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Quantum Mechanics 2

Ch. 5 Approximation Methods Lecture Notes

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Time Independent Perturbation Theory

For the unperturbed eigenstate equation

$$\mathcal{H}_0 |m^{(0)}\rangle = E_m^{(0)} |m^{(0)}\rangle$$

where $\sum |m^{(0)}\rangle\langle m^{(0)}| = \mathbb{1}$ is the completeness relation for a known complete basis of eigenstates of $\mathcal{H}_0$.

In the presence of a perturbation, the eigenvalue equation becomes :

$$(\mathcal{H}_0 + \lambda V)|m\rangle_\lambda = E_m^{(\lambda)} |m\rangle_\lambda$$

where $E_m^{(\lambda)}$ is the perturbed eigenvalue and $|m\rangle_\lambda$ the corresponding eigenstate. The energy shift of the m^{th} ket is :

$$\Delta_m = E_m^{(\lambda)} - E_m^{(0)}$$

and hence,

$$(\mathcal{H}_0 + \lambda V)|m\rangle = (E_m^{(0)} + \Delta_m)|m\rangle$$

$$\Rightarrow \qquad (E_m^{(0)} - \mathcal{H}_0)|m\rangle = (\lambda V - \Delta_m)|m\rangle \qquad (1)$$

Hence,

$$\langle m^{(0)}|(E_m^{(0)} - \mathcal{H}_0)|m\rangle = \langle m^{(0)}|(\lambda V - \Delta_m)|m\rangle = 0 \qquad (2)$$

Therefore we say

$$\Delta_m = \lambda \langle m^{(0)}|V|m\rangle \qquad (3)$$

Expanding $|m\rangle$ and Δ_m in powers of λ,

$$|m\rangle = \sum_{k=0}^{\infty} \lambda^k |m^{(k)}\rangle \quad , \quad \Delta_m = \sum_{k=1}^{\infty} \lambda^k \Delta_m^{(k)} \qquad (3.1)$$

$$\Delta_m^{(1)} = \langle m^{(0)}|V|m^{(0)}\rangle$$

$$\Rightarrow \qquad \Delta_m^{(2)} = \langle m^{(0)}|V|m^{(1)}\rangle$$

$$\vdots$$

$$\Delta_m^{(N)} = \langle m^{(0)}|V|m^{(N-1)}\rangle$$

Also, from (2), $[(\lambda V - \Delta_m)|m\rangle]$ is orthogonal to $|m^{(0)}\rangle$.

From this we can say

$$(\lambda V - \Delta_m)|m\rangle = \phi_m (\lambda V - \Delta_m)|m\rangle \tag{4}$$

Where

$$\varphi_m = \mathbb{1} - |m^{(0)}\rangle\langle m^{(0)}| = \sum_{k \neq m} |k^{(0)}\rangle\langle k^{(0)}|$$

is the complementory projection operator,

$$\frac{1}{E_m^{(0)} - \mathcal{H}_0}\phi_m = \sum_{k \neq m} \frac{1}{E_m^{(0)} - E_k^{(0)}} |k^{(0)}\rangle\langle k^{(0)}| \tag{5}$$

From (1),

$$|m\rangle = \frac{1}{E_m^{(0)} - \mathcal{H}_0}\varphi_m (\lambda V - \Delta_m)|m\rangle + C_m\lambda|m^{(0)}\rangle$$

With $C_m(\lambda) = \langle m^{(0)}|m\rangle$.

For convenience, we set $C_m(\lambda) = 1$ and normalize $|m\rangle$ at the end.

