University of Strasbourg

Tutorial III

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Reminder

EXERCISE I : Introduction to time-dependent perturbation theory

We assume a physical system described by a time-independent Hamiltonian H_0 with eigenstates $|\varphi_n\rangle$ and eigenvalues E_n. The system is then subjected to a perturbation $V(t)$ for $0 \leq t \leq \tau$. The wavefunction describing the state of the system at time t can be written as a function of the eigenstates of H_0 according to :

$$|\Psi(t)\rangle = \sum_n b_n(t) e^{-iE_n t/\hbar} |\varphi_n\rangle$$

this ansatz is sometimes called the "method of variation of constants" introduced by Dirac for time-dependent perturbation theory.

1. Write the system of differential equations for the coefficients $b_n(t)$.

Let's write,

$$c_n(t) = b_n(t) e^{-iE_n t/\hbar}$$

So, we can write,

$$|\Psi(t)\rangle = \sum_k c_k(t) |\varphi_k\rangle$$

We can write time-dependent Schrödinger's equation,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$$
$$i\hbar \sum_k \frac{\mathrm{d}}{\mathrm{d}t} c_k(t) |\varphi_k\rangle = \sum_k c_k(t) H(t) |\varphi_k\rangle$$

We can perform a pre-multiplication by $\langle\varphi_n|$, and then we know that $\langle\varphi_n|\varphi_k\rangle = \delta_{nk}$,

$$\begin{aligned}
\langle\varphi_n| i\hbar \sum_k \frac{\mathrm{d}}{\mathrm{d}t} c_k(t) |\varphi_k\rangle &= \langle\varphi_n| \sum_k c_k(t) H(t) |\varphi_k\rangle \\
\frac{\mathrm{d}}{\mathrm{d}t} c_n(t) &= -\frac{i}{\hbar} \sum_k c_k(t) \langle\varphi_n| H(t) |\varphi_k\rangle \\
&= -\frac{i}{\hbar} \sum_k c_k(t) \left[\langle\varphi_n| H_0 |\varphi_k\rangle + \langle\varphi_n| V |\varphi_k\rangle\right] \\
&= -\frac{i}{\hbar} E_n c_n(t) - \frac{i}{\hbar} \sum_k c_k(t) \langle\varphi_n| V |\varphi_k\rangle
\end{aligned}$$

And now we can perform the substitution from $c_n(t)$ to $b_n(t)$,
Left-hand-side gives us

$$\frac{\mathrm{d}}{\mathrm{d}t} c_n(t) = \frac{\mathrm{d}}{\mathrm{d}t}(b_n(t)) e^{-iE_n t/\hbar} - \frac{i}{\hbar} E_n b_n(t) e^{-iE_n t/\hbar}$$

right-hand-side gives us

$$-\frac{i}{\hbar}E_n c_n(t) - \frac{i}{\hbar}\sum_k c_k(t)\langle\varphi_n| V |\varphi_k\rangle = -\frac{i}{\hbar}E_n b_n(t)e^{-iE_nt/\hbar} - \frac{i}{\hbar}\sum_k b_k(t)e^{-iE_kt/\hbar}\langle\varphi_n| V |\varphi_k\rangle$$

Meaning we get,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}b_n(t) &= -\frac{i}{\hbar}\sum_k b_k(t)e^{-i(E_k-E_n)t/\hbar}\langle\varphi_n| V |\varphi_k\rangle \\ &= -\frac{i}{\hbar}\sum_k b_k(t)e^{i\omega_{nk}t}V_{nk}(t) \qquad\qquad \omega_{nk} = \frac{E_n - E_k}{\hbar}\end{aligned}$$

Where $V_{nk}(t)$ is a matrix element.

2. Describe the time evolution of the system for $t < 0$.

For $t < 0$,

$$V(t < 0) = 0$$

Using the equation for $\dot{b}_n(t)$, it gives us,

$$\frac{\mathrm{d}}{\mathrm{d}t}b_n(t) = 0$$

meaning $b_n(t)$ for $t < 0$ is a constant.

