130B Quantum Physics

Part IV. 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 exact solutions and make the most of them.
- *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 $\hat{H}_0$, find the *spectrum* of $\hat{H} = \hat{H}_0 + \lambda\, \hat{V}$, in power series of λ (given that λ is small).
- **Time-dependent perturbation**: given the (bare) *propagator* $\hat{U}_0(t) = e^{-i\, \hat{H}_0\, t}$, find the *propagator*

$$\begin{aligned} \hat{U}(t) &= \mathcal{T} \exp\left(-i \int_0^t d\, t'\, \hat{H}(t')\right), \\ \hat{H}(t) &= \hat{H}_0 + \lambda\, \hat{V}(t), \end{aligned} \tag{1}$$

in power series of λ (given that λ 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 … (what theorists cares about)
- Practically: to calculate scattering amplitudes, response functions, spectral weights … (what experimentalists measures)

Qubit Model and its Exact Solution

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

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda\, \hat{V}, \tag{2}$$

where $\hat{H}_0 = \hat{\sigma}^z$ and $\hat{V} = \hat{\sigma}^x$, s.t. $\hat{H}(\lambda)$ can be more explicitly written as (in the $\{|0\rangle, |1\rangle\}$ basis)

$$\begin{aligned}\hat{H}(\lambda) &= \hat{\sigma}^z + \lambda\, \hat{\sigma}^x \\ &\doteq \begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix}.\end{aligned} \tag{3}$$

What are the eigenenergies and eigenstates of $\hat{H}(\lambda)$?

$$\hat{H}(\lambda)\, |\psi_\pm(\lambda)\rangle = E_\pm(\lambda)\, |\psi_\pm(\lambda)\rangle. \tag{4}$$

Exact solutions:

- Eigenenergies

$$E_\pm(\lambda) = \pm \sqrt{1+\lambda^2}\,. \tag{5}$$

- Eigenstates

$$\begin{aligned}|\psi_+(\lambda)\rangle &= \frac{\left(1+\sqrt{1+\lambda^2}\right)|0\rangle + \lambda\, |1\rangle}{\sqrt{2\left(1+\lambda^2+\sqrt{1+\lambda^2}\right)}}, \\ |\psi_-(\lambda)\rangle &= \frac{\left(1+\sqrt{1+\lambda^2}\right)|1\rangle - \lambda\, |0\rangle}{\sqrt{2\left(1+\lambda^2+\sqrt{1+\lambda^2}\right)}}.\end{aligned} \tag{6}$$

Taylor Expansion

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

- As a reminder, the **Taylor expansion** of a function $f(\lambda)$ is given by

$$\begin{aligned}f(\lambda) &= \sum_{k=0}^{\infty} \frac{\partial_\lambda^k f(0)}{k!}\, \lambda^k \\ &= f(0) + f'(0)\,\lambda + \frac{f''(0)}{2}\,\lambda^2 + \frac{f^{(3)}(0)}{6}\,\lambda^3 + \ldots.\end{aligned} \tag{7}$$

- Applying Eq. (7) to Eq. (5) and Eq. (6), we get

$$E_\pm = \pm\left(1 + \frac{\lambda^2}{2} - \frac{\lambda^4}{8} + \ldots\right), \tag{8}$$

$$
\begin{aligned}
|\psi_+(\lambda)\rangle &= |0\rangle + \frac{\lambda}{2}\,|1\rangle - \frac{\lambda^2}{8}\,|0\rangle - \frac{3\,\lambda^3}{16}\,|1\rangle + \frac{11\,\lambda^4}{128}\,|0\rangle + \ldots, \\
|\psi_-(\lambda)\rangle &= |1\rangle - \frac{\lambda}{2}\,|0\rangle - \frac{\lambda^2}{8}\,|1\rangle + \frac{3\,\lambda^3}{16}\,|0\rangle + \frac{11\,\lambda^4}{128}\,|1\rangle + \ldots.
\end{aligned} \tag{9}
$$

Goal: obtain these power series *without* first calculating the exact solution! - This can be done as long as we know how to evaluate the **derivatives** $\partial_\lambda^n E(0)$ and $\partial_\lambda^n |\psi_\pm(0)\rangle$.

The **perturbation theory** is essentially an *iterative algorithm* to calculate these derivatives *order by order*, based on our knowledge about $\hat{H}_0$ and $\hat{V}$.

Non-Degenerate Perturbation Theory

Problem Setup

The starting point is the following Hamiltonian (*linearly* parameterized by λ)

$$\boxed{\hat{H}(\lambda) = \hat{H}_0 + \lambda\,\hat{V}.} \tag{10}$$

- This implies

$$
\begin{aligned}
&\hat{H}(0) = \hat{H}_0, \\
&\partial_\lambda \hat{H}(0) = \hat{V}, \\
&\partial_\lambda^2 \hat{H}(0) = \partial_\lambda^3 \hat{H}(0) = \ldots = 0.
\end{aligned} \tag{11}
$$

- To simplify the notation, we will suppress the argument λ if it is evaluated at $\lambda = 0$.

$$
\begin{aligned}
&\hat{H} = \hat{H}_0, \\
&\partial_\lambda \hat{H} = \hat{V}, \\
&\partial_\lambda^2 \hat{H} = \partial_\lambda^3 \hat{H} = \ldots = 0.
\end{aligned} \tag{12}
$$

Rule: Everything depends on λ. But if the dependence on λ is not spelt out explicitly, we assume it to be the evaluated at $\lambda = 0$, i.e. $\hat{H} \equiv \hat{H}\,|_{\lambda=0} = \hat{H}(0)$.

