PERTURBATION THEORY (TIME-INDEPENDENT) 3

We left a couple of open questions open in our treatment of perturbation theory. They clearly stare at us when we look at our results. A short reminder of our issue:

- we know exactly the solutions of an Hamiltonian H^0, i.e., we know all its eigenstates ψ_n^0 and corresponding eigenvalues E_n^0, such that
$$\underbrace{H^0}_{\text{operator}}\psi_n^0 = \underbrace{E_n^0}_{\text{number}}\psi_n^0$$
- we now consider a perturbation $\lambda H'$ to our Hamiltonian H^0, which gives us a new Hamiltonian $H = H^0 + \lambda H'$
- we finally ask ourselves what we can say about the eigenstates ψ_n and eigenvalues E_n of the new Hamiltonian H

We wrote ψ_n and E_n as a power series in λ:

$$\psi_n = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots$$
$$E_n = E_n^0 + \lambda E_n^1 + \underbrace{\lambda^{2}}_{\text{exponent}} \underbrace{E_n^{2}}_{\text{index}} + \dots$$

and found a nice expression for the <u>first</u> order corrections:

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$
$$\psi_n^1 = \sum_{m\neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$$

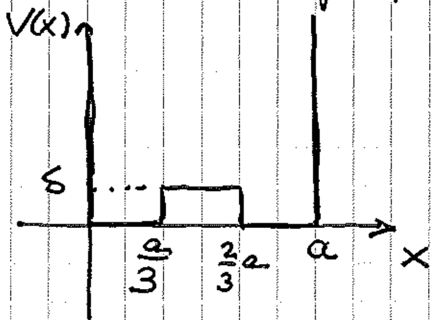
Two requirements come naturally up, for perturbation theory to be valid:

1) $|E_n^1| \ll |E_n^0|$
2) $|\langle \psi_m^0 | H' | \psi_n^0 \rangle| \ll |E_n^0 - E_m^0|$

i.e., corrections ought to be <u>small</u>

Let us do, from A to Z, an example, to see what these conditions mean. Let me also anticipate one point we will see later. Technically speaking, we are doing <u>non-degenerate</u> perturbation theory. If $E_n^0 = E_m^0$ for some value of $m \neq n$ (i.e., there are more than one eigenstates of H^0 with the same eigenvalue), then my system collapses: $\frac{1}{E_n^0 - E_m^0} = \infty$! (in some cases, it also happens that $\langle \psi_m^0 | H' | \psi_n^0 \rangle = 0$, but let's say that the situation is still unpleasant). We will in due time see how to formally solve the problem of degeneracy.

Here is an example, similar to the one you can find in Griffith's textbook:



Particle of mass m inside infinite square well with width <u>a</u>.

Perturbation: a bump in the middle of the well, by an amount δ.

Then:

$$H^0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & x < 0 \text{ or } x > a \end{cases}$$

Unperturbed solutions and corresponding eigenvalues:

$$\psi_n^0 = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), & 0 < x < a \\ 0, & x < 0 \text{ or } x > a \end{cases} \qquad E_n^0 = \frac{\pi^2 \hbar^2}{2ma^2} n^2$$

<u>Perturbation:</u>

$$H' = \begin{cases} \delta, & \frac{a}{3} < x < \frac{2}{3}a \\ 0, & x < \frac{a}{3} \text{ or } x > \frac{2}{3}a \end{cases}$$

Let us calculate E_1^1 and ψ_1^1, the corrections to the ground state:
i.e., $n=1$

$$E_1^1 = \langle \psi_1^0 | H' | \psi_1^0 \rangle = \frac{2}{a}\int_{\frac{a}{3}}^{\frac{2}{3}a} \delta \cdot \sin^2\left(\frac{\pi x}{a}\right) dx =$$

$$= \frac{2\delta}{a}\int_{\frac{a}{3}}^{\frac{2}{3}a}\left(\frac{1}{2}-\frac{1}{2}\cos\left(\frac{2\pi x}{a}\right)\right)dx = \frac{2\delta}{a}\left[\frac{1}{2}x - \frac{a}{4\pi}\sin\left(\frac{2\pi x}{a}\right)\right]_{\frac{1}{3}a}^{\frac{2}{3}a} =$$

$$= \frac{2\delta}{a}\cdot\left[\frac{1}{6}a - \frac{a}{4\pi}\underbrace{\sin\left(\frac{4\pi}{3}\right)}_{-\sqrt{3}/2} + \frac{a}{4\pi}\underbrace{\sin\left(\frac{2\pi}{3}\right)}_{+\sqrt{3}/2}\right] =$$

$$= \delta\cdot\left(\frac{1}{3}+\frac{\sqrt{3}}{2\pi}\right) \approx 0.61\,\delta$$

if $\delta > 0$, the ground state is lifted up; if $\delta < 0$, it is pushed down.

We obtain:

$$E_1^0 = \frac{\hbar^2\pi^2}{2ma^2} \Longrightarrow E_1 = \underbrace{\frac{\hbar^2\pi^2}{2ma^2}}_{E_1^0} + \underbrace{\delta\left(\frac{1}{3}+\frac{\sqrt{3}}{2\pi}\right)}_{E_1^1} + \underbrace{\ldots}_{E_1^2\ ?}$$

The smallness condition becomes:

$$\boxed{\frac{\hbar^2\pi^2}{2ma^2} >> 0.61\,|\delta|}$$: this sets a limit to δ.

$$(E_1^0 >> E_1^1)$$

Let us now move to the ground state wavefunction:

$$\psi_1^0 = \sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi x}{a}\right)$$

The first order correction is:

$$\psi_1^1 = \sum_{m\neq 1}\frac{\langle \psi_m^0 | H' | \psi_1^0\rangle}{E_1^0 - E_m^0}\,\psi_m^0$$

