

Physics 137B Lecture 6

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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 29 - Second order and Degenerate Perturbation Theory

Recap

- We've been trying to develop **Perturbation Theory** in order to solve problems with Hamiltonians of the form:

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{known sol.}} + \lambda \hat{H}'$$

- We did so by assuming we could parametrize the Eigen-states and Eigen-energies as functions of some small parameter λ

$$|n^{(\lambda)}\rangle = \sum_j \lambda^j |n^{(j)}\rangle$$

$$E_n^{(\lambda)} = \sum_j \lambda^j E_n^{(j)}$$

(If this cannot be done, then the system we are studying is non-perturbative).

- So far, we've found the **Leading order corrections** for **non-degenerate systems** to be

$$E_n^{(1)} = \langle n^{(0)} | \hat{H}' | n^{(0)} \rangle$$

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

1.1 Second Order Perturbation Theory

In second order PT, we also grab the λ^2 coefficients:

$$\mathcal{O}(\lambda^2) : \lambda^2 \left[(\hat{H}_0 - E_n^{(0)}) |n^{(2)}\rangle + (\hat{H}' - E_n^{(1)}) |n^{(1)}\rangle - E_n^{(2)} |n^{(0)}\rangle \right] = 0$$

Once again, we act on the equation with $|n^{(0)}\rangle$:

$$\begin{aligned} \implies & \underbrace{\langle n^{(0)} | (\hat{H}_0 - E_n^{(0)}) | n^{(2)} \rangle}_{=0} + \langle n^{(0)} | \hat{H}' | n^{(1)} \rangle - E_n^{(1)} \underbrace{\langle n^{(0)} | n^{(1)} \rangle}_{=0} = 0 \\ \implies & \boxed{E_n^{(2)} = \langle n^{(0)} | \hat{H}' | n^{(1)} \rangle} \end{aligned}$$

Using the expression we get for $|n^{(1)}\rangle$:

$$\implies E_n^{(2)} = \sum_{n \neq k} \frac{\langle n^{(0)} | \hat{H}' | k^{(0)} \rangle \langle k^{(0)} | \hat{H}' | n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$$

[Write about the possible interpretation as the state being propagated and then returning back above by watching recording]

Interesting fact: When we were finding the states using 1st order PT we wrote

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle$$

and said we wouldn't worry about normalization, but in fact they are normalized up to second order corrections:

$$\begin{aligned} \Rightarrow \langle n|n\rangle &= \langle n^{(0)}|n^{(0)}\rangle + \lambda \left(\underbrace{\langle n^{(0)}|n^{(1)}\rangle}_0 + \underbrace{\langle n^{(1)}|n^{(0)}\rangle}_0 \right) + \mathcal{O}(\lambda^2) \\ &= 1 + \mathcal{O}(\lambda^2) \end{aligned}$$

This came about because we had $|n^{(1)}\rangle = \sim_{k \neq n} (stuff)$ summing over states k not equal to n .

Now, what about $|n^{(2)}\rangle$? We have two choices:

Choice #1: Once again sum over states $k \neq n$

$$|n^{(2)}\rangle = \sum_{k \neq n} |k^{(0)}\rangle c_{nk}^{(2)}$$

In this case, we yet again get normalized states

Choice #2: Include $k = n$

$$|n^{(2)}\rangle = \sum_k |k^{(0)}\rangle c_{nk}^{(2)}$$

In this case, we can determine $c_{nn}^{(2)}$ from the normalization condition

$$\langle n|n\rangle = 1 + \mathcal{O}(\lambda^3)$$

For now, we will follow Choice #1. So, let

$$|n^{(2)}\rangle = \sum_{k \neq n} |k^{(0)}\rangle c_{nk}^{(2)}$$

Then

$$\Rightarrow \left(\hat{H}_0 - E_n^{(0)} \right) \sum_{k \neq n} |k^{(0)}\rangle c_{nk}^{(2)} + \left(\hat{H}' - E_n^{(0)} \right) |n^{(1)}\rangle - E_n^{(2)} |n^{(0)}\rangle = 0$$

Let $l \neq n$. Then,

$$\begin{aligned} &\sum_{k \neq n} \langle l^{(0)}|k^{(0)}\rangle c_{nk}^{(2)} \left(E_k^{(0)} - E_n^{(0)} \right) + \langle l^{(0)}| \left(\hat{H}' - E_n^{(0)} \right) |n^{(1)}\rangle - E_n^{(2)} \underbrace{\langle l^{(0)}|n^{(0)}\rangle}_0 = 0 \\ \Rightarrow c_{nk}^{(2)} &= \sum_{k \neq n} \frac{E_n^{(1)}}{E_n^{(0)} - E_l^{(0)}} + \sum_{k \neq n} \sum_{l \neq n} \frac{\langle k^{(0)}|\hat{H}'|l^{(0)}\rangle \langle l^{(0)}|\hat{H}'|n^{(0)}\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(2)} - E_l^{(0)})} \end{aligned}$$

[THE ABOVE ARE DUBIOUS; DOUBLE-CHECK THE CALCULATIONS LATER]

1.2 Degenerate Perturbation Theory

So far, we've assumed that our systems have stationary states which are non-degenerate. However, in many situations we have orthogonal states $|a^{(0)}\rangle$ and $|b^{(0)}\rangle$ with $\langle a^{(0)}|b^{(0)}\rangle = 0$ but with

$$\begin{aligned}\hat{H}^{(0)}|a^{(0)}\rangle &= E^{(0)}|a^{(0)}\rangle \\ \hat{H}^{(0)}|b^{(0)}\rangle &= E^{(0)}|b^{(0)}\rangle\end{aligned}$$

So, we'll have to tweak our approach. We will try to use the parameter λ to split the energies.