CAS PY 452 — Quantum Physics II

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Discussion Notes

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Time-dependent perturbation theory for the two-level system

Problem: Consider a two-level system with energy eigenstates $|0\rangle, |1\rangle$ and energy eigenvalues E_0, E_1, respectively. That is, it's Hamiltonian in the basis $|0\rangle, |1\rangle$ is,

$$\hat{H} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix} = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}. \tag{1}$$

The system is then subject to a time-dependent perturbation $\hat{V}(t)$ which couples the unperturbed states:

$$\hat{V}(t) = \left(\begin{cases} \frac{1}{2}\alpha\eta e^{\eta t} & t < 0 \\ \frac{1}{2}\alpha\eta e^{-\eta t} & t \geq 0 \end{cases} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\alpha}{2}\eta e^{-\eta|t|} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2}$$

Assume that $\eta > 0$, $\alpha \ll \hbar$ and $\hbar\eta \ll E_0, E_1$ so that we can apply first-order time-dependent perturbation theory. Given that the system is in state $|0\rangle$ at $t \to -\infty$, find the probability that the state will be in state $|1\rangle$ at $t \to \infty$ using time-dependent perturbation theory. Analyze these results as $\eta \to 0$ and $\eta \to \infty$. What type of perturbation does $\hat{V}(t)$ look like as $\eta \to \infty$?

Reminder: In time-dependent perturbation theory, we attempt to solve $i\hbar\partial_t |\psi(t)\rangle = (\hat{H} + \hat{V}(t))|\psi(t)\rangle$. We find a systematic method by moving to the interaction representation:

$$|\psi(t)\rangle_I = e^{i\hat{H}t/\hbar}|\psi(t)\rangle, \qquad \hat{V}_I(t) = e^{i\hat{H}t/\hbar}\hat{V}(t)e^{-i\hat{H}t/\hbar}, \tag{3}$$

so the TDSE becomes,

$$i\hbar\partial_t |\psi(t)\rangle_I = \hat{V}_I(t)|\psi(t)\rangle_I. \tag{4}$$

If we write $|\psi(t)\rangle_I = \sum_n c_n(t)|n\rangle$, where $|n\rangle$ is the nth stationary state, then $\langle m| i\hbar\partial_t |\psi(t)\rangle_I = \langle m| \hat{V}_I(t)|\psi(t)\rangle_I$, becomes,

$$i\hbar\partial_t c_m(t) = \sum_n V_{mn}(t)e^{i\omega_{mn}t}c_n(t), \tag{5}$$

where $V_{mn}(t) = \langle m|\hat{V}(t)|n\rangle$ and $\omega_{mn} = (E_m - E_n)/\hbar$. If a system begins in state $|i\rangle$, we can form a perturbative approximation by solving iteratively. This approximation gives $c_n(t) = c_n^{(0)} + c_n^{(1)} + c_n^{(2)} + \cdots$, where,

$$c_n^{(0)}(t) = \delta_{ni}, \tag{6}$$

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt' e^{i\omega_{ni}t'}V_{ni}(t') \tag{7}$$

$$c_n^{(2)}(t) = \left(-\frac{i}{\hbar}\right)\sum_m \int_{t_0}^{t} dt' e^{i\omega_{nm}t'}V_{nm}(t')\left(-\frac{i}{\hbar}\right)\int_{t_0}^{t'} dt'' e^{i\omega_{mi}t''}V_{mi}(t''). \tag{8}$$

This is called the Dyson series.[1]

[1] The Dyson series is related to Feynman diagrams. If you're curious about this connection, consider reading these notes (`https://web2.ph.utexas.edu/~vadim/Classes/2022f/dyson.pdf`) from a class at UT Austin.

Solution: To find the transition probability, we compute the integral:

$$\begin{aligned}
c_1^{(1)}(t\to\infty) &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' e^{i\omega_{10}t'}\,\langle 1|\hat{V}(t)|0\rangle = -\frac{i\alpha\eta}{2\hbar}\int_{-\infty}^{\infty} dt' e^{i\omega_{10}t'} e^{-\eta|t|} \\
&= -\frac{i\alpha\eta}{2\hbar}\left(\int_{-\infty}^{0} dt e^{(i\omega_{10}+\eta t)t} + \int_{0}^{\infty} dt e^{(i\omega_{10}-\eta t)t}\right) = -\frac{i\alpha\eta}{2\hbar}\left(\int_{0}^{\infty} dt e^{-(i\omega_{10}+\eta)t} + \int_{0}^{\infty} dt e^{-(-i\omega_{10}+\eta)t}\right) \\
&= -\frac{i\alpha\eta}{2\hbar}\left(\frac{1}{\eta+i\omega_{10}} + \frac{1}{\eta-i\omega_{10}}\right) = -\frac{i\alpha}{\hbar}\left(\frac{\eta^2}{\eta^2+\omega_{10}^2}\right).
\end{aligned} \tag{9}$$