Defining

$$\frac{1}{E_m^{(0)} - \mathcal{H}_0}\varphi_m \longrightarrow \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0}$$

we have

$$|m\rangle = |m^{(0)}\rangle + \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0}(\lambda V - \Delta_m)|m\rangle \tag{6}$$

From (3),

$$|m^{(0)}\rangle + \lambda|m^{(1)}\rangle + \lambda^2|m^{(2)}\rangle + \dots = |m^{(0)}\rangle + \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0}(\lambda V - \lambda\Delta_m^{(1)} - \lambda^2\Delta_m^{(2)}) \times (|m^{(0)}\rangle + \lambda|m^{(1)}\rangle + \lambda^2|m^{(2)}\rangle + \dots)$$

We have:

$$|m^{(1)}\rangle = \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}} V|m^{(0)}\rangle$$

given that $\phi_m\Delta_m^{(1)}|m^{(0)}\rangle = \Delta_m^{(1)}\phi_m|m^{(0)}\rangle = 0$. Hence,

$$\Delta_m^{(2)} = \langle m^{(0)}|V|m^{(1)}\rangle = \langle m^{(0)}| V \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0} V|m^{(0)}\rangle$$

$$\Rightarrow \qquad \Delta_m^{(2)} = \sum_{k \neq m} \frac{|V_{km}|^2}{E_m^{(0)} - E_k^{(0)}} \tag{7}$$

With

$$V_{km} \equiv \langle k^{(0)} | V | m^{(0)} \rangle$$

Therefore,

$$|m^{(1)}\rangle = \sum_{k \neq m} \frac{V_{km}}{E_m^{(0)} - E_k^{(0)}} |k^{(0)}\rangle \qquad (8)$$

With this result, we get the second order connection in $|m^{(2)}\rangle$ from the λ^2 terms

$$|m^{(2)}\rangle = \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0} V \frac{\varphi_m}{E_m - \mathcal{H}_0} V |m^{(0)}\rangle - \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0} \langle m^{(0)} | V | m^{(0)} \rangle \frac{\varphi_m}{E_m^{(0)} - \mathcal{H}_0} V | m^{(0)} \rangle$$

We can re-write the above as

$$|m^{(2)}\rangle = \sum_{\substack{k \neq m \\ \ell \neq m}} |k^{(0)}\rangle \frac{V_{k\ell} V_{\ell m}}{(E_m^{(0)} - E_k^{(0)})(E_m^{(0)} - E_\ell^{(0)})} - \sum_{k \neq m} |k^{(0)}\rangle \frac{V_{mm} V_{km}}{(E_m^{(0)} - E_k^{(0)})^2}$$

and so on.

<u>Wave function</u> <u>Normalization</u>

The wavefunction normalization is defined as:

$$|\bar{m}\rangle = Z_m^{1/2} |m\rangle,$$

Such that $\langle \bar{m} | \bar{m} \rangle = 1$

$$Z_m^{-1/2} = \langle m^{(0)} | \bar{m} \rangle$$

Since $\langle m^{(0)} | m \rangle = 1$. Hence,

$$\langle \bar{m} | \bar{m} \rangle = Z_m \langle m | m \rangle = 1 \quad \therefore \quad Z_m^{-1} = \langle m | m \rangle$$

Where we can further say

$$Z_m^{-1} = (\langle m^{(0)}| + \lambda \langle m^{(1)} | + \dots)(|m^{(0)}\rangle + \lambda |m^{(1)}\rangle + \dots) = 1 + \lambda^2 \langle m^{(1)} | m^{(1)} \rangle + \mathcal{O}(\lambda^3)$$

$$= 1 + \lambda^2 \sum_{k \neq m} \frac{|V_{km}|^2}{(E_m^{(0)} - E_k^{(0)})^2} + \mathcal{O}(\lambda^3) \quad \therefore \quad Z_m = 1 - \lambda^2 \sum_{k \neq m} \frac{|V_{km}|^2}{(E_m^{(0)} - E_k^{(0)})^2}$$

<u>Degenerate</u> <u>Perturbation</u> <u>Theory</u>

If the spectrum of the unperturbed system is degenerate, we can change the $|m^{(0)}\rangle$ basis such that the matrix elements in the degenerate states is zero.

$$\frac{V_{mk}}{E_m^{(0)} - E_k^{(0)}} = 0 \quad \text{for} \quad E_m^{(0)} = E_k^{(0)}$$

For that, we can define a new set of eigenstates,

$$|\ell^{(0)}\rangle = \sum_{\mu \in \{a_m\}} \langle \mu^{(0)}|\ell^{(0)}\rangle |\mu^{(0)}\rangle$$