Consider the **eigen equation**

$$\hat{H}(\lambda)\,|n(\lambda)\rangle = E_n(\lambda)\,|n(\lambda)\rangle. \tag{13}$$

For each given λ, there is a different $\hat{H}(\lambda)$, 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 nth energy level. It is a real number depending on λ.
- $|n(\lambda)\rangle$ is the nth eigenstate (in correspondence to $E_n(\lambda)$). It is a state vector in the Hilbert space that can change with λ. Note: The notation $|n(\lambda)\rangle$ does *not* imply that the index n is λ dependent, it should be understood as

$$|n(\lambda)\rangle = \sum_m \psi_{nm}(\lambda)\,|m\rangle. \tag{14}$$

We assume a *discrete* spectrum *without degeneracy*, such that the "nth" 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* $\lambda = 0$,

$$\boxed{\hat{H}\,|n\rangle = E_n\,|n\rangle,} \tag{15}$$

- and what the perturbation is: $\hat{V} = \partial_\lambda \hat{H}$,

$$\boxed{V_{mn} = \langle m|\,\hat{V}\,|n\rangle = \langle m|\,\partial_\lambda \hat{H}\,|n\rangle,} \tag{16}$$

we want to calculate $E_n(\lambda)$ and $|n(\lambda)\rangle$ in power series of λ (to any desired order) in terms of E_n, V_{mn} and $|n\rangle$ (at $\lambda = 0$).

Hellmann-Feynman Theorems

- Applying ∂_λ to both sides of $\hat{H}\,|n\rangle = E_n\,|n\rangle$,

$$\partial_\lambda \hat{H}\,|n\rangle + \hat{H}\,|\partial_\lambda n\rangle = \partial_\lambda E_n\,|n\rangle + E_n\,|\partial_\lambda n\rangle. \tag{17}$$

  - Note: $|\partial_\lambda n\rangle$ stands for the derivative of the state $|n\rangle$ (not the index n)

$$|\partial_\lambda n\rangle \equiv \partial_\lambda |n\rangle = \left(\sum_m \partial_\lambda \psi_{nm}(\lambda)\,|m\rangle\right)_{\lambda=0}. \tag{18}$$

  It does *not* imply that the integer index n can be differentiated.

- Overlap with $\langle m|$ from the left,

$$\langle m|\,\partial_\lambda \hat{H}\,|n\rangle + \langle m|\,\hat{H}\,|\partial_\lambda n\rangle = \partial_\lambda E_n\,\langle m \mid n\rangle + E_n\,\langle m \mid \partial_\lambda n\rangle. \tag{19}$$

  Using $\langle m|\,\hat{H} = \langle m|\,E_m$,

$$\begin{aligned}&\langle m|\,\partial_\lambda \hat{H}\,|n\rangle + E_m\,\langle m \mid \partial_\lambda n\rangle = \partial_\lambda E_n\,\langle m \mid n\rangle + E_n\,\langle m \mid \partial_\lambda n\rangle\\ &\Rightarrow \langle m|\,\partial_\lambda \hat{H}\,|n\rangle = \partial_\lambda E_n\,\langle m \mid n\rangle + (E_n - E_m)\,\langle m \mid \partial_\lambda n\rangle.\end{aligned} \tag{20}$$

- Note that $\partial_\lambda \hat{H} = \hat{V}$ and $\langle m \mid n\rangle = \delta_{mn}$,

$$\boxed{V_{mn} = \langle m|\,\hat{V}\,|n\rangle = \partial_\lambda E_n\,\delta_{mn} + (E_n - E_m)\,\langle m \mid \partial_\lambda n\rangle.} \tag{21}$$

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

$$\boxed{\partial_\lambda E_n = V_{nn}.} \tag{22}$$

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

- When $m \neq n$, Eq. (21) implies

$$\begin{aligned} \langle m \mid \partial_\lambda n\rangle &= \frac{V_{mn}}{E_n - E_m}, \\ \langle \partial_\lambda m \mid n\rangle &= \frac{V_{mn}}{E_m - E_n}. \end{aligned} \tag{23}$$

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 $\langle\partial_\lambda m|$ can be expressed in terms of E_n and V_{mn} which do not contain ∂_λ. ⇒ This effectively *reduces* the order of ∂_λ 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,

$$E_n(\lambda) = \sum_{k=0}^{\infty} \frac{\partial_\lambda^k E_n}{k!} \lambda^k = E_n + (\partial_\lambda E_n)\,\lambda + \frac{1}{2}\left(\partial_\lambda^2 E_n\right)\lambda^2 + \ldots. \tag{24}$$

Applying Hellmann-Feynman theorems, the energy derivatives are

$$\begin{aligned} \partial_\lambda E_n &= V_{nn}, \\ \partial_\lambda^2 E_n &= 2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n - E_m}, \\ &\ldots \end{aligned} \tag{25}$$

Exc 1

> Evaluate Eq. (25).

so the perturbative correction to the eigenenergy is given by

$$\boxed{E_n(\lambda) = E_n + V_{nn}\,\lambda + \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n - E_m} \lambda^2 + \ldots.} \tag{26}$$

State Corrections

According to the Taylor expansion,

$$|n(\lambda)\rangle = \sum_{k=0}^{\infty} \frac{\left|\partial_\lambda^k n\right\rangle}{k!} \lambda^k = |n\rangle + |\partial_\lambda n\rangle \lambda + \frac{1}{2} \left|\partial_\lambda^2 n\right\rangle \lambda^2 + \ldots. \tag{27}$$

