Quantum mechanics I : tutorial solutions

2021.11.25 / self-study pack 5

1) Review your lecture notes to make sure you know where the expressions given at the beginning of the movie come from. Note: there is one other expression you should know, for the second-order change in energy.

the expressions at the beginning are:

- perturbation theory 1st order NON-DEGENERATE

$$E_n^{(1)} = \int_{\text{all space}} dV \, u_n^{(0)*} \, \hat{H}' \, u_n^{(0)} \equiv H'_{nn}$$

1st order change in energy

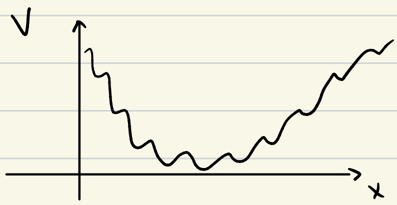
for $m \neq n$

$$a_{nm} = \frac{\int dV \, u_m^{(0)*} \hat{H}' u_n^{(0)}}{E_n^{(0)} - E_m^{(0)}} = \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}$$

1st order change in the wave function coefficients.

How do we find these?

Suppose we have a complicated potential in our system.



We can think of changing it to a simpler one and add a small perturbation to it.

$$\underbrace{\hat{H}}_{\text{unsolvable}} = \underbrace{\hat{H}^{(0)}}_{\text{solvable}} + \underbrace{\hat{H}'}_{\text{perturbation}}$$

the solutions to the solvable model are

$$\hat{H}^{(0)} u_n^{(0)} = E_n^{(0)} u_n^{(0)}$$

the system rewritten with the perturbation is

$$\hat{H} = \hat{H}^{(0)} + \beta \hat{H}'$$

with this β, we can set our perturbation strength

We expect the energies & wavefunctions of $\hat{H}$ to be perturbed by $\hat{H}'$

$$E_n = E_n^{(0)} + \beta E_n^{(1)} + \beta^2 E_n^{(2)} + \dots$$

$$u_n = u_n^{(0)} + \beta u_n^{(1)} + \beta^2 u_n^{(2)} + \dots$$

Since this is 1^{st} order perturbation theory, we need only the 1^{st} order corrections.

$$\hat{H} u_n = E_n u_n$$

$$(H^{(0)} + \beta H')(u^{(0)} + \beta u_n^{(1)} + \beta^2 u_n^{(2)} + \dots) =$$

$$= (E_n^{(0)} + \beta E_n^{(1)} + \beta^2 E_n^{(2)} + \dots)(u^{(0)} + \beta u_n^{(1)} + \beta^2 u_n^{(2)} + \dots)$$

$$\hat{H}^{(0)} u_n^{(0)} + \beta (H^{(0)} u_n^{(1)} + H' u^{(0)}) + O(\beta^2)$$

$$= E_n^{(0)} u_n^{(0)} + \beta (E^{(0)}_n u_n^{(1)} + E^{(1)}_n u^{(0)}) + O(\beta^2)$$

$$ax^2 + bx^1 + c = dx^2 + fx + g$$

Since this has to hold for any value of β, terms on the LHS & RHS w/ same power of β have to be equal,

$$\beta^0 \longrightarrow \hat{H}^{(0)} u_n^{(0)} = E_n^{(0)} u_n^{(0)}$$

$$\beta^1 \longrightarrow \hat{H}^{(0)} u_n^{(1)} + \hat{H}^1 u_n^{(0)} = E_n^{(0)} u_n^{(1)} + E_n^{(1)} u_n^{(0)}$$

& so on for 2^{nd} order, 3^{rd} order ...

We stop to the 1^{st} order.

$$(\hat{H}^1 - E_n^{(1)}) u_n^{(0)} = (E_n^{(0)} - \hat{H}^{(0)}) u_n^{(1)}$$

we write $u_n^{(1)}$ as

$$u_n^{(1)} = \sum_{\substack{k \\ k \neq n}} a_{nk} u_k^{(0)}$$

} the perturbed eig. vect. expressed as a sum of the unperturbed ones

Not exactly a matrix product but you can see it as:

$$\begin{array}{c} u_n^{(1)} \\ \begin{bmatrix} | & | & | \\ | & | & | \\ | & | & | \end{bmatrix} \end{array} = \begin{array}{cc} & k \\ n & \begin{bmatrix} \cdots & a_{nk} & \cdots \end{bmatrix} \end{array} \begin{array}{c} u_k^{(0)} \\ \begin{bmatrix} | & | & | \\ | & | & | \\ | & | & | \end{bmatrix} \end{array}$$

we have

$$(\hat{H}^1 - E_n^{(1)}) u_n^{(0)} = (E_n^{(0)} - \hat{H}^{(0)}) \sum_{\substack{k \\ k \neq n}} a_{nk} u_k^{(0)}$$