Defining

$$P_0 \equiv \sum_{\mu \in \{\alpha_m\}} |\mu^{(0)}\rangle\langle\mu^{(0)}|$$

as the projector in the degenerate space, and $P_1 = 1 - P_0$. The complementary projector is then

$$0 = (E - \mathcal{H}_0 - \lambda V)|\ell\rangle = (E - E_D^{(0)} - \lambda V) P_0|\ell\rangle + (E - \mathcal{H}_0 - \lambda V)P_1|\ell\rangle$$

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Degenerate Space:

$$|\ell^{(0)}\rangle = \sum_{\mu \in \alpha_m} \langle \mu^{(0)}|\ell^{(0)}\rangle |\mu^{(0)}\rangle$$

The projector is then

$$P_0 \equiv \sum_{\mu^0 \in \alpha_m} |\mu^{(0)}\rangle\langle\mu^{(0)}| \quad \text{(Projector in the degenerate space)}$$

We also have

$$P_1 \equiv \mathbb{1} - P_0 \quad \text{(Complementary projector)}$$

In general,

$$0 = (E_\ell - \mathcal{H}_0 - \lambda V)(P_0 + P_1)|\ell\rangle = (E_\ell - E_D^{(0)} - \lambda V)P_0|\ell\rangle + (E_\ell - \mathcal{H}_0 - \lambda V)P_1|\ell\rangle$$

Applying P_0 and P_1 on the left,

$$(E_\ell - E_D^{(0)} - \lambda P_0 V)P_0|\ell\rangle - \lambda P_0 V P_1|\ell\rangle = 0 \qquad (1)$$

and

$$-\lambda P_1 V P_0|\ell\rangle + (E_\ell - \mathcal{H}_0 - \lambda P_1 V)P_1|\ell\rangle = 0 \qquad (2)$$

Solving (2),

$$P_1|\ell\rangle = \frac{\lambda}{E_\ell - \mathcal{H}_0 - \lambda P_1 V P_1} P_1 V P_0 |\ell\rangle \qquad (3)$$

To first order in λ, $E_\ell \approx E_D^{(0)}$

$$P_1|\ell^{(1)}\rangle = \sum_{K \neq D} \frac{V_{K\ell}}{E_D^{(0)} - E_K^{(0)}} |K^{(0)}\rangle \qquad (4)$$

Replacing (4) into (1),

$$\left[E_\ell^{(1)} - E_D^{(0)} - \lambda P_0 V P_0\right] P_0 |\ell^{(1)}\rangle + \mathcal{O}(\lambda^2) = 0$$

To leading order in λ,

$$\text{Det}\left[\lambda \bar{V} - (E_\ell^{(1)} - E_D^{(0)})\right] = 0$$

Where $\bar{V} = P_0 V P_0$ is the projection of V inside the degenerate space.

<u>Example</u>: <u>Stark Effect</u>

The $n=2$ levels of the Hydrogen atom are degenerate in the absence of spin orbit and time. structure connections ($\ell = 0, 1$)

Applying a uniform electric field as a perturbation,

$$V = -e z |\vec{E}|$$

the matrix elements of V in the $|2\ell m\rangle$ basis are:

$$\langle 2\ell' m' | V | 2\ell m\rangle = -eE \underbrace{\langle 2\ell' m' | z | 2\ell m\rangle}_{\propto T_0^1}$$

From the Wigner Eckart theorem the only matrix elements are $m = m' = 0$ and $\ell = 1$, $\ell' = 0$ or $\ell = 0$, $\ell' = 1$ (Parity sum rule).

$$V = \begin{array}{cc} & \begin{array}{cccc} |200\rangle & |210\rangle & |211\rangle & |21\text{-}1\rangle \end{array} \\ & \begin{pmatrix} 0 & -|V_0| & 0 & 0 \\ -|V_0| & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \begin{array}{l} |200\rangle \\ |210\rangle \\ |211\rangle \\ |21\text{-}1\rangle \end{array}$$