3. For $0 \leq t \leq \tau$, express the solution for $b_n(t)$ using first order time-dependent perturbation theory (by iteration).

$$b_n(t) = b_n(0) + \text{perturbation}$$

$$\begin{aligned}\int_0^t \frac{\mathrm{d}}{\mathrm{d}t'}b_n(t')\mathrm{d}t' &= -\frac{i}{\hbar}\sum_k \int_0^t b_k(t')e^{i\omega_{nk}t'}V_{nk}(t')\mathrm{d}t' \\ b_n(t) - b_n(0) &= -\frac{i}{\hbar}\sum_k \int_0^t b_k(t')e^{i\omega_{nk}t'}V_{nk}(t')\mathrm{d}t' \\ b_n(t) &= b_n(0) - \frac{i}{\hbar}\sum_k \int_0^t b_k(t')e^{i\omega_{nk}t'}V_{nk}(t')\mathrm{d}t'\end{aligned}$$

We can now iteratively plug this expression of $b_n(t)$ in the $b_k(t')$ expression, meaning at first order it will be

$$b_n(t) = b_n(0) - \frac{i}{\hbar}\sum_k \int_0^t \mathrm{d}t_1 V_{nk}(t_1)e^{i\omega_{nk}t_1}b_k(0)$$

> At second order it would be,
>
> $$b_n(t) = b_n(0) - \frac{1}{\hbar^2}\sum_k \sum_l \int_0^{t_1}\int_0^{t_2} \mathrm{d}t_1 \mathrm{d}t_2 V_{nk}(t_1)V_{nl}(t_2)e^{i(\omega_{nk}t_1 - \omega_{nl}t_2)}b_l(0)$$

4. Write an expression for the probability $\mathcal{P}^{(1)}_{i\to f}$ for the system to be in the state $|\varphi_f\rangle$ after the perturbation ($t \geq \tau$) if it was initially in the state $|\varphi_i\rangle$ for $t < 0$ ($i \neq f$).

$$\mathcal{P}_{i\to f} = |\langle\varphi_f|\Psi(t\geq\tau)\rangle|^2$$

$$\dot{b}_n = -\frac{i}{\hbar}\sum_k b_k(t)e^{i\omega_{nk}t}\langle\varphi_n|V|\varphi_k\rangle$$

if φ_k is an eigenstate of V,

$$\langle\varphi_n|V|\varphi_k\rangle = V\delta_{nk}$$

Meaning,

$$\dot{b}_n = -\frac{i}{\hbar}b_n(t)e^{i\omega_{nn}t}V = -\frac{i}{\hbar}b_n(t)V$$

Meaning,

$$b_n(t) = b_n(0)e^{-iVt/\hbar}$$

And so,

$$|\Psi(t\geq\tau\rangle = \sum_n b_n(\tau)e^{-iE_nt/\hbar}|\varphi_n\rangle$$

And we know that

$$b_n(\tau) \approx b_n(0) - \frac{i}{\hbar}\sum_k \int_0^{\tau} \mathrm{d}t_1 V_{nk}(t_1)e^{i\omega_{nk}t_1}b_k(0)$$

$$
\begin{aligned}
\mathcal{P}_{i\to f} &= |\langle\varphi_f|\Psi(t\geq\tau)\rangle|^2 \\
&= \left|\sum_n b_n(\tau)e^{-iE_nt/\hbar}\langle\varphi_f|\varphi_n\rangle\right|^2 \\
&= \left|\sum_n b_n(\tau)e^{-iE_nt/\hbar}\delta_{fn}\right|^2 \\
&\approx \left|\sum_n b_n(0)e^{-iE_nt/\hbar}\delta_{fn} - \frac{i}{\hbar}e^{-iE_nt/\hbar}\sum_k\int_0^\tau \mathrm{d}t_1 V_{nk}(t_1)e^{i\omega_{nk}t_1}b_k(0)\delta_{fn}\right|^2 \\
&= \frac{1}{\hbar^2}\left|\sum_k\int_0^\tau \mathrm{d}t_1 V_{fk}e^{i\omega_{fk}t_1}\delta_{ki}\right|^2 \\
&= \frac{1}{\hbar^2}\left|\int_0^\tau \mathrm{d}tV_{fi}(t)e^{i\omega_{fi}t}\right|^2
\end{aligned}
$$

Remark : it does looks like a Fourrier transform of the perturbation.

