Time-dependent Perturbation Theory [1]

A.V. Camposano[2]

21 March 2018

[1] extended notes from the class of Dr. Bernido

[2] University of San Carlos, Philippines

an extended lecture notes from my graduate class on Quantum Mechanics, added some topics not covered during the class. Detailed calculations are added for future reference and to make the life of the reader easier. Life is too short.

In quantum mechanics, **perturbation theory** is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one. The idea is to start with a simple system for which a mathematical solution is known, and add an additional "perturbing" Hamiltonian representing a weak disturbance to the system. If the disturbance is not too large, the various physical quantities associated with the perturbed system (e.g. its energy levels and eigenstates) can be expressed as "corrections" to those of the simple system. [3]

[3] copied from wiki, I like this definition of perturbation theory, it emphasizes the idea that complicated systems can be studied by examining the simpler ones

Hamiltonian Approximations

Perturbation theory is an important tool for describing real quantum systems, as it turns out to be very difficult to find exact solutions to the Schrodinger equation for Hamiltonians of even moderate complexity. The Hamiltonians to which we know exact solutions, such as the hydrogen atom, the quantum harmonic oscillator and the particle in a box, are too idealized to adequately describe most systems. Using perturbation theory, we can use the known solutions of these simple Hamiltonians to generate solutions for a range of more complicated systems.[4]

[4] copied from wiki again!

Time-dependent Perturbation Theory

Consider the Hamiltonian,

$$H = H_0 + H_1 \tag{1}$$

where the perturbing Hamiltonian is explicitly time-dependent,

$$H_1 = H_1(t)$$

e.g. $H_1 = cos(\omega t), H_1 = \exp(-i\omega t)$

From the Schrodinger equation, [5]

[5] $\Psi(\mathbf{r}, t)$ is the wavefunction of the unperturbed Hamilton H_0

$$H\Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} \tag{2}$$

$$\underbrace{(H_0 + H_1)}_{H} \Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} \tag{3}$$

We worked with the unperturbed solutions of the time-independent eigenvalue equation.

$$H_0 \Psi_n^0 = E_n \Psi_n^0 \tag{4}$$

where ψ_n^0 form a complete orthonormal sets!

We let $\Psi(t)$ be the state of the perturbed system at time t. We can make the expansion: [6]

[6] $\Psi(t)$ is wavefunction of the perturbed Hamiltion $H = H_0 + H_1$

$$\Psi(t) = \sum_n c_n(t) \exp(-i\omega_n t) \Psi_n^0 \tag{5}$$

where $\omega_n = E_n/\hbar$ (an energy eigenvalue of the unperturbed Hamiltonian H_0), and $|c_n(t)|^2$ is the probability of finding the system in the state $|n\rangle$ at time t.

The time-dependent wavefunction obeys the Schrodinger equation,

$$\underbrace{(H_0 + H_1)}_{H} \Psi(t) = i\hbar \frac{\partial \Psi(t)}{\partial t} \tag{6}$$

We then substitute equation (5) to equation (6),

$$\begin{aligned} &(H_0 + H_1) \sum c_n(t) \exp(-i\omega_n t) |\Psi_n^0\rangle \\ &\qquad = i\hbar \frac{\partial}{\partial t} (\sum c_n(t) \exp(-i\omega_n t) |\Psi_n^0\rangle) \\ &H_0 \sum c_n(t) \exp(-i\omega_n t) |\Psi_n^0\rangle + H_1 \sum c_n(t) \exp(-i\omega_n t) |\Psi_n^0\rangle \\ &\quad = i\hbar \sum_n \left((-i\omega_n t) \exp(-i\omega_n t) |\Psi_n^0\rangle + \frac{dc_n}{dt} \exp(-i\omega_n t) |\Psi_n^0\rangle \right) \end{aligned}$$

We then multiply the results with $\langle \Psi_m^0 |$ (on the left side), [7]

[7] please note we've shifted to Dirac notation

$$\begin{aligned} &\langle \Psi_m^0 | H_0 \sum c_n(t) \exp(-i\omega_n t) |\Psi_n^0\rangle + \langle \Psi_m^0 | H_1 \sum c_n(t) \exp(-i\omega_n t) |\Psi_n^0\rangle \\ &= i\hbar \sum_n \left((-i\omega_n t) \exp(-i\omega_n t) \langle \Psi_m^0 | \Psi_n^0 \rangle + \frac{dc_n}{dt} \exp(-i\omega_n t) \langle \Psi_m^0 | \Psi_n^0 \rangle \right) \\ &\sum c_n(t) \exp(-i\omega_n t) \langle \Psi_m^0 | H_0 |\Psi_n^0\rangle + \sum c_n(t) \exp(-i\omega_n t) \langle \Psi_m^0 | H_1 |\Psi_n^0\rangle \\ &= i\hbar \sum_n \left((-i\omega_n t) \exp(-i\omega_n t) \langle \Psi_m^0 | \Psi_n^0 \rangle + \frac{dc_n}{dt} \exp(-i\omega_n t) \langle \Psi_m^0 | \Psi_n^0 \rangle \right) \end{aligned}$$

To simplify the equation, we use equation (4), the definition of ω_n and the orthonormality of the wavefunctions, [8]