To account for the effect of the perturbation in the degenerate space, we calculate the determinant,

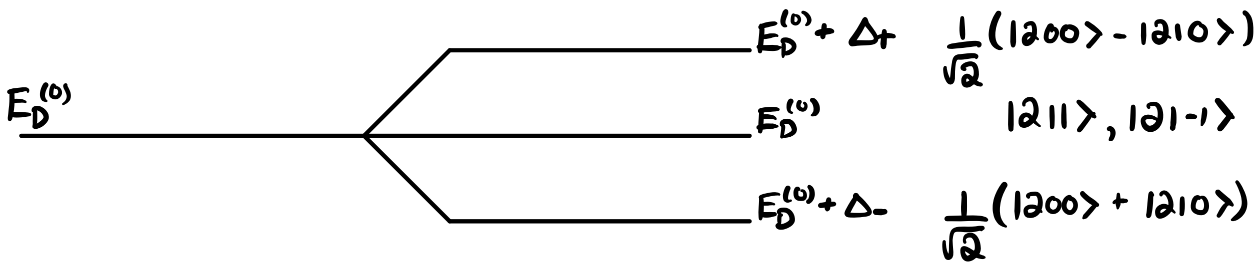
$$\det\left[E^{(1)} - E_D^{(0)} - P_0 V P_0\right] = 0$$

$$\Rightarrow \begin{vmatrix} \Delta & |V_0| & 0 & 0 \\ |V_0| & \Delta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix} = 0 \Rightarrow \Delta^2 \begin{vmatrix} \Delta & |V_0| \\ |V_0| & \Delta \end{vmatrix} = \Delta^2(\Delta^2 - V_0^2) \Rightarrow \Delta = 0,\ \Delta_\pm = \pm|V_0|$$

With eigenvectors:

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|200\rangle \mp |210\rangle) \qquad |211\rangle, |21{-1}\rangle$$

We can look at this pictorally as



Interaction Representation (Dirac)

In the Schrödinger picture,

$$\mathcal{H}_S = \mathcal{H}_0 + V$$

the time evolution of a ket $|\psi(t)\rangle$ is

$$i\hbar \partial_t |\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle = (\mathcal{H}_0 + V)|\psi(t)\rangle$$

In the interaction representation

$$|\psi_D(t)\rangle \equiv e^{\frac{i}{\hbar}\mathcal{H}_0 t}|\psi(t)\rangle$$

The time evolution of $|\psi_D(t)\rangle$ is:

$$i\hbar\partial_t|\psi_D(t)\rangle = -\mathcal{H}_0 e^{\frac{i}{\hbar}\mathcal{H}_0 t}|\psi(t)\rangle + e^{\frac{i}{\hbar}\mathcal{H}_0 t}(\mathcal{H}_0 + V)|\psi(t)\rangle = e^{i/\hbar\,\mathcal{H}_0 t}\, V e^{-i/\hbar\,\mathcal{H}_0 t}|\psi_D(t)\rangle$$

We can then move forward and say

$$i\hbar\partial_t|\psi_D(t)\rangle = V_D(t)|\psi_D(t)\rangle$$

we can then finally say

$$V_D(t) = e^{i/\hbar\,\mathcal{H}_0 t}\, V e^{-i/\hbar\,\mathcal{H}_0 t}$$

Is the interaction in the Dirac representation, the operators transform in the same way.

Elaborating some more we can say

$$\Omega_D(t) = e^{i/\hbar \mathcal{H}_0 t}\,\Omega(t)\,e^{-i/\hbar \mathcal{H}_0 t}$$