Applying Hellmann-Feynman theorems, the state derivatives are

$$\begin{aligned} |\partial_\lambda n\rangle &= \sum_{m\neq n} |m\rangle \frac{V_{mn}}{E_n - E_m}, \\ \left|\partial_\lambda^2 n\right\rangle &= \sum_{m\neq n} \left(\sum_{l\neq n} 2\,|m\rangle \frac{V_{ml}\, V_{ln}}{(E_n - E_m)\,(E_n - E_l)} - 2\,|m\rangle \frac{V_{mn}\, V_{nn}}{(E_n - E_m)^2} - |n\rangle \frac{V_{nm}\, V_{mn}}{(E_n - E_m)^2} \right), \\ &\ldots \end{aligned} \tag{28}$$

Exc 2 Evaluate Eq. (28).

so the perturbative correction to the eigenstate is given by

$$\boxed{\begin{aligned} |n(\lambda)\rangle = |n\rangle + \sum_{m\neq n} |m\rangle \frac{V_{mn}}{E_n - E_m} \lambda + \\ \left(\sum_{m\neq n} \sum_{l\neq n} |m\rangle \frac{V_{ml}\, V_{ln}}{(E_n - E_m)\,(E_n - E_l)} - \sum_{m\neq n} |m\rangle \frac{V_{mn}\, V_{nn}}{(E_n - E_m)^2} - \frac{1}{2} \sum_{m\neq n} |n\rangle \frac{V_{nm}\, V_{mn}}{(E_n - E_m)^2} \right) \lambda^2 + \ldots. \end{aligned}} \tag{32}$$

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).

Summary of Results

Sometimes, it is simpler to redefine $\lambda \hat{V}$ as $\hat{V}$

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{V} \to \hat{H}_0 + \hat{V}. \tag{33}$$

Rule: whenever we encounter λV_{mn} we rewrite it as V_{mn}.

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

$$\boxed{\begin{aligned} E_n(V) &= E_n + V_{nn} + \sum_{m\neq n} \frac{V_{nm}\, V_{mn}}{E_n - E_m} + \ldots, \\ |n(V)\rangle &= |n\rangle + \sum_{m\neq n} |m\rangle \frac{V_{mn}}{E_n - E_m} + \ldots. \end{aligned}} \tag{34}$$

To summarize, given the unperturbed Hamiltonian $\hat{H}_0$ and the perturbation $\hat{V}$ (represented in the eigenbasis of $\hat{H}_0$),

$$\hat{H}_0 = \sum_n |n\rangle\, E_n\, \langle n|,\;\; \hat{V} = \sum_{m,n} |m\rangle\, V_{mn}\, \langle n|, \tag{35}$$

the **perturbation theory** allows us to construct the *spectral decomposition* of the *perturbed* Hamiltonian $\hat{H}_0 + \hat{V}$ (i.e. its corrected eigenenergies and eigenstates)

$$\hat{H}_0 + \hat{V} = \sum_n |n(V)\rangle\, E_n(V)\, \langle n(V)|. \tag{36}$$

Physical Intuitions

In matrix form, $\hat{H}_0$ is diagonal in its eigenbasis, but $\hat{V}$ is not.

$$\hat{H}_0 + \hat{V} \simeq \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & E_n + V_{nn} & \cdots & V_{nm} & \cdots \\ & \vdots & & \vdots & \\ \cdots & V_{mn} & \cdots & E_m + V_{mm} & \cdots \\ & \vdots & & \vdots & \end{pmatrix}, \tag{37}$$

we will need to **re-diagonalize** the new Hamiltonian $\hat{H}_0 + \hat{V}$. But if the off-diagonal elements are weak ($V \to 0$), $\hat{H}_0 + \hat{V}$ is *close to* diagonal, such that re-diagonalization only requires a small effort, that is why the new eigenenergies and eigenstates can be obtained from *perturbative corrections* based on eigensystem of $\hat{H}_0$.

- To the 1st order, $E_n(V)$ simply takes out the *diagonal* matrix element of $\hat{H}_0 + \hat{V}$, which amounts to re-evaluating the **energy expectation value** on the old eigenstate $|n\rangle$:

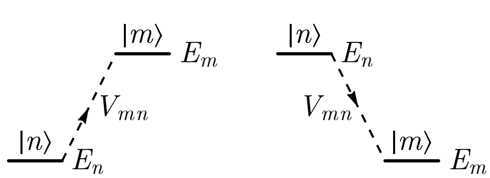
$$E_n + V_{nn} = \langle n|\, \hat{H}_0 + \hat{V}\, |n\rangle. \tag{38}$$

- **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}.

$$|n(V)\rangle = |n\rangle + \sum_{m\neq n} |m\rangle \frac{V_{mn}}{E_n - E_m} \tag{39}$$

  The **hybridization coefficient** is

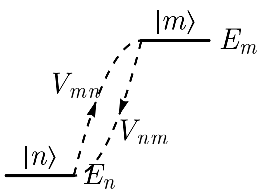
  - proportional to the **transition rate** V_{mn},
  - inversely proportional to the energy **level spacing** $(E_n - E_m)$.