This means the probability of transition is,

$$p_{0\to 1} = |c_1^{(1)}(t\to\infty)|^2 = \frac{\alpha^2}{\hbar^2}\left(\frac{1}{1+(\omega_{10}/\eta)^2}\right)^2. \tag{10}$$

We can see that as $\eta \to 0$, the probability of transition goes to zero: $c_1^{(1)}(t\to\infty)\to 0$. When $\eta\to\infty$, $\alpha\eta e^{-\eta|t|}/2 \to \alpha\delta(t)$, so we have a delta-function perturbation at $t = 0$. The integral $\alpha\int_{-\infty}^{\infty}\delta(t)e^{i\omega_{10}t}dt = \alpha$ is consistent with $c_1^{(1)}(t\to\infty) = -i\alpha/\hbar$ as $\eta\to\infty$.

Time-dependent perturbation theory for the quantum harmonic oscillator

Problem: Consider the quantum harmonic oscillator:

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2, \tag{11}$$

which is being perturbed by a linear electric field $\mathcal{E}(t)$ that is turned on and then turned back off:

$$\hat{V}(t) = q\mathcal{E}(t)\hat{x}, \tag{12}$$

where,

$$\mathcal{E}(t) = \frac{\mathcal{E}_0}{\tau\sqrt{\pi}}e^{-(t/\tau)^2}, \tag{13}$$

where $q\mathcal{E}_0 \ll \sqrt{m\omega\hbar}$. If the system starts in the ground state $|0\rangle$ at $t \to -\infty$, find the probability the state will be in an excited state $|n\rangle$ using first-order time-dependent perturbation theory. Examine the behavior when $\tau \ll 1/\omega$ and $\tau \gg 1/\omega$.

Solution: As usual, we introduce ladder operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p}), \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p}), \tag{14}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}), \qquad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a}), \tag{15}$$

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \qquad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \qquad \hat{a}\,|0\rangle = 0. \tag{16}$$

This makes the relevant matrix elements of $\hat{V}(t)$:

$$\begin{aligned} V_{mn}(t) &= \langle m|\hat{V}(t)|n\rangle = q\mathcal{E}(t)\,\langle m|\,\hat{x}\,|n\rangle = q\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\,\langle m|\,(\hat{a}^\dagger + \hat{a})\,|n\rangle = q\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\,\langle m|\,(\sqrt{n+1}\,|n+1\rangle + \sqrt{n}\,|n-1\rangle) \\ &= q\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1}\right). \end{aligned} \tag{17}$$

For the ground state,

$$V_{n0}(t) = q\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{1}\delta_{n1} + \sqrt{0}\delta_{n,-1}\right) = q\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\delta_{n1}. \tag{18}$$

Note that $\omega_{0n} = \omega n$, where ω is the frequency of the oscillator. We are left to compute the integral,

$$\begin{aligned} c_n^{(1)}(t\to\infty) &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt e^{i\omega_{n0}t}V_{n0}(t) = -iq\delta_{n1}\sqrt{\frac{1}{2m\omega\hbar}}\int_{-\infty}^{\infty} dt e^{in\omega t}\mathcal{E}(t) \\ &= -i\delta_{n1}\frac{q\mathcal{E}_0}{\tau}\sqrt{\frac{1}{2\pi m\omega\hbar}}\int_{-\infty}^{\infty} dt e^{in\omega t - t^2/\tau^2} = -i\delta_{n1}\frac{q\mathcal{E}_0}{\tau}\sqrt{\frac{1}{2\pi m\omega\hbar}}e^{-n^2\tau^2\omega^2/4}\int_{-\infty}^{\infty} dt e^{-(t/\tau - in\tau\omega/2)^2} \qquad (19) \\ &= -i\delta_{n1}\frac{q\mathcal{E}_0}{\tau}\sqrt{\frac{1}{2\pi m\omega\hbar}}e^{-n^2\tau^2\omega^2/4}\int_{-\infty}^{\infty} dt e^{-(t/\tau)^2} = -i\delta_{n1}q\mathcal{E}_0\sqrt{\frac{1}{2m\omega\hbar}}e^{-n^2\tau^2\omega^2/4}. \qquad (20) \end{aligned}$$