The dynamical equation is:

$$i\hbar \frac{d}{dt}\Omega_D(t) = -\mathcal{H}_0 e^{i/\hbar \mathcal{H}_0 t}\Omega(t)e^{-i/\hbar \mathcal{H}_0 t} + e^{i/\hbar \mathcal{H}_0 t}\Omega(t)\mathcal{H}_0 e^{-i/\hbar \mathcal{H}_0 t}$$
$$+ i\hbar e^{i/\hbar \mathcal{H}_0 t}\partial_t \Omega(t) e^{-i/\hbar \mathcal{H}_0 t} = [\Omega_D(t), \mathcal{H}_0] + i\hbar \frac{\partial}{\partial t}\Omega_D(t)$$

where

$$\frac{\partial}{\partial t}\Omega_D(t) \equiv e^{i/\hbar \mathcal{H}_0 t}\frac{\partial}{\partial t}\Omega(t)\,e^{-i/\hbar \mathcal{H}_0 t}$$

Therefore

$$i\hbar \frac{\partial}{\partial t}|\psi_D(t)\rangle = V_D(t)|\psi_D(t)\rangle$$

$\Rightarrow$ The kets evolve with the potential $V_D(t)$, whereas the operators evolve with $\mathcal{H}_0$.

From now on we are ommitting the "D" index from the kets.

<u>Definition</u>: <u>Time</u> <u>Evolution</u> <u>Operator</u>

$$\mathcal{U}(t,t_0)|\psi(t_0)\rangle = |\psi(t)\rangle$$

$\Rightarrow$ $$i\hbar\,\partial_t\, \mathcal{U}(t,t_0)|\psi(t_0)\rangle = V_D(t)\,\mathcal{U}(t,t_0)|\psi(t)\rangle$$

We can in turn say

$$i\hbar \partial_t \mathcal{U}(t,t_0) = V_D(t)\,\mathcal{U}(t,t_0) \tag{5}$$

With the boundary condition

$$\mathcal{U}(t,t) = \mathbb{1} \tag{6}$$

The $\mathcal{U}$ operator has the properties

$$\mathcal{U}(t,t_0)\,\mathcal{U}(t_0,t') = \mathcal{U}(t,t') \quad \& \quad \mathcal{U}(t,t_0) = \mathcal{U}^*(t_0,t) = \mathcal{U}^{-1}(t_0,t)$$

The solution of the differential equation (5) & (6) has the form

$$\mathcal{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, V_D(t')\,\mathcal{U}(t',t_0)$$

Which can be solved iteratively.

The Dirac notation is useful when the interaction is localized in time and the asymptotic states at $t=\pm\infty$ are free.

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The time evolution operator is

$$\mathcal{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} V_D(t')\mathcal{U}(t',t_0)\, dt' \qquad (1)$$

Where

$$|\psi(t)\rangle = \mathcal{U}(t,t_0)\,|\psi(t)\rangle \qquad \text{(time evolution operator)}$$

Let us define an initial state

$$|\varphi_i\rangle \equiv \lim_{t\to\infty} |\psi(t)\rangle$$

Which is a superposition of eigenstates of $\mathcal{H}_0$, and a final state

$$\lim_{t\to\infty} |\psi(t)\rangle$$

Which evolves freely.

The probability amplitude of scattering between an initial $|\varphi_i\rangle$ and a final state $|\varphi_f\rangle$ is

$$\lim_{t_2\to\infty} \langle\varphi_f|\psi(t_2)\rangle = \lim_{t_2\to\infty}\ \lim_{t_1\to-\infty} \langle\varphi_f|\mathcal{U}(t,t_0)|\varphi_i\rangle$$

This limit defines the scattering matrix (S matrix), with matrix elements

$$S_{fi} = \lim_{t_2\to\infty}\ \lim_{t_1\to\infty} \langle\varphi_f|\mathcal{U}(t_2,t_1)|\varphi_i\rangle$$

With a short notation of

$$S \equiv \mathcal{U}(\infty,-\infty)$$

Solving equation (1), the lowest order approximation is:

$$\mathcal{U}(t,t_0) \simeq 1$$

Replacing in (1),

$$\mathcal{U}(t,t_0) \approx \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} V_D(t')\,dt'$$

In higher order

$$\mathcal{U}(t,t_0) = \mathbb{1} + \left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} V_D(t_1)\,dt_1 + \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t} V_D(t_1)\,dt_1\int_{t_0}^{t_1} V_D(t_2)\,dt_2 + \cdots\cdots$$

where we can write

$$I_n = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \, V_D(t_1)V_D(t_2)\cdots V_D(t_n)$$

$$= \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, \Theta(t_1-t_2)\Theta(t_2-t_3)\cdots\Theta(t_{n-1}-t_n)V_D(t_1)V_D(t_2)\cdots V_D(t_n)$$