  - When $E_n - E_m \to 0$ (energy levels become degenerated) ⇒ the hybridization coefficient diverges ⇒ 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).

$$E_n + \sum_m \frac{|V_{nm}|^2}{E_n - E_m} \begin{cases} < E_n & \text{if } E_n < E_m, \\ > E_n & \text{if } E_n > E_m. \end{cases} \tag{40}$$



Application: the Qubit Model

$$\hat{H}_0 + \hat{V} \doteq \begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix}. \tag{41}$$

- Unperturbed spectrum. $|0\rangle$: $E_0 = +1$, $|1\rangle$: $E_1 = -1$.
- State hybridization:

$$\begin{aligned} |0\rangle' &= |0\rangle + \frac{V_{10}}{E_0 - E_1} |1\rangle + \ldots = |0\rangle + \frac{\lambda}{2} |1\rangle + \ldots, \\ |1\rangle' &= |1\rangle + \frac{V_{01}}{E_1 - E_0} |0\rangle + \ldots = |1\rangle - \frac{\lambda}{2} |0\rangle + \ldots. \end{aligned} \tag{42}$$

- Level repulsion:

$$\begin{aligned} E_0' &= E_0 + \frac{V_{01}\ V_{10}}{E_0 - E_1} + \ldots = +1 + \frac{\lambda^2}{2} + \ldots, \\ E_1' &= E_1 + \frac{V_{10}\ V_{01}}{E_1 - E_0} + \ldots = -1 - \frac{\lambda^2}{2} + \ldots. \end{aligned} \tag{43}$$

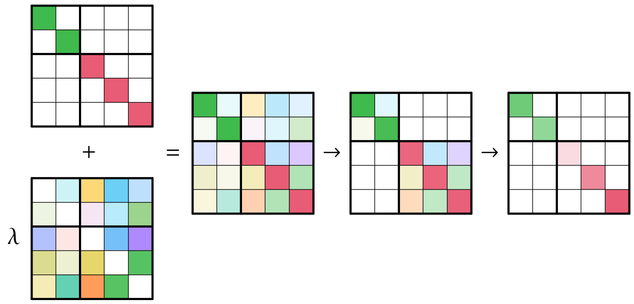
Here we use a $'$ to denote the *corrected* states $|n\rangle' \equiv |n(V)\rangle$ and energies $E_n' \equiv E_n(V)$.

Degenerate Perturbation Theory

General Ideas

How do we deal with degeneracies in $\hat{H}_0$ spectrum?

Strategy: **divide and conquer**.



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* → **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* $\hat{H}_0$ has degenerate levels, we use *two* indices to label the basis state

$$|n\rangle \xrightarrow{\text{generalize}} |n\alpha\rangle \tag{44}$$

- n: **principal** quantum number, labels degenerate subspaces.
- α: **secondary** quantum number, labels orthogonal degenerate state within each subspace.

The states with the same index n are degenerated:

$$\boxed{\hat{H}_0 \, |n\alpha\rangle = E_n \, |n\alpha\rangle,} \tag{45}$$

such that the eigenenergy E_n only depends on n.

- $|n\alpha\rangle$ form a set of *orthonormal* basis: $\langle m\alpha \mid n\beta\rangle = \delta_{mn}\,\delta_{\alpha\beta}$.
- The *perturbation operator* V can be represented in this basis:

$$\boxed{\hat{V} = \sum_{m\alpha,n\beta} |m\alpha\rangle\ V_{m\alpha,n\beta}\ \langle n\beta|.} \tag{46}$$

However, once the perturbation $\hat{V}$ is included,

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda\ \hat{V}, \tag{47}$$

the degeneracy in each subspace can no longer be maintained in general. Instead, we will only require the perturbed Hamiltonian $\hat{H}(\lambda)$ to be *block-diagonalized* in the $|n\alpha(\lambda)\rangle$ basis, meaning that

$$\boxed{\hat{H}(\lambda)\ |n\beta(\lambda)\rangle = \sum_{\alpha} |n\alpha(\lambda)\rangle\ E_{n,\alpha\beta}(\lambda).} \tag{48}$$

- $E_{n,\alpha\beta}(\lambda)$ is the matrix element of the **effective Hamiltonian** in the nth degenerate subspace.
  - When $\lambda = 0$, $E_{n,\alpha\beta}(\lambda)$ should fall back to

$$E_{n,\alpha\beta} \equiv E_{n,\alpha\beta}(0) = E_n\ \delta_{\alpha\beta}, \tag{49}$$

  to recover Eq. (45) in the unperturbed limit.
- The Hermitian conjugate version of Eq. (48) reads

$$\langle m\gamma(\lambda)|\ \hat{H}(\lambda) = \sum_{\delta} \langle m\delta(\lambda)|\ E^*_{m,\delta\gamma}(\lambda) = \sum_{\delta} E_{m,\gamma\delta}(\lambda)\ \langle m\delta(\lambda)|, \tag{50}$$

  where we have assumed that the effective Hamiltonian is *Hermitian*: $E^*_{m,\delta\gamma}(\lambda) = E_{m,\gamma\delta}(\lambda)$.

Applying ∂_λ on both sides of Eq. (48) and overlapping with $\langle m\gamma|$, we obtain

$$\begin{aligned} \langle m\gamma|\ \partial_\lambda \hat{H}\ |n\beta\rangle &= \sum_{\alpha} \partial_\lambda E_{n,\alpha\beta}\ \langle m\gamma \mid n\alpha\rangle + \sum_{\alpha} \langle m\gamma \mid \partial_\lambda n\alpha\rangle\ E_{n,\alpha\beta} - \sum_{\delta} E_{m,\gamma\delta}\ \langle m\delta \mid \partial_\lambda n\beta\rangle \\ &= \partial_\lambda E_{n,\gamma\beta}\ \delta_{mn} + (E_n - E_m)\ \langle m\gamma \mid \partial_\lambda n\beta\rangle \end{aligned} \tag{51}$$

- When $m = n$, the **first Hellmann-Feynman** theorem:

$$\boxed{\partial_\lambda E_{n,\alpha\beta} = \langle n\alpha|\ \partial_\lambda \hat{H}\ |n\beta\rangle = V_{n\alpha,n\beta}.} \tag{52}$$

