (107) and Eq. (110), we have

$$U(t) = \sum_{k=0}^{\infty} (-i)^k$$

$$\int_0^t dt_k \int_0^{t_k} dt_{k-1} ... \int_0^{t_2} dt_1 G_0(t, t_k) G_0(t_k, t_{k-1}) V(t_{k-1}) ... G_0(t_2, t_1) V(t_1) G_0(t_1, 0).$$

Further define the **dressed Green’s function** (or the **dressed propagator**) as

$$G(t, t') = U(t) U^r(t'),$$

then Eq. (111) can be written as

$$G(t, t_0) = \sum_{k=0}^{\infty} (-i)^k \int_0^t dt_k \int_0^{t_k} dt_{k-1} ...$$

$$\int_0^{t_2} dt_1 G_0(t, t_k) G_0(t_k, t_{k-1}) V(t_{k-1}) ... G_0(t_2, t_1) V(t_1) G_0(t_1, t_0),$$

where we have generalized the initial time to $t_0$. This is the **Dyson series** for Green’s function.

- $G(t, t')$ can be calculated in **power series** of $V(t)$ given $G_0(t, t')$.
- Since $U(t) = G(t, 0)$, we also know how to calculate $U(t)$ in power series of $V(t)$.

So we have reached our goal!

**Feynman Diagrams**

However, the formula Eq. (113) looks complicated. Let us develop some physical intuitions using **Feynman diagrams**.
• A directed single-line link: the bare Green’s function from one time to another,
\[ \overrightarrow{t \rightarrow t'} = G_0(t, t'). \]  
(114)

The arrow specifies the direction of time (from past to future).

• A solid node: the perturbation operator at a particular time,
\[ \bullet t = -i \ V(t). \]  
(115)

• Connecting links and nodes: identifying the time together
\[ \overrightarrow{t_0 \rightarrow t_1 \rightarrow t_2} = G_0(t_2, t_1) (-i \ V(t_1)) G_0(t_1, t_0). \]  
(116)

Note: in the diagram, the time flows along the arrow from left to right; but in the operator product, the operator acts in sequence from right to left. Things are mirror image (left-right reversed) to each other with respect to the “⇔” sign.

• If the time is not labeled explicitly, then
  • the time of the outmost node (the initial and final nodes) is fixed, (convention: \( t_0 \) - the initial time, \( t \) - the final time),
  • the time of the internal node will be automatically integrated over, and the integration goes through all possible arrangements preserving the time-ordering.
\[ \overrightarrow{t} = G_0(t, t_0), \]
\[ \overrightarrow{t_0 \rightarrow t_1 \rightarrow t_2} = (-i) \int_{t_0}^{t_1} dt_1 \ G_0(t, t_1) \ V(t_1) \ G_0(t_1, t_0), \]
\[ \overrightarrow{t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow t_3} = (-i)^2 \int_{t_0}^{t_1} dt_2 \ \int_{t_0}^{t_1} dt_1 \ G_0(t, t_2) \ V(t_2) \ G_0(t_2, t_1) \ V(t_1) \ G_0(t_1, t_0), \]  
(117)

\[ \ldots \]

• A directed double-line link: the dressed Green’s function from one time to another,
\[ \overleftarrow{\bullet \bullet} = G(t, t_0). \]  
(118)

With the diagrammatic representations in Eq. (117) and Eq. (118), we can rewrite Eq. (113) as
\[ \overrightarrow{t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow t_3} = \overrightarrow{t_0 \rightarrow t_1} + \overrightarrow{t_1 \rightarrow t_2 \rightarrow t_3} + \overrightarrow{t_2 \rightarrow t_3 \rightarrow t_0} \ldots \]  
(119)

• If we turn off the perturbation, i.e. \( V(t) = 0 \) or \( \bullet = 0 \), Eq. (119) reduces to
\[ \overrightarrow{t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow t_3} = \overrightarrow{t_0 \rightarrow t_1}, \]  
(120)

as all the diagrams containing the node will vanish. This simply restores \( G(t, t_0) = G_0(t, t_0) \) in the absence of perturbation.