Doing some simplifying we can say

$$I_n \equiv \frac{1}{n!}\int_{t_0}^{t} dt_1 \cdots dt_n \times T\left[V_D(t_1)\cdots V_D(t_n)\right]$$

where T is the time ordering operator

$$T\left[V_D(t_1)V_D(t_2)\cdots V_D(t_n)\right] \equiv \sum_{\sigma} \Theta(t_{\sigma(1)}-t_{\sigma(2)})\cdots\Theta(t_{\sigma(n-1)}-t_{\sigma(n)})V_D(t_{\sigma(1)})\cdots V_D(t_{\sigma(n)})$$

This then becomes

$$T\left[V_D(t_1)V_D(t_2)\cdots V_D(t_n)\right] = V_D(t_i)\cdots V_D(t_j)\cdots V_D(t_k)$$

where $t_i > \cdots > t_j > \cdots > t_k$. For equal times

$$T\left[V_D(t)V_D(t)\right] = V_D(t)V_D(t)$$

In general,

$$\mathcal{U}(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1\cdots dt_n \, T\left[V_D(t_1)\cdots V_D(t_n)\right]$$

$$= T\left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n\left(\int_{t_0}^{t} V_D(t')\,dt'\right)^n\right] = T\left[\exp\left(\frac{-i}{\hbar}\int_{t_0}^{t} V_D(t')\,dt'\right)\right]$$

<u>Time Dependent Perturbation Theory</u>

Let us consider a perturbation that is turned on and off adibatically, such that

$$\mathcal{H}(t=\pm\infty) = \mathcal{H}_0$$

and at $t=0$,

$$\mathcal{H} = \mathcal{H}_0 + \lambda V_0.$$

If $|l_m^{(0)}\rangle$ are eigenfunctions of $\mathcal{H}_0$, then

$$\mathcal{H}_0 |l_m^0\rangle = E_m^0 |l_m^0\rangle$$

In the same way, we define $|l,m\rangle$ as the eigenstates of $\mathcal{H}$, such that

$$\mathcal{H}|l,m\rangle = E_m |l,m\rangle$$

In perturbation theory we assume that the perturbed and unperturbed states are adiabatically connected to each other in such way that

i)
$$\lim_{\lambda\to 0} |l,m\rangle = |l_m^{(0)}\rangle$$

ii)
$$\lim_{\lambda\to 0} E_m = E_m^{(0)}$$

The transition probability measures the likelihood that the system will evolve from a given initial state before the perturbation was turned on to some final state after the perturbation is turned off

Transition Probability

The time of the initial state in the interaction picture is:

$$|i,t\rangle = \mathcal{U}(t,t_0)|i\rangle = \sum_m C_m(t)|m\rangle$$

Where

$$C_m(t) = \langle m|\mathcal{U}(t,t_0)|i\rangle$$

The transition probability $|i\rangle \to |m\rangle$ between two eigenstates of $\mathcal{H}_0$ are:

$$|C_m(t)|^2 = |\langle m|\mathcal{U}(t,t_0)|i\rangle|^2$$

Since:

$$\mathcal{U}(t,t_0) = \sum_{m=0}^{\infty} \left(\frac{-i}{\hbar}\right)^m \lambda^m \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{m-1}} V(t_1)\cdots V(t_m)\, dt_m$$

Is the time evolution operator, then expanding $\mathcal{U}$ in powers of λ

$$C_m^{(0)}(t) = \delta_{mi} \quad , \quad C_m^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^{t} \langle m|V_D(t')|i\rangle = \frac{-i}{\hbar}\int_{t_0}^{t} e^{i\omega_{mi}} V_{mi}(t')\, dt'$$

where $\exp(i(E_\mu - E_i)t/\hbar) \equiv \exp(i\omega_{\mu i})$. In the same way

$$C_\mu^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_l \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, e^{i\omega_{\mu l}t} V_{\mu l}(t_1)\, V_{li}(t_2)\, e^{i\omega_{li}t}$$