- When $m \neq n$, the **second Hellmann-Feynman** theorem:

$$\boxed{\begin{aligned} \langle m\alpha \mid \partial_\lambda n\beta\rangle &= \frac{\langle m\alpha|\ \partial_\lambda \hat{H}\ |n\beta\rangle}{E_n - E_m} = \frac{V_{m\alpha,n\beta}}{E_n - E_m}, \\ \langle \partial_\lambda m\alpha \mid n\beta\rangle &= \frac{\langle m\alpha|\ \partial_\lambda \hat{H}\ |n\beta\rangle}{E_m - E_n} = \frac{V_{m\alpha,n\beta}}{E_m - E_n}. \end{aligned}} \tag{53}$$

■ Effective Hamiltonian

Using Eq. (52), Eq. (53) and the techniques we have developed previously, the following derivatives can be calculated

$$\begin{aligned}
\partial_\lambda E_{n,\alpha\beta} &= V_{n\alpha,n\beta}, \\
\partial_\lambda^2 E_{n,\alpha\beta} &= 2 \sum_{m\neq n} \sum_\gamma \frac{V_{n\alpha,m\gamma} V_{m\gamma,n\beta}}{E_n - E_m}, \\
|\partial_\lambda n\alpha\rangle &= \sum_{m\neq n} \sum_\beta |m\beta\rangle \frac{V_{m\beta,n\alpha}}{E_n - E_m}.
\end{aligned} \tag{54}$$

With these, we can obtain:

- (the matrix element of) the **effective Hamiltonian** to the 2nd order in λ

$$\boxed{E_{n,\alpha\beta}(\lambda) = E_n \delta_{\alpha\beta} + V_{n\alpha,n\beta} \lambda + \sum_{m\neq n} \sum_\gamma \frac{V_{n\alpha,m\gamma} V_{m\gamma,n\beta}}{E_n - E_m} \lambda^2 + \ldots,} \tag{55}$$

- the corrected **basis state** to the 1st order in λ

$$\boxed{|n\alpha(\lambda)\rangle = |n\alpha\rangle + \sum_{m\neq n} \sum_\beta |m\beta\rangle \frac{V_{m\beta,n\alpha}}{E_n - E_m} \lambda + \ldots.} \tag{56}$$

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

Eq. (55) and Eq. (56) allow us to construct the **effective Hamiltonian** in operator form

$$\boxed{\hat{H}_n^{\text{eff}}(\lambda) = \sum_{\alpha,\beta} |n\alpha(\lambda)\rangle E_{n,\alpha\beta}(\lambda) \langle n\beta(\lambda)|.} \tag{57}$$

The **full Hamiltonian**: summation of effective Hamiltonians over degenerate subspaces $\hat{H}(\lambda) = \oplus_n \hat{H}_n^{\text{eff}}(\lambda)$.

Application: A Spin-1 Model*

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

$$\boxed{\hat{H}(t) = \hat{H}_0 + \hat{V}(t).} \tag{70}$$

- The spectrum of $\hat{H}_0$ is known

$$\hat{H}_0 \, |n\rangle = E_n \, |n\rangle. \tag{71}$$

The basis states $|n\rangle$ are fixed (time-independent), because $\hat{H}_0$ is time-independent.

- All the time dependence is ascribed to the operator $\hat{V}(t)$, which can be represented in the eigenbasis of $\hat{H}_0$

$$\hat{V}(t) = \sum_{m,n} |m\rangle \; V_{mn}(t) \, \langle n|. \tag{72}$$

$V_{mn}(t)$ is expected to be small (compared to the energy scale of $\hat{H}_0$) 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):

$$\boxed{i \, \partial_t |\psi(t)\rangle_S = \hat{H}(t) \, |\psi(t)\rangle_S = \left(\hat{H}_0 + \hat{V}(t)\right) |\psi(t)\rangle_S.} \tag{73}$$

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

$$\boxed{|\psi(t)\rangle_S = \hat{U}(t) \, |\psi(0)\rangle_S.} \tag{74}$$

- This defines the *unitary* operator $\hat{U}(t)$, called the **time-evolution operator**. Once we know $\hat{U}(t)$, 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. (74) to Eq. (73) leads to an equation for $\hat{U}(t)$,

$$\boxed{i \, \partial_t \, \hat{U}(t) = \hat{H}(t) \, \hat{U}(t),} \tag{75}$$

subject to the *initial condition*: $\hat{U}(0) = \mathbb{1}$. 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 $\hat{V}(t) = 0$, where

$$i\,\partial_t\,\hat{U}_0(t) = \hat{H}_0\,\hat{U}_0(t). \tag{76}$$

The solution is given by

$$\boxed{\hat{U}_0(t) = e^{-i\,\hat{H}_0\,t} = \sum_n |n\rangle\, e^{-i\,E_n\,t}\,\langle n|.} \tag{77}$$

Now suppose $\hat{V}(t)$ is *small* (as a perturbation), $\hat{H}(t)$ is only slightly modified from $\hat{H}_0$, thus we expect that $\hat{U}(t)$ is also close to $\hat{U}_0(t)$ up to perturbative corrections. The goal of the **time-dependent perturbation theory** is to calculate these *corrections* in *power series* of $\hat{V}(t)$.

$$\begin{array}{ccc} \hat{H}_0 & \xrightarrow{+\hat{V}(t)} & \hat{H}(t) \\ \downarrow & & \downarrow \\ \hat{U}_0(t) & \xrightarrow{+???} & \hat{U}(t) \end{array}$$

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 $\hat{V}(t)$ perturbation.