This means that the probability of transition to state $|1\rangle$ is,

$$p_{0\to1} = |c_1^{(1)}(t\to\infty)|^2 = \frac{q^2\mathcal{E}_0^2}{2m\omega\hbar}e^{-\tau^2\omega^2/2}, \tag{21}$$

and the probability of transition to any other excited state is 0. When $\tau \to 0$ (i.e., $\tau \ll 1/\omega$), $V(t)$ becomes a delta perturbation and $c_1^{(1)}(t\to\infty) = -iq\mathcal{E}_0/\sqrt{2m\omega\hbar}$ which is consistent with the integral $-(i\mathcal{E}_0 q/\sqrt{2m\omega\hbar})\int_{-\infty}^{\infty} dt e^{i\omega t}\delta(t)$. When $\tau \gg 1/\omega$, we see $|\mathcal{E}'(t)| = \frac{2|t|\mathcal{E}_0 e^{-\frac{t^2}{\tau^2}}}{\sqrt{\pi}\tau^3} \le \sqrt{\frac{2}{e\pi}}\frac{\mathcal{E}_0}{\tau^2}$, so the perturbation is varied very slowly. In this case, $c_1^{(1)}(t\to\infty) = 0$, so there is no change made after a long time. This can be seen as a case of the adiabatic theorem.

Appendix: How do we know what functions have δ-distribution behavior as a limit?

The δ-distribution function is defined so that $\delta(x) = 0$ for all $x \neq 0$, and for all functions g,

$$\int_{-\infty}^{\infty} \delta(x)g(x)dx = g(0). \tag{22}$$

Equivalently,

$$\int_{-\varepsilon}^{\varepsilon} \delta(x)g(x)dx = g(0), \tag{23}$$

for all $\varepsilon > 0$. If f_η is a collection of functions parameterized by η, f_η converges to a δ distribution function as $\eta \to a$ if,

$$\lim_{\eta\to a} \int_{-\infty}^{\infty} g(x)f_\eta(x)dx = g(0), \tag{24}$$

for all functions g. In most cases, $a = \infty$ or 0. Here are two nice ways to check this behavior:

Taylor series: If we play fast-and-loose mathematically, we can say that all functions g of interest can be written as,

$$g(x) = g(0) + \sum_{n=1}^{\infty} g^{(n)}(0)\frac{x^n}{n!}, \tag{25}$$

in some neighborhood of $x = 0$. Therefore, if we can show,

$$\lim_{\eta\to a} f_\eta(x) = 0, \qquad x \neq 0 \tag{26}$$

$$\lim_{\eta\to a} \int_{-\infty}^{\infty} f_\eta(x)dx = 1 \tag{27}$$

$$\lim_{\eta\to a} \int_{-\infty}^{\infty} f_\eta(x)x^n dx = 0, \qquad n \geq 1 \tag{28}$$

then,

$$\lim_{\eta\to a} \int_{-\infty}^{\infty} g(x)f_\eta(x) = g(0) \lim_{\eta\to a} \int_{-\infty}^{\infty} f_\eta(x)dx + \sum_{n=1}^{\infty} \frac{g^n(0)}{n!} \lim_{\eta\to a} \int_{-\infty}^{\infty} f_\eta(x)x^n dx = g(0). \tag{29}$$

Fourier transform: Consider that,

$$\int_{-\infty}^{\infty} e^{-2\pi ikx}\delta(x)dx = 1, \tag{30}$$

which says that the Fourier transform of the δ distribution function is 1, so by the Fourier inversion theorem,

$$\delta(x) = \int_{-\infty}^{\infty} e^{2\pi ikx}dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx}dk. \tag{31}$$

Therefore, f_η converges to a δ distribution function as $\eta \to a$ if,

$$\lim_{\eta\to a} \mathcal{F}[f_\eta](k) = \lim_{\eta\to a} \int_{-\infty}^{\infty} e^{ikx}f_\eta(k)dk = \frac{1}{\sqrt{2\pi}}. \tag{32}$$