Since H' and ψ_1^0 are even with respect to $\frac{a}{2}$, while ψ_2^0 is odd, it is easy to show that the first term $\neq 0$ in the sum is the one with $m = 3$ (well, all terms with m even will be $\emptyset$ as well...):

$$C_3^{(1)} = \frac{\langle \psi_3^0 | H' | \psi_1^0 \rangle}{E_1^0 - E_3^0} = \frac{1}{E_1^0 - E_3^0} \cdot \int_{\frac{1}{3}a}^{\frac{2}{3}a} \frac{2}{a} \delta \sin\left(\frac{3\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx =$$

$H' = 0$ outside $\frac{1}{3}a < x < \frac{2}{3}a$ interval

$1 - m^2, m = 3$

$$= \frac{2ma^2}{\hbar^2 \pi^2} \cdot \left(-\frac{1}{8}\right) \frac{2\delta}{a} \cdot \int_{\frac{1}{3}a}^{\frac{2}{3}a} \frac{1}{2} \left(\cos\left(\frac{2\pi x}{a}\right) - \cos\left(\frac{4\pi x}{a}\right)\right) dx =$$

$$= -\frac{ma\delta}{4\hbar^2\pi^2} \cdot \left[\frac{a}{2\pi} \sin\left(\frac{2\pi x}{a}\right) - \frac{a}{4\pi} \sin\left(\frac{4\pi x}{a}\right) \right]_{\frac{1}{3}a}^{\frac{2}{3}a} =$$

$$= -\frac{ma\delta}{4\hbar^2\pi^2} \left[\frac{a}{2\pi} \cdot \left(-\frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} \right) - \frac{a}{4\pi} \left(\frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2} \right) \right] =$$

$$= \frac{ma^2\delta}{16\pi^3\hbar^2} \cdot 3\sqrt{3}$$

NOTE: I need to calculate $C_m^{(1)}$ for all odd m in order to get the complete form of ψ_1^1, which is just the first order correction to the wavefunction.

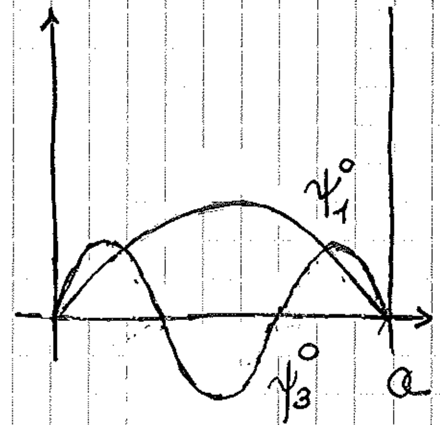
$$\psi_1^1 = \sum_{\substack{m \neq 1 \\ \text{odd}}} C_m^{(1)} \psi_m^0 = \frac{ma^2\delta}{16\pi^3\hbar^2} 3\sqrt{3} \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right) + \overset{C_5^{(1)}\psi_5^0}{\ldots} + \ldots$$

Finally:

$$\psi_1 \cong \psi_1^0 + \psi_1^1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) + \underbrace{\frac{ma^2\delta}{16\pi^3\hbar^2} 3\sqrt{3} \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right)}_{\text{first term of } \psi_1^1 \text{ expansion}} + \underbrace{\ldots}_{\text{other terms in } \psi_1^1 \text{ expansion}}$$

only to first order, I am leaving ψ_1^2 out

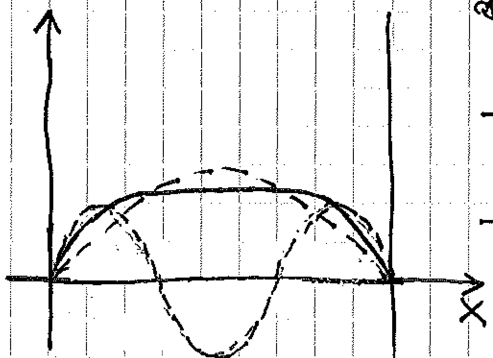
How does the correction look?



$$\psi_1 \simeq \psi_1^0 + \psi_1^1 = \psi_1^0 + c_3^{(1)} \psi_3^0 + \dots$$

$$\underline{\underline{c_3^{(1)} \propto \delta}}$$

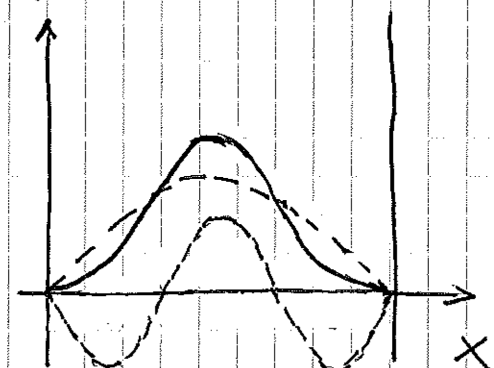
If $\boxed{\delta > 0}$, I am adding a bump in the middle of the well: ψ_3^0 is negative in that region, and the effect of the bump is that the wavefunction ψ_1 gets "pushed away":



--- unperturbed ψ_1^0 and ψ_3^0

—— $\psi_1 \simeq \psi_1^0 + \underbrace{c_3^{(1)}}_{>0} \psi_3^0$

If $\boxed{\delta < 0}$, I am digging a hole in the middle of the well: $c_3^{(1)} < 0$, hence ψ_3^0 gets a negative coefficient; the effect is that the wavefunction ψ_1 gets "sucked" towards the center of the well:



--- unperturbed ψ_1^0 and $-\psi_3^0$

—— $\psi_1 \simeq \psi_1^0 + \underbrace{c_3^{(1)}}_{<0} \psi_3^0$