

Physics 137B Lecture 5

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These are notes taken from lectures on Quantum Mechanics delivered by Professor Raúl A. Briceño for UC Berkeley's Physics 137B class in the Spring 2024 semester.

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1 January 26 - Perturbation Theory continued...

Last time, we left off while trying to extract $|n^{(0)}\rangle$.

To extract $|n^{(0)}\rangle$, we make use of the fact that $\{|l^{(0)}\rangle\}$ is orthonormal. Act using another stationary state $|l^{(0)}\rangle$ where $l \neq n$.

$$\begin{aligned} \Rightarrow \sum_{k \neq n} c_{nk}^{(1)} (E_k^{(0)} - E_n^{(0)}) \underbrace{\langle l^{(0)} | k^{(0)} \rangle}_{\delta_{lk}} + \langle l^{(0)} | \hat{H}' | n^{(0)} \rangle - E_n^{(1)} \underbrace{\langle l^{(0)} | n^{(0)} \rangle}_0 &= 0 \\ \Rightarrow (E_l^{(0)} - E_n^{(0)}) c_{nl}^{(1)} = -\langle l^{(0)} | \hat{H}' | n^{(0)} \rangle \end{aligned}$$

Again, for emphasis, we are currently dealing with a special case: **Non-degenerate Perturbation Theory** wherein $E_n^{(0)} = E_l^{(0)}$ iff $n = l$. So, rearranging the equation, we finally get

$$c_{nl}^{(1)} = \frac{\langle l^{(0)} | \hat{H}' | n^{(0)} \rangle}{(E_n^{(0)} - E_l^{(0)})}$$

This gives us the first order correction for the state i.e.

$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{\langle l^{(0)} | \hat{H}' | n^{(0)} \rangle}{(E_n^{(0)} - E_l^{(0)})} |k^{(0)}\rangle$$

Before moving on to second-order PT and degenerate PT, let's see some nice examples.

1.1 Example: 1D Infinite Square Well with a δ -potential

The known potential is

$$\hat{H}_0 = \frac{\hat{P}^2}{2m} + V_0(x); \quad V_0(x) = \begin{cases} 0 & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ \infty & \text{otherwise} \end{cases}$$

and we have $\hat{H}' = \alpha \delta(x)$

The goal is to find $E_n^{(1)}$ and $|n^{(1)}\rangle$. We follow the standard procedure:

1. Find $|n^{(0)}\rangle$ and $E_n^{(0)}$
2. Use $E_n^{(1)} = \langle n^{(0)} | \hat{H}' | n^{(0)} \rangle$
3. Use $|n^{(1)}\rangle = \sum_{k \neq n} \frac{\langle k^{(0)} | \hat{H}' | n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})} |k^{(0)}\rangle$
4. "think" : do your solutions make sense?

Step 1: To get the *unperturbed* eigenstates and eigenenergies, we set up the TISE:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n^{(0)}(x) = E_n^{(0)} \psi_n^{(0)}$$

and impose the *boundary conditions*.

Doing so, we obtain

$$\psi_n^{(0)}(x) = \begin{cases} \frac{2}{L} \cos\left(\frac{n\pi x}{L}\right) & n = 2n' + 1 \\ \frac{2}{L} \sin\left(\frac{n\pi x}{L}\right) & n = 2n' \end{cases}$$

and

$$E_n^{(0)} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n^2$$

Step 2:

The energy correction is

$$\begin{aligned} E_n^{(1)} &= \langle n^{(1)} | \hat{H}' | n^{(0)} \rangle \\ &= \int dx \langle n^{(0)} | x \rangle \langle x | \hat{H}' | x' \rangle \langle x' | n^{(0)} \rangle \\ &= \int dx \psi(x)^* \alpha \delta(x) \psi(x) \\ &= \alpha |\psi_n(0)|^2 \\ &= \begin{cases} \frac{\alpha^2}{L} & n = \text{odd} \\ 0 & n = \text{even} \end{cases} \end{aligned}$$

So, the overall eigenenergy is given by

$$E_n^{(0)} = \left(\frac{\pi\hbar}{L}\right)^2 \frac{n^2}{2m} + \begin{cases} \alpha \frac{L}{2} & \text{iff } n = \text{odd} \\ 0 & \text{iff } n = \text{even} \end{cases}$$

Note that this makes sense if and only if

$$\begin{aligned} \alpha \frac{L}{2} &< \left(\frac{\pi\hbar}{L}\right)^2 \frac{n^2}{2m} \\ \implies \alpha &< \frac{2}{L} \left(\frac{\pi\hbar}{L}\right)^2 \frac{n^2}{2m} \end{aligned}$$

So, if experimental values of α tell us that the 1st order correction is bigger than the 0-order correction, we most definitely have a problem and our system may be *non-perturbative*.

Step 3:

The eigenstate correction is

$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{\langle k^{(0)} | \hat{H}' | n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})} |k^{(0)}\rangle$$