Such that $(\mu \neq i)$

$$|C_\mu(t)|^2 = |C_\mu^{(1)} + C_\mu^{(2)} + \ldots|^2$$

Example:

The potential is defined as

$$V(t) = \begin{cases} 0 & \text{for } t < 0 \\ V & \text{for } t > 0 \end{cases}$$

The transition amplitude between $|i\rangle \to |\mu\rangle$ is

$$C_\mu^{(0)} = \delta_{\mu i} \quad , \quad C_\mu^{(1)}(t) = \frac{-i}{\hbar} V_{\mu i} \int_0^t \exp(i\omega_{\mu i}t')\, dt' = \frac{V_{\mu i}}{E_\mu - E_i}\left(1 - e^{i\omega_{\mu i}t}\right)$$

$$= \frac{V_{\mu i}}{E_\mu - E_i}\, 2i\, e^{\frac{i\omega_{\mu i}t}{2}} \sin\left(\frac{\omega_{\mu i}t}{2}\right)$$

Hence, for $m \neq i$,

$$|C_\mu(t)|^2 = \frac{4|V_{\mu i}|^2}{(E_\mu - E_i)^2} \sin^2\left(\frac{\omega_{\mu i}t}{2}\right)$$

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Adiabatic Switch

Let's assume that our potential is slowly turned on from the initial state at $t_0 = -\infty$,

$$V(t) = Ve^{\eta t} \qquad t < 0$$

With $\eta \to 0_+$ at the end, and $V = \text{const}$. For $\eta \neq i$

$$C_\eta^{(0)}(t) = 0 \quad , \quad C_\eta^{(1)} = -\frac{i\lambda}{\hbar} V_{\eta i} \int_{-\infty}^{t} dt'\, e^{\eta t'} e^{i\omega_{\eta i}t} = -\frac{i\lambda}{\hbar} V_{\eta i} \frac{e^{(\eta + i\omega_{\eta i})t}}{\eta + i\omega_{\eta i}}$$

Therefore to lowest order in perturbation, the probability of transition is:

$$|C_\eta(t)|^2 = \frac{|V_{\eta i}|^2}{\hbar^2} \frac{e^{2\eta t}}{\eta^2 + \omega_{\eta i}^2} \lambda^2 \Rightarrow \frac{d}{dt}|C_\eta(t)|^2 = 2\frac{|V_{\eta i}|^2}{\hbar^2}\left(\frac{\eta e^{2\eta t}}{\eta^2 + \omega_{\eta i}^2}\right)$$

For $\eta \to 0$,

$$\lim_{\eta \to 0} \frac{\eta}{\eta^2 + \omega_{\eta i}^2} = \pi \delta(\omega_{\eta i}) = \pi \hbar \, \delta(E_\eta - E_i)$$

The transition rate is :

$$W_{i \to \eta} \equiv \frac{d}{dt} | C_n(t) |^2 = \frac{2\pi}{\hbar} |V_{\eta i}|^2 \delta(E_\eta - E_i) \quad w/ \quad i \neq \eta$$

Which gives the Fermi Golden rule.

For an harmonic potential,

$$V(t) = v e^{i\omega t} + v^{\dagger} e^{-i\omega t}$$

we make the replacements

$$\omega_{\eta i} = \omega_{\eta i} \pm \omega$$

and the Fermi golden rule becomes

$$W_{i \to \eta} = \frac{2\pi \lambda^2}{\hbar} \left[|V_{\eta i}|^2 \delta(E_\eta - E_i + \omega) + |V_{\eta i}^{\dagger}|^2 \delta(E_\eta - E_i - \omega) \right]$$

For $i = \eta$, potential (1) gives

$$c_i^{(0)} = 1 \quad , \quad c_i^{(1)} = \frac{-i}{\hbar} \lambda \int_{-\infty}^{t} dt' \, V_{ii} \, e^{\eta t'} = \frac{-i\lambda}{\hbar \eta} V_{11} \, e^{\eta t}$$