EXERCISE II : A sudden perturbation with constant amplitude

As a specific example we now consider a constant amplitude perturbation $V(t) = V_0$ that is suddenly applied at $t = 0$ and switched off again at $t = \tau$.

1. Calculate the probability $\mathcal{P}^{(1)}_{i\to f}$ as a function of $\omega_{fi} = (E_f - E_i)/\hbar$. We assume that $V_{if} = V_{fi} = \langle\varphi_f| V_0 |\varphi_i\rangle \neq 0$ and $V_{ff} = V_{ii} = 0$.

$$\begin{aligned}
\mathcal{P}_{i\to f} &= \frac{|V_{fi}|^2}{\hbar^2}\left|\frac{1}{i\omega_{fi}}\left(e^{i\omega_{fi}\tau} - 1\right)\right|^2 \\
&= \frac{|V_{fi}|^2}{\hbar^2}\left|\frac{2e^{i\omega_{fi}\tau/2}}{\omega_{fi}}\frac{e^{i\omega_{fi}\tau/2} - e^{-i\omega_{fi}\tau/2}}{2i}\right|^2 \\
&= \frac{\tau^2|V_{fi}|^2}{\hbar^2}\left|\frac{\sin(\omega_{fi}\tau/2)}{\omega_{fi}\tau/2}\right|^2 \\
&= \frac{\tau^2|V_{fi}|^2}{\hbar^2}\left|\mathrm{sinc}(\omega_{fi}\tau/2)\right|^2
\end{aligned}$$

> We know that the sinc is the Fourier transform of the rectangular pulse.

2. Suppose $H_0' = H_0 + V_0$ (independent of time) and we denote $|\varphi_n'\rangle$ and E_n' the eigenstates and eigenenergies of H_0'. For $0 \leq t \leq \tau$, the state vector $|\Psi(t)\rangle$ of the system can be decomposed in this basis according to :

$$|\Psi(t)\rangle = \sum_n b_n'(t)e^{-iE_n't/\hbar}|\varphi_n'\rangle$$

   (a) Show that the coefficients $b_n'(t)$ are time-independent (for $0 \leq t < \tau$). Express these coefficients as a function of $|\Psi(t = 0\rangle$.

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = -\frac{i}{\hbar}H_0'|\Psi(t)\rangle$$

$$\sum_n\left[\frac{\mathrm{d}}{\mathrm{d}t}b_n'(t)\right]e^{-iE_n't/\hbar}|\varphi_n'\rangle - \cancel{\frac{i}{\hbar}E_n'b_n'(t)e^{-iE_n't/\hbar}}|\varphi_n'\rangle = \cancel{-\frac{i}{\hbar}\sum_n E_n'b_n'(t)e^{-iE_n't/\hbar}}|\varphi_n'\rangle$$

Meaning that,

$$\sum_n\left[\frac{\mathrm{d}}{\mathrm{d}t}b_n'(t)\right]e^{-iE_n't/\hbar}|\varphi_n'\rangle = 0$$

Which is true for

$$\frac{\mathrm{d}}{\mathrm{d}t} b'_n(t) = 0$$

$$|\Psi(t=0)\rangle = \sum_k b'_k |\varphi'_k\rangle = \sum_k b_k |\varphi_k\rangle$$

This is equivalent to a change of basis. We can apply $\langle \varphi'_n|$,

$$\langle \varphi'_n| \sum_k b'_k |\varphi'_k\rangle = \langle \varphi'_n| \sum_k b_k |\varphi_k\rangle$$