[8] use orthonormality equation: $\langle \Psi_m^0 | \Psi_n^0 \rangle = \delta_{mn}$

$$\cancel{\sum E_n c_n(t) \exp(-i\omega_n t)\delta_{mn}} + \sum c_n(t) \exp(-i\omega_n t) \langle \Psi_m^0 | H_1 | \Psi_n^0 \rangle = \cancel{\sum E_n c_n(t) \exp(-i\omega_n t)\delta_{mn}} + i\hbar \sum \frac{dc_n}{dt} \exp(-i\omega_n t)\delta_{mn}$$

$$\sum c_n(t) \exp(-i\omega_n t) \langle \Psi_m^0 | H_1 | \Psi_n^0 \rangle = i\hbar \sum \frac{dc_n}{dt} \exp(-i\omega_n t)\delta_{mn}$$

Manipulating the equation above, we have:

$$\frac{dc_m}{dt} = -\frac{i}{\hbar} \sum_n c_n(t) \langle m | H_1 | n \rangle \exp(-i(\omega_m - \omega_n)t) \tag{7}$$

This exact results enables us to determine the time dependence of the coefficients $c_n(t)$ and the wavefunctions.

$$c_m(t) = -\frac{i}{\hbar} \sum_n \int_0^t c_n(t) \langle m | H_1 | n \rangle e^{(-i(\omega_m - \omega_n)t)} dt \tag{8}$$

Several important results follows from this, such as **Fermi's Golden Rule** which relates the rate of transitions between quantum states to the density of states at particular energies.

If H_1 is small,

$$\frac{dc_n}{dt} << 1$$

at $t = 0$, at state $|n\rangle$, we have $c_n(0) = 1$ and for all $c_m = 0; m \neq n$. We can rewrite equation (8) as,

$$c_m(t) \approx -\frac{i}{\hbar} \int_0^t \langle m | H_1 | n \rangle e^{-i(\omega_m - \omega_n)t} \underbrace{c_n(0)}_{1} dt \tag{9}$$

Special Cases

CASE 1: Sudden approximation

Suppose the perturbation has acted for finite duration, $t = 0$ to $t = \tau$.

The amplitude for $t > \tau$ may be obtained by extending the domains of integration.

$$c_m(t) \approx -\frac{i}{\hbar} \int_{-\infty}^{+\infty} \langle m | H_1 | n \rangle e^{-i(\omega_m - \omega_n)t} dt \tag{10}$$

This integral is just a Fourier transform integral:

$$\mathcal{F}[\, \langle m | H_1 | n \rangle \,]$$

CASE 2: Adiabatic approximation

Suppose $\langle m | H_1 | n \rangle$ is 'approximately' constant for $t > 0$, then we have,

$$c_m(t) \approx -\frac{i}{\hbar} \langle m | H_1 | n \rangle \int_0^t e^{-i(\omega_m - \omega_n)t} dt \tag{11}$$

$$\begin{aligned} c_m(t) &\approx -\frac{i}{\hbar}\langle m|H_1|n\rangle \int_0^t e^{-i(\omega_m-\omega_n)t}dt \\ &\approx -\frac{i}{\hbar}\langle m|H_1|n\rangle \frac{e^{-i(\omega_m-\omega_n)t}}{-i(\omega_m-\omega_n)} \\ &\approx \langle m|H_1|n\rangle \frac{e^{-i(\omega_m-\omega_n)t}}{(E_m-E_n)} \end{aligned}$$

The probability of reaching the state $|m\rangle$:

$$\begin{aligned} P_m(t) &= |c_m(t)|^2 \\ &= |\langle m|H_1|n\rangle|^2 \left[\frac{e^{i\omega_{mn}t}-1}{(E_m-E_n)}\right]\left[\frac{e^{-i\omega_{mn}t}-1}{(E_m-E_n)}\right] \\ &= |\langle m|H_1|n\rangle|^2 \left[\frac{sin^2(\frac{1}{2}\omega_{mn}t)}{\frac{1}{2}\hbar\omega_{mn})}\right] \end{aligned}$$

Dependence on the frequency is given by,

$$P(\omega_{mn}) = \frac{4sin^2(\frac{1}{2}\omega_{mn}t)}{\omega_{mn}^2} \tag{12}$$

As $t \to \infty$ while $\omega \to 0$, $P(\omega_{mn})$ becomes more peaked at $w_{mn} = 0$. The limiting behavior is,

$$lim_{t\to\infty}\left[\frac{sin^2(\frac{1}{2}\omega_{mn}t)}{\frac{1}{2}\omega_{mn}^2)}\right] = 2\pi\hbar t\delta(E_m-E_n) \tag{13}$$

Thus,

$$P(\omega_{mn}) = \frac{2\pi}{\hbar}|\langle m|H_1|n\rangle|^2\delta(E_m-E_n)t \tag{14}$$

The transition rate is then given by:

$$\Gamma_{n\to m} = \frac{dP(\omega_{mn})}{dt} = \frac{2\pi}{\hbar}|\langle m|H_1|n\rangle|^2\delta(E_m-E_n) \tag{15}$$

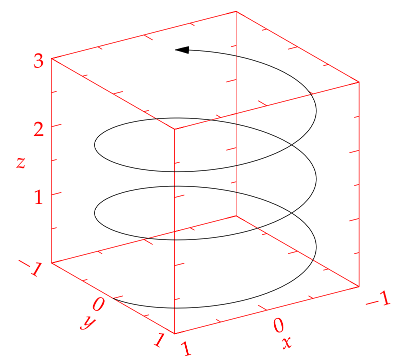

Figure 1: This is a margin figure. The helix is defined by $x = \cos(2\pi z)$, $y = \sin(2\pi z)$, and $z = [0, 2.7]$. The figure was drawn using Asymptote (`http://asymptote.sf.net/`).