PHYs 487: Lecture # 7

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Lecture Span

- Time independent perturbation theory (non degenerate)

Non degenerate time independent perturbation theory

Consider a Hamiltonian

$$H = H^{(s)} + H' \tag{1}$$

Where $H^{(s)}$ is the standard Hamiltonian of an infinite square well and H' is a perturbation to that Hamiltonian.

Approach for PT

1. We know: $H^{(0)} \left|\psi_n^{(0)}\right\rangle = E_n \left|\psi_n^{(0)}\right\rangle$ with $\left\langle \psi_n^{(0)} \middle| \psi_m^{(0)} \right\rangle = \delta_{nm}$
2. But we want $H \left|\psi_n\right\rangle = E_n \left|\psi_n\right\rangle$ (solutions to the perturbed Hamiltonian H)

Write: $H = H^{(0)} + \lambda H$ where λ is a tuning parameter. We will use it to keep track of the orders of PT. We write $\left|\psi_n\right\rangle$ as a power series:

$$\left|\psi_n\right\rangle = \left|\psi_n^{(0)}\right\rangle + \lambda \left|\psi_n^{(1)}\right\rangle + \lambda^2 \left|\psi_n^{(2)}\right\rangle + \dots \tag{2}$$

Same for the energies

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \dots \tag{3}$$

We plug this ansatz into bullet point (2), and we obtain

$$\left(H^{(0)} + \lambda H'\right) \left[\left|\psi_n^{(0)}\right\rangle + \lambda \left|\psi_n^{(1)}\right\rangle + \dots\right] = \left(E_n^{(0)} + \lambda E_n^{(1)} + \dots\right) \left[\left|\psi_n^{(0)}\right\rangle + \lambda \left|\psi_n^{(1)}\right\rangle + \dots\right] \tag{4}$$

We can collect like powers of λ. Equations by order:

$$\lambda^0 = H^{(0)} \left|\psi_n^{(0)}\right\rangle = E_n^{(0)} \left|\psi_n^{(0)}\right\rangle \tag{5}$$

$$\lambda^1 = H^{(0)} \left|\psi_n^{(1)}\right\rangle + H' \left|\psi_n^{0}\right\rangle = E_n^{(0)} \left|\psi_n^{1}\right\rangle + E_n^{(1)} \left|\psi_n^{(0)}\right\rangle \tag{6}$$

$$\lambda^2 = H^{(0)} \left|\psi_n^{(2)}\right\rangle + H' \left|\psi_n^{1}\right\rangle = E_n^{(0)} \left|\psi_n^{2}\right\rangle + E_n^{(1)} \left|\psi_n^{1}\right\rangle + E_n^{(2)} \left|\psi_n^{(0)}\right\rangle \tag{7}$$

First order correction in E, $E_n^{(1)}$, multiply by λ^1 equation with $\left\langle \psi_n^{(0)} \right|$:

$$\langle \psi_n^{(0)} | H^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle = E_n^{(0)} \left\langle \psi_n^{(0)} \middle| \psi_n^{(1)} \right\rangle + E_n^{(1)} \left\langle \psi_n^{(0)} \middle| \psi_n^{(0)} \right\rangle \tag{8}$$

Note that

$$\langle \psi_n^{(0)} | H^{(0)} | \psi_n^{(1)} \rangle = E_n^{(0)} \left\langle \psi_n^{(0)} \middle| \psi_n^{(1)} \right\rangle \tag{9}$$

Therefore, we get a simple expression for the first order correction to the energy:

$$E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle \tag{10}$$

Now, we consider the first order correction to the state. We rewrite the λ^1 equation:

$$(H^{(0)} - E_n^{(0)}) \left| \psi_n^1 \right\rangle = -(H' - E_n^{(1)}) \left| \psi_n^{(0)} \right\rangle \tag{11}$$