Use $\hat{U}_0(t)$ to transform everything to the **Interaction picture**.

- **State-level** formalism.

$$\boxed{|\psi(t)\rangle_I = \hat{U}_0^\dagger(t)\,|\psi(t)\rangle_S = e^{i\,H_0\,t}\,|\psi(t)\rangle_S,} \tag{78}$$

Define the perturbation in the interaction picture:

$$\boxed{V_I(t) = U_0^\dagger(t)\;V(t)\;U_0(t) = \sum_{m,n} |m\rangle\;V_{mn}(t)\,e^{i(E_m-E_n)\,t}\,\langle n|.} \tag{79}$$

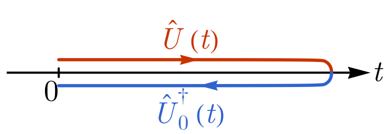
The time-evolution of $|\psi(t)\rangle_I$ is described by

$$\boxed{i\,\partial_t|\psi(t)\rangle_I = V_I(t)\,|\psi(t)\rangle_I.} \tag{80}$$

Exc 3 Show Eq. (80).

- **Operator-level** formalism.

$$\boxed{\hat{U}_I(t) = \hat{U}_0^\dagger(t)\;\hat{U}(t).} \tag{82}$$



$\hat{U}_I(t)$ captures the "additional" unitary evolution implemented by $\hat{U}(t)$ compared to the reference $\hat{U}_0(t)$. Following the similar derivation in Eq. (81), we can show that $\hat{U}_I(t)$ is governed by

$$\boxed{i\,\partial_t\,\hat{U}_I(t) = \hat{V}_I(t)\,\hat{U}_I(t),} \tag{83}$$

subject to the initial condition: $\hat{U}_I(0) = \mathbb{1}$. The solution of $\hat{U}_I(t)$ can be used

- to provide the universal solution for $|\psi(t)\rangle_I = \hat{U}_I(t)\,|\psi(0)\rangle_I$,
- and to construct $\hat{U}(t) = \hat{U}_0(t)\,\hat{U}_I(t)$.

There is no explicit dependence on $\hat{H}_0$ in either Eq. (80) or Eq. (83), which allows us to focus on the perturbation $\hat{V}_I(t)$.

■ Dyson Series

Integrating both sides of Eq. (83) in time

$$i\,\hat{U}_I(t) - i\,\hat{U}_I(0) = i\int_0^t d\,t'\,\partial_{t'}\,\hat{U}_I(t') = \int_0^t d\,t'\,\hat{V}_I(t')\,\hat{U}_I(t'), \tag{84}$$

plugging in the initial condition $\hat{U}_I(0) = \mathbb{1}$, we obtain an *integral equation*, equivalent to the *differential equation* Eq. (83),

$$\boxed{\hat{U}_I(t) = \mathbb{1} - i\int_0^t d\,t'\,\hat{V}_I(t')\,\hat{U}_I(t').} \tag{85}$$

This provides a *self-consistent* equation for $\hat{U}_I(t)$. If we take this expression and substitute $\hat{U}_I(t')$ under the integrand, we obtain

$$\hat{U}_I(t) = \mathbb{1} - i\int_0^t d\,t'\,\hat{V}_I(t') + (-i)^2\int_0^t d\,t'\,\hat{V}_I(t')\int_0^{t'} d\,t''\,\hat{V}_I(t'')\,\hat{U}_I(t''). \tag{86}$$

Iterating this procedure, we obtain a formal solution in power series of $\hat{V}_I$, known as the **Dyson series**:

$$\boxed{\hat{U}_I(t) = \sum_{k=0}^{\infty}(-i)^k\int_0^t d\,t_k\int_0^{t_k} d\,t_{k-1}\ldots\int_0^{t_2} d\,t_1\,\hat{V}_I(t_k)\,\hat{V}_I(t_{k-1})\ldots\hat{V}_I(t_1).} \tag{87}$$

where the $k = 0$ term corresponds to $\mathbb{1}$. The operators $\hat{V}_I(t)$ are organized in a *time-ordered* sequence with $0 \le t_1 \le \ldots \le t_{k-1} \le t_k \le t$. Rule: *earlier* operator on the *right*, *later* operator on the *left*.

■ Green's Function

Let us take a closer look at the product of $\hat{V}_I$ in the Dyson series. By definition $\hat{V}_I(t) = \hat{U}_0^\dagger(t)\,\hat{V}(t)\,\hat{U}_0(t)$,

$$\begin{aligned}&\hat{V}_I(t_k)\,\hat{V}_I(t_{k-1})\ldots\hat{V}_I(t_1)\\&=\hat{U}_0^\dagger(t_k)\,\hat{V}(t_k)\,\hat{U}_0(t_k)\,\hat{U}_0^\dagger(t_{k-1})\,\hat{V}(t_{k-1})\,\hat{U}_0(t_{k-1})\ldots\hat{U}_0^\dagger(t_1)\,\hat{V}(t_1)\,\hat{U}_0(t_1).\end{aligned}\tag{88}$$

This motivates us to introduce the unitary operator $\hat{G}_0(t, t')$, known as the **bare Green's function** or the **bare propagator**,

$$\boxed{\hat{G}_0(t, t') = \hat{U}_0(t)\,\hat{U}_0^\dagger(t') = \sum_n |n\rangle\, e^{-i\,E_n(t-t')}\,\langle n|,}\tag{89}$$