• In the presence of \( V(t) \), the propagator is dressed order-by-order by scattering with the perturbation \( \bullet \). For example, \( \overrightarrow{t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow t_3} \) describes that the system is first propagated to an intermediate time, acted by the perturbation operator, and then continued to propagate to the final time. Other diagrams describe higher order processes. The full propagation is the sum of all possible processes.
## Energy Level Transitions

### Transition Probability

If a system is prepared in an initial state $|\psi\rangle$ at time $t_0$, at a subsequent time $t$, the initial state will evolve to $G(t, t_0) |\psi\rangle$. Then the probability to find the system in a final state $|f\rangle$ should be given by

$$P_{i\rightarrow f} = |\langle f | G(t, t_0) |\psi\rangle|^2.$$  \hspace{1cm} (121)

$P_{i\rightarrow f}$ is known as the **transition probability**.

To the 1st order in $V(t)$, Eq. (113) reads

$$G(t, t_0) \approx G_0(t, t_0) - i \int_{t_0}^{t} dt_1 G_0(t, t_1) V(t_1) G_0(t_1, t_0) + \ldots,$$  \hspace{1cm} (122)

where $G_0(t, t') = \sum_n |n\rangle e^{-i E_n (t-t')} \langle n|$ is given in Eq. (109). Suppose $|\psi\rangle$ and $|f\rangle$ are eigenstates of $H_0$, we have

$$\langle f | G(t, t_0) |\psi\rangle \approx \langle f | G_0(t, t_0) |\psi\rangle - i \int_{t_0}^{t} dt_1 \langle f | G_0(t, t_1) V(t_1) G_0(t_1, t_0) |\psi\rangle$$

$$\quad = e^{-i (E_f + E_i, t_0)} \delta_{fi} - i \int_{t_0}^{t} dt_1 e^{-i E_i (t-t_1)} \langle f | V(t_1) |\psi\rangle e^{-i E_f (t_1 - t_0)}$$

$$\quad = e^{-i (E_f + E_i, t_0)} \left( \delta_{fi} - i \int_{t_0}^{t} dt_1 \langle f | V(t_1) |\psi\rangle e^{i (E_f - E_i) t_1} \right).$$  \hspace{1cm} (123)

For $i \neq f$, the transition probability is given by

$$P_{i\rightarrow f}(t, t_0) = \frac{1}{\hbar^2} \left| \int_{t_0}^{t} dt_1 \langle f | V(t_1) |\psi\rangle e^{i \omega_{fi} t_1} \right|^2,$$  \hspace{1cm} (124)

here we have restored the Planck constant $\hbar$ and rewrite the energy difference as $E_f - E_i = \hbar \omega_{fi}$. Note that as a probability, $P_{i\rightarrow f}$ is dimensionless.

### Fermi’s Golden Rule

### Adiabatic Process

Consider the perturbation is gradually turn on following an exponential grow from the infinite past (and switch off after $t = 0$)

$$V(t) = \begin{cases} V e^{\epsilon t} & t < 0 \\ 0 & t \geq 0 \end{cases},$$  \hspace{1cm} (130)
Suppose the system is prepared in state $|\psi\rangle$ in the infinite past ($t_0 \to -\infty$), what is the probability for the system to transit to the state $|f\rangle$ at $t = 0$?

According to Eq. (124),

$$P_{i\rightarrow f} = \frac{1}{\hbar^2} \left| \int_{-\infty}^{0} dt_1 \langle f | V | \psi \rangle e^{i/t_1 \omega_{\psi} t_1} \right|^2 \quad \text{(131)}$$

The transition probability exhibits a resonance around $\omega_f = \omega_i$: states are more likely to hybridize when they are closer in energy.

In the adiabatic limit of $\tau \to \infty$, the perturbation is turned on very slowly, such that the $H_0$ eigenstate $|\psi\rangle$ simply evolves to the corresponding eigenstate of $H = H_0 + V$, which is given by

$$|\psi(V)\rangle = |\psi\rangle + \sum_{m \neq i} \frac{V_{mi}}{E_i - E_m} + \ldots, \quad \text{(132)}$$

according to the time-independent perturbation, c.f. Eq. (44). Then the probability to observe the system in the state $|f\rangle$ will be

$$\langle f | \psi(V) \rangle^2 = \frac{|V_{fi}|^2}{(E_f - E_i)^2}. \quad \text{(133)}$$

which matches the result of time-dependent perturbation Eq. (131) in the limit of $\tau \to \infty$. Thus we have verified that the time-dependent perturbation falls back to the time-independent perturbation if the perturbation changes slow enough in time.

On the other hand, for any realistic physical process, the time scale $\tau$ can not be infinitely long. A finite $\tau$ sets an energy resolution $\hbar \tau^{-1}$ (due to the uncertainty principle), below which the energy level resonance is smoothed out. So the singularity of the energy denominator in the time-
independent perturbation do not actually occur in reality.