Which we can write,

$$b'_n = \sum_k \langle \varphi'_n|\varphi_k\rangle b_k = \sum_k c_{nk} b_k$$

This does represent the state in a different basis.
Because b'_n is time-independant, we can write

$$|\varphi_i\rangle \rightarrow \sum_n b'_n(0) e^{-iE'_n t/\hbar} |\varphi'_n\rangle$$

(b) Express the probability $\mathcal{P}_{i\rightarrow f}$ of finding the system in the state $|\varphi_f\rangle$ for $t \geq \tau$, in terms of $|\varphi_i\rangle$, $|\varphi_f\rangle$, $|\varphi'_n\rangle$ and E'_n. Assume the system was in the state $|\varphi_i\rangle$, $(i \neq f)$ for $t \leq 0$.

$$\begin{aligned}
\mathcal{P}_{i\rightarrow f} &= |\, \langle \varphi_f|\Psi(t)\rangle \,|^2 \\
&= |\, \langle \varphi_f| \sum_n b'_n(0) e^{-iE'_n t/\hbar} |\varphi'_n\rangle \,|^2 \\
&= |\, \langle \varphi_f| \sum_n \sum_k \langle \varphi'_n|\varphi_k\rangle \, \delta_{ki} e^{-iE'_n t/\hbar} |\varphi'_n\rangle \,|^2 \\
&= |\, \langle \varphi_f| \sum_n \langle \varphi'_n|\varphi_i\rangle \, e^{-iE'_n t/\hbar} |\varphi'_n\rangle \,|^2 \\
&= |\, \sum_n \langle \varphi'_n|\varphi_i\rangle \, e^{-iE'_n t/\hbar} \langle \varphi_f|\varphi'_n\rangle \,|^2
\end{aligned}$$

We do not have an expression for the $|\varphi'_n\rangle$ so we can't perform the calculation now.

3. Evaluate $\mathcal{P}_{i\rightarrow f}$ using first order time-independent perturbation theory. Start by writing down the eigenstates and eigenvalues of H'_0 assuming that the matrix elements of V_0 are small compared to the (non-degenerate) energy level differences of H0. How does your result compare with the result obtained in question II.1 ?

$$\begin{cases} |\varphi'_n\rangle = |\varphi_n\rangle + \sum_{k\neq n} \frac{V_{kn}}{E_n - E_k} |\varphi_k\rangle \\ E'_n = E_n + V_{nn} \end{cases}$$

Where

$$V_{kn} = \langle\varphi_k| V_0 |\varphi_n\rangle \qquad\qquad V_{nn} = \text{ diaognal element}$$

$$\begin{aligned} \langle\varphi_f|\varphi'_n\rangle &= \delta_{fn} + \sum_{k\neq n} \frac{V_{kn}}{E_n - E_k} \langle\varphi_f|\varphi_k\rangle \\ &= \delta_{fn} + \sum_{k} \frac{V_{kn}}{E_n - E_k} \langle\varphi_f|\varphi_k\rangle - \frac{V_{fn}}{E_n - E_f}\delta_{fn} \\ &= \delta_{fn} + \frac{V_{fn}}{E_n - E_f}(1 - \delta_{fn}) \end{aligned}$$

$$\langle\varphi_i|\varphi'_n\rangle = \delta_{in} + \frac{V_{in}}{E_n - E_i}(1 - \delta_{in})$$

Meaning,

$$\begin{aligned} \mathcal{P}_{i\to f} &= \left| \sum_n \left[\delta_{in} + \frac{V_{in}}{E_n - E_i}(1 - \delta_{in})\right] e^{-i(E_n + V_{nn})t/\hbar} \left[\delta_{fn} + \frac{V_{fn}}{E_n - E_f}(1 - \delta_{fn})\right] \right|^2 \\ &= \left| \frac{V_{fi}}{E_i - E_f} e^{-iE_i t/\hbar} + \frac{V_{if}}{E_f - E_i} e^{-iE_f t/\hbar} \right|^2 \\ &= \frac{|V_{fi}|^2}{\hbar^2\omega_{fi}^2} \left| e^{-i\omega_{fi}\tau} - 1 \right|^2 \end{aligned}$$

It is the same result as we found before.