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

$$\begin{aligned}&\hat{V}_I(t_k)\,\hat{V}_I(t_{k-1})\ldots\hat{V}_I(t_1)\\&=\hat{U}_0^\dagger(t)\,\hat{G}_0(t, t_k)\,\hat{V}(t_k)\,\hat{G}_0(t_k, t_{k-1})\,\hat{V}(t_{k-1})\ldots\hat{G}_0(t_2, t_1)\,\hat{V}(t_1)\,\hat{G}_0(t_1, 0).\end{aligned}\tag{90}$$

The left most $\hat{U}_0^\dagger(t)$ can be canceled out if we consider the *time-evolution operator* in the *Schrödinger picture*, i.e. $\hat{U}(t) = \hat{U}_0(t)\,\hat{U}_I(t)$. According to Eq. (87) and Eq. (90), we have

$$\begin{aligned}\hat{U}(t) = \sum_{k=0}^{\infty}(-i)^k\int_0^t d\,t_k\\ \int_0^{t_k}d\,t_{k-1}\ldots\int_0^{t_2}d\,t_1\,\hat{G}_0(t, t_k)\,\hat{V}(t_k)\,\hat{G}_0(t_k, t_{k-1})\,\hat{V}(t_{k-1})\ldots\hat{G}_0(t_2, t_1)\,\hat{V}(t_1)\,\hat{G}_0(t_1, 0).\end{aligned}\tag{91}$$

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

$$\boxed{\hat{G}(t, t') = \hat{U}(t)\,\hat{U}^\dagger(t'),}\tag{92}$$

then Eq. (91) can be written as

$$\boxed{\begin{aligned}\hat{G}(t, t_0) = \sum_{k=0}^{\infty}(-i)^k\int_{t_0}^t d\,t_k\int_{t_0}^{t_k}d\,t_{k-1}\ldots\\ \int_{t_0}^{t_2}d\,t_1\,\hat{G}_0(t, t_k)\,\hat{V}(t_k)\,\hat{G}_0(t_k, t_{k-1})\,\hat{V}(t_{k-1})\ldots\hat{G}_0(t_2, t_1)\,\hat{V}(t_1)\,\hat{G}_0(t_1, t_0),\end{aligned}}\tag{93}$$

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

- $\hat{G}(t, t')$ can be calculated in *power series* of $\hat{V}(t)$ given $\hat{G}_0(t, t')$.
- Since $\hat{U}(t) = \hat{G}(t, 0)$, we also know how to calculate $\hat{U}(t)$ in power series of $\hat{V}(t)$.

So we have reached our goal!

Feynman Diagrams

However, the formula Eq. (93) 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,

$$t' \rightarrow t = \hat{G}_0(t, t'). \tag{94}$$

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

- A solid node: the perturbation operator at a particular time,

$$\bullet_t = -i\ \hat{V}(t). \tag{95}$$

- Connecting links and nodes: identifying the time together

$$\underset{t_0\quad t_1\quad t_2}{\rightarrow\bullet\rightarrow} = \hat{G}_0(t_2, t_1)\left(-i\ \hat{V}(t_1)\right)\hat{G}_0(t_1, t_0). \tag{96}$$

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*.

$$\begin{aligned}
&\rightarrow = \hat{G}_0(t, t_0),\\
&\rightarrow\bullet\rightarrow = (-i)\int_{t_0}^{t} d t_1\ \hat{G}_0(t, t_1)\ \hat{V}(t_1)\ \hat{G}_0(t_1, t_0),\\
&\rightarrow\bullet\rightarrow\bullet\rightarrow = (-i)^2\int_{t_0}^{t} d t_2\int_{t_0}^{t_2} d t_1\ \hat{G}_0(t, t_2)\ \hat{V}(t_2)\ \hat{G}_0(t_2, t_1)\ \hat{V}(t_1)\ \hat{G}_0(t_1, t_0),\\
&\ldots
\end{aligned} \tag{97}$$

- A directed *double-line* link: the *dressed* Green's function from one time to another,

$$\Rightarrow = \hat{G}(t, t_0). \tag{98}$$

With the diagrammatic representations in Eq. (97) and Eq. (98), we can rewrite Eq. (93) as

$$\boxed{\Rightarrow\ =\ \rightarrow\ +\ \rightarrow\bullet\rightarrow\ +\ \rightarrow\bullet\rightarrow\bullet\rightarrow\ +\ \ldots.} \tag{99}$$

- If we turn off the perturbation, i.e. $V(t) = 0$ or $\bullet = 0$, Eq. (99) reduces to

$$\Rightarrow\ =\ \rightarrow, \tag{100}$$

as all the diagrams containing the node will vanish. This simply restores $\hat{G}(t, t_0) = \hat{G}_0(t, t_0)$ 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, $\rightarrow\bullet\rightarrow$ 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** $|i\rangle$ at time t_0, at a subsequent time t, the initial state will evolve to $\hat{G}(t, t_0)\,|i\rangle$. Then the *probability* to find the system in a **final state** $|f\rangle$ should be given by

$$\boxed{P_{i\to f} = \left|\langle f|\, \hat{G}(t, t_0)\,|i\rangle\right|^2.} \tag{101}$$

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

To the 1st order in $\hat{V}(t)$, for $i \neq f$, the transition probability reads

$$\boxed{P_{i\to f}(t, t_0) = \left|\int_{t_0}^{t} d t_1 \,\langle f|\, \hat{V}(t_1)\,|i\rangle\, e^{i\,\omega_{fi}\,t_1}\right|^2,} \tag{102}$$

where $\omega_{fi} = E_f - E_i$ is the energy difference.