We can write

$$\left| \psi_n^{(0)} \right\rangle = \sum_{m \neq n} c_{nm} \left| \psi_m^{(0)} \right\rangle \tag{12}$$

Here, we want to ignore the current state because we want more interesting corrections.

$$\sum_{m \neq n} \left(E_m^{(0)} - E_n^{(0)} \right) c_{nm} \left| \psi_m^{(0)} \right\rangle = -(H' - E_n^{(1)}) \left| \psi_n^{(0)} \right\rangle \tag{13}$$

Multiply both sides by $\left\langle \psi_k^{(0)} \right|$, and we obtain

$$\sum_{m \neq n} (E_m^{(0)} - E_n^{(0)}) c_{nm} \left\langle \psi_k^{(0)} \middle| \psi_m^{(0)} \right\rangle = \langle \psi_k^{(0)} | H' | \psi_n^0 \rangle + E_n^{(1)} \langle \psi_k^{(0)} | \psi_n^{(0)} \rangle \tag{14}$$

Here, if $k = n$, then it just reduces to the first order energy correction. For $k \neq n$:

$$\left(E_k^{(0)} - E_n^{(0)} \right) c_{nk} = -\langle \psi_k^{(0)} | H' | \psi_n^{(0)} \rangle \tag{15}$$

Therefore,

$$\left| \psi_n^{(1)} \right\rangle = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | H' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \left| \psi_m^{(0)} \right\rangle \tag{16}$$

Second order

1. λ^2 equation, multiply by $\left\langle \psi_n^{(0)} \right|$

Then we get

$$\begin{aligned} E_n^{(2)} &= \langle \psi_n^{(0)} | H' | \psi_n^{(1)} \rangle \\ &= \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | H' | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \end{aligned}$$

Example 0

Infinite square well; then just move the bottom of the well down. This is a diagonal perturbation with V_0, therefore

$$H = \frac{p^2}{2m} + V_0 \tag{17}$$

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} \right) \tag{18}$$

$$E_n^{(1)} = \langle \psi_n^{(0)} | V_0 | \psi_n^{(0)} \rangle = V_0 \tag{19}$$

Then

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | V_0 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \left| \psi_m^{(0)} \right\rangle = 0 \tag{20}$$

Example 1

So now, let's consider a well with only half its floor raised up by V_0 with length $a/2$. Here,

$$
\begin{aligned}
E_n^{(1)} &= \int_0^{a/2} \psi_n^{(0)} V_0 \psi_n^{(0)} \\
&= 2\frac{V_0}{a} \int_0^{a/2} \sin^2\left(\frac{n\pi x}{a}\right) \\
&= \frac{2V_0}{a}\left(\frac{a}{4}\right) \\
&= \frac{V_0}{2}
\end{aligned}
$$

Here, we consider

$$
\begin{aligned}
\psi_1^{(1)}(x) &= \sum_{m\neq n} \frac{\langle \psi_m^{(0)} | H' | \psi_1^{(0)} \rangle}{(E_1^{(0)} - E_m^{(0)})} \psi_m^{(0)}(x) \\
&= \frac{2V_0 m \cos\left(\frac{m\pi}{2}\right)}{\pi(1-m^2)}
\end{aligned}
$$

Also,

$$
E_1^{(0)} - E_m^{(0)} = \frac{\pi^2\hbar^2}{2(\text{mass})a^2}(1-m^2) \tag{21}
$$

Example 2

Consider $H' = \alpha\delta(x - a/2)$ in an infinite square well. Here, the odd functions will probably not be affected since they are 0 at $a/2$. But the even functions are likely to see this change. Energy corrections

$$
\begin{aligned}
E_n^{(1)} &= \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle \\
&= \frac{2\alpha}{a} \int_0^a \sin^2\left(\frac{n\pi x}{a}\right)\delta(x - a/2)dx \\
&= \frac{2\alpha}{a}\sin^2(\frac{n\pi}{2})
\end{aligned}
$$