We can then say $c_i^{(2)}$ is

$$c_i^{(2)} = \left(\frac{-i}{\hbar}\right)^2 \sum_{\eta} |V_{\eta i}|^2 \int_{-\infty}^{t} dt' \, e^{i\omega_{i\eta} t + \eta t} \times \int_{-\infty}^{t'} dt'' \, e^{i\omega_{\eta i} t'' + \eta t''}$$

$$= \left(\frac{-i\lambda}{\hbar}\right)^2 |V_{11}|^2 \frac{e^{2\eta t}}{2\eta^2} + \left(\frac{-i\lambda}{\hbar}\right)^2 \lambda^2 \sum_{\eta \neq i} \frac{e^{2\eta t}}{2\eta (E_i - E_\eta + i\hbar\eta)}$$

In second order,

$$c_1(t) \cong 1 - \frac{i\lambda}{\hbar \eta} V_{ii} e^{\eta t} + \left(\frac{-i\lambda}{\hbar}\right)^2 |V_{ii}| \frac{e^{2\eta t}}{2\eta^2} + \left(\frac{-i}{\hbar}\right) \lambda^2 \sum_{\eta \neq i} \frac{|V_{\eta i}|^2 e^{2\eta t}}{2\eta (E_i - E_\eta + i\hbar\eta)} + \mathcal{O}(\lambda^3)$$

Defining $\dot{c}_i(t) \equiv \frac{d}{dt} c_i(t)$, for $\eta \to 0$

$$\dot{c}_1(t) = \frac{-i\lambda}{\hbar} V_{11} e^{\eta t} + \left(\frac{-i\lambda}{\hbar}\right)^2 |V_{11}|^2 \frac{e^{2\eta t}}{\eta} - \frac{i}{\hbar} \lambda^2 \sum_{\eta \neq i} \frac{|V_{\eta i}|^2 e^{2\eta t}}{(E_i - E_\eta + i\hbar\eta)}$$

should be μ

not same as η in exp!!

Since we know $(1/(1+x)) \approx 1-x$, then

$$\frac{\dot{c}_i}{c_i} \sim \frac{-i}{\hbar} V_{ii}\lambda - \frac{i}{\hbar}\lambda^2 \sum_{m\neq i} \frac{|V_{mi}|^2}{E_i - E_m + i\hbar\eta} \equiv \Delta_i^{(1)} + \Delta_i^{(2)}$$

where we define $\Delta_i = \Delta_i^{(1)}\lambda + \Delta_i^{(2)}\lambda^2 + \dots\dots$

The solution of the differential equation is:

$$\frac{\dot{c}_i(t)}{c_i(t)} = \frac{-i}{\hbar}\Delta_i \qquad (2)$$

Where we can then say

$$c_i(t) = e^{-i\Delta_i t/\hbar} \qquad (3)$$

Where $\Delta_i^{(1)} = V_{ii}$ and

$$\Delta_i^{(2)} = \sum_{m\neq i} \frac{|V_{mi}|^2}{E_i - E_m + i\hbar\eta}$$

Since

$$\frac{1}{a + i0_+} = P\frac{1}{a} - i\pi\delta(a)$$

where P is the principal part.

$$\Rightarrow \quad \Delta_i^{(2)} = P\sum_{m\neq i} \frac{|V_{mi}|^2}{E_i - E_m} - \underbrace{i\pi \sum_{m\neq i} |V_{mi}|^2 \delta(E_i - E_m)}_{Im(\Delta_i)}$$

Where

$$\frac{P_i}{\hbar} \equiv -\frac{2}{\hbar} Im(\Delta_i) = \sum_{m\neq i} W_{i\to m}$$

defines the decay rate, which is set by Fermi's Golden rule. From (3)

$$|c_i(t)|^2 = e^{2Im(\Delta_i)t/\hbar} = e^{-P_i t/\hbar}$$

Which gives the rate at which the initial state fades away due to transitions to other states.