Exc 4 Prove Eq. (102)

Fermi's Golden Rule

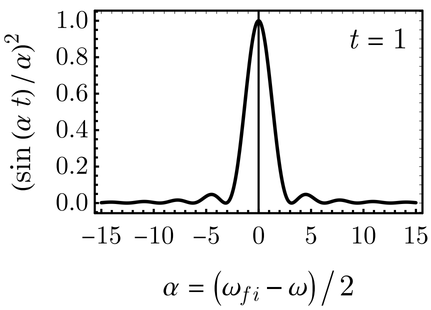
Consider a system prepared in an initial state $|i\rangle$ and perturbed by a periodic operator abruptly switched on at time $t_0 = 0$.

$$\hat{V}(t) = \begin{cases} \hat{V}\, e^{-i\,\omega\,t} & t > 0 \\ 0 & t \leq 0 \end{cases}. \tag{105}$$

What is the probability that, at some later time t, the system is found to be in the state $|f\rangle$. From Eq. (102), we have

$$\begin{aligned} P_{i\to f}(t) &= \left|\int_0^t d t_1 \,\langle f|\, \hat{V}\,|i\rangle\, e^{i(\omega_{fi}-\omega)\,t_1}\right|^2 \\ &= \left|\langle f|\, \hat{V}\,|i\rangle\, \frac{e^{i(\omega_{fi}-\omega)\,t} - 1}{i(\omega_{fi}-\omega)}\right|^2 \\ &= \left|\langle f|\, \hat{V}\,|i\rangle\right|^2 \left(\frac{\sin((\omega_{fi}-\omega)\,t/2)}{(\omega_{fi}-\omega)/2}\right)^2 \end{aligned} \tag{106}$$

Setting $\alpha = (\omega_{fi} - \omega)/2$, the transition probability takes the form of $(\sin(\alpha\,t)/\alpha)^2$ with a peak at $\alpha = 0$, with maximum value t^2 and width of order $1/t$ giving a total weight of order t.



In the **long-time limit** of $t \to \infty$,

$$\lim_{t\to\infty} \frac{1}{t}\left(\frac{\sin \alpha\, t}{\alpha}\right)^2 = \pi\, \delta(\alpha) = 2\,\pi\, \delta(2\,\alpha). \tag{107}$$

This leads to the following expression for the **transition rate**,

$$\boxed{W_{i\to f} = \lim_{t\to\infty} \frac{P_{i\to f}(t)}{t} = 2\,\pi \left|\langle f|\, \hat{V}\, |i\rangle\right|^2 \delta\big(E_f - E_i - \omega\big).} \tag{108}$$

This is known as **Fermi's golden rule**.

- One might worry that in the $t \to \infty$ limit, the transition probability is in fact diverging. How can we justify the use of perturbation theory? For a transition with $\omega_{fi} \neq \omega$, the "long time" limit is reached when $t \gg 1/(\omega_{fi} - \omega)$, a value that can still be very short compared with the mean transition time, which is set by the matrix element $1 \Big/ \left|\langle f|\, \hat{V}\, |i\rangle\right|$.
- Energy conservation is enforced in the long-time limit

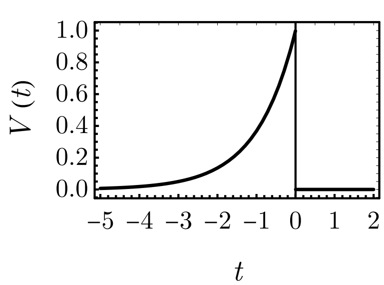
  $$E_f - E_i = \omega, \tag{109}$$

  such that transition occurs between levels in resonant with the the frequency of the perturbation.

Adiabatic Process

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

$$\hat{V}(t) = \begin{cases} \hat{V}\, e^{t/\tau} & t < 0 \\ 0 & t \geq 0 \end{cases}. \tag{110}$$

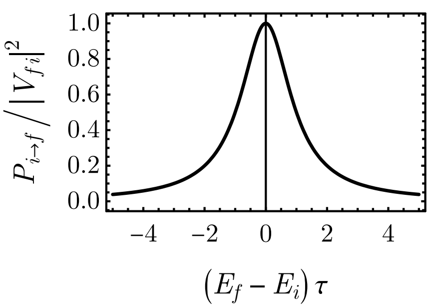


Suppose the system is prepared in state $|i\rangle$ in the infinite past ($t_0 \to -\infty$), what is the probability for the system to transit to the state $|f\rangle$ at $t = 0$?

According to Eq. (102),

$$\begin{aligned} P_{i\to f} &= \left| \int_{-\infty}^{0} d\, t_1 \langle f | \, \hat{V} \, | i \rangle \, e^{t_1/\tau} \, e^{i\,\omega_{fi}\, t_1} \right|^2 \\ &= \frac{\left| \langle f | \, \hat{V} \, | i \rangle \right|^2}{\left(E_f - E_i\right)^2 + 1 / \tau^2}. \end{aligned} \tag{111}$$

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 $\hat{H}_0$ eigenstate $|i\rangle$ simply evolves to the corresponding eigenstate of $\hat{H} = \hat{H}_0 + \hat{V}$, which is given by

$$|i(V)\rangle = |i\rangle + \sum_{m \neq i} |m\rangle \frac{V_{mi}}{E_i - E_m} + \ldots, \tag{112}$$

according to the *time-independent* perturbation, c.f. Eq. (34). Then the probability to observe the system in the state $|f\rangle$ will be

$$|\langle f \mid i(V) \rangle|^2 = \frac{\left| V_{fi} \right|^2}{\left(E_i - E_f\right)^2}, \tag{113}$$

which matches the result of time-dependent perturbation Eq. (111) in the limit of $\tau \to \infty$. Thus we have verified that the *time-dependen*t 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 τ can not be infinitely long. A finite τ sets an *energy resolution* τ^{-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.