we can apply $H^{(0)}$ on the eigenstates,

$$(\hat{H}' - E_n^{(1)})\, u_n^{(0)} = \sum_{\substack{k \\ k\neq n}} (E_n^{(0)} - E_k^{(0)})\, a_{nk}\, u_k^{(0)}$$

if we multiply for $\boxed{u_n^{(0)*}}$ & integrate,

$$\int dV\, u_n^{(0)*} \hat{H}' u_n^{(0)} - E_n^{(1)} \cancelto{1}{\int dV\, u_n^{(0)*} u_n^{(0)}} =$$

$$= \sum_{\substack{k \\ k\neq n}} (E_n^{(0)} - E_k^{(0)})\, a_{nk} \cancelto{0}{\int dV\, u_n^{(0)*} u_k^{(0)}}$$

where we used the fact that the set of $u_i^{(0)}$ is ORTHONORMAL. We obtained,

$$E_n^{(1)} = \int dV\, u_n^{(0)*} \hat{H}' u_n^{(0)}$$

the 1st order correction of the EIGENVALUES is the expectation value of $\hat{H}'$ on the UNPERTURBED states $u_i^{(0)}$

from $*$, which is

$$(\hat{H}' - E_n^{(1)})\, u_n^{(0)} = \sum_{\substack{k \\ k\neq n}} (E_n^{(0)} - E_k^{(0)})\, a_{nk}\, u_k^{(0)}$$

if we multiply by $\boxed{u_m^{(0)*}}$ & integrate ,

$$\int dV\, u_m^{(0)*}\, \hat{H}'\, u_n^{(0)} - E_n^{(1)} \cancelto{0}{\int dV\, u_m^{(0)*}\, u_n^{(0)}} =$$

$$= \sum_{\substack{k \\ k\neq n}} (E_n^{(0)} - E_k^{(0)})\, a_{nk} \cancelto{\delta_{m,k}}{\int dV\, u_m^{(0)*}\, u_k^{(0)}}$$

we used again the ORTHONORMALITY ,

$$\int dV\, u_m^{(0)*}\, \hat{H}'\, u_n^{(0)} = (E_n^{(0)} - E_m^{(0)})\, a_{nm}$$

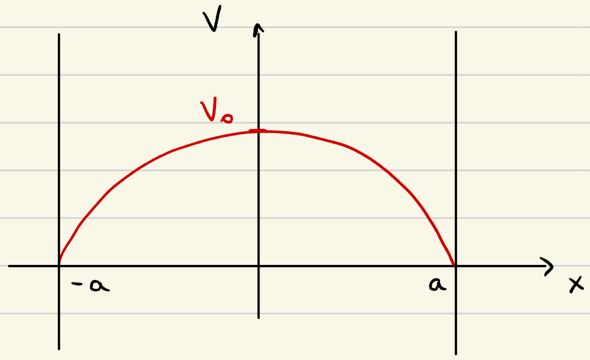
matrix element m, n

$$\Rightarrow \quad a_{nm} = \frac{\int dV\, u_m^{(0)*}\, \hat{H}'\, u_n^{(0)}}{E_n^{(0)} - E_m^{(0)}} = \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}$$

which is the 1st order correction in the coefficients of the eigenvectors

2) Do the integrals which I left for you in the first exercise (question 2 from the Exercises for Week 10). There should be sufficient hints in the movie for you to do this – if not consult your maths notes.

- integral from week 10 exercise 2.



$$\hat{H}' = V_0 \cos\left(\frac{\pi}{2a} x\right)$$

the correction to the 1^{st} order in the eigenenergies is

$$E_n^{(1)} = \int dV \, u_n^{(0)*} \, \hat{H}' \, u_n^{(0)}$$

Recalling the ground state of the infinite well,

$$u^{(0)} = \frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a} x\right)$$

we can set up the 1^{st} order correction

$$E_{n=1}^{(1)} = \int dV \, u_n^{(0)*} \, \hat{H}' \, u_n^{(0)}$$

$$= \int dx \, \frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a} x\right) V_0 \cos\left(\frac{\pi}{2a} x\right) \frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a} x\right)$$

$$= \frac{V_0}{a} \int dx \quad \cos^3\left(\frac{\pi}{2a} x\right)$$

I change variable, $y = \frac{\pi}{2a} x$, $dy = \frac{\pi}{2a} dx$

$$= \frac{V_0}{a} \frac{2a}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} dy \quad \cos^3(y)$$

$$= \frac{2V_0}{\pi} \int dy \quad \cos^3(y)$$

$$\int dy \quad \cos y \quad (1 - \sin^2 y)$$

$$= \int dy \cos y \quad - \int dy \quad \cos y \sin^2 y$$

Since $\quad d(\sin y) = \cos y \, dy$

$$= \int dy \cos y \quad - \int d(\sin y) \sin^2 y$$

$$= \sin y \Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}} - \frac{\sin^3 y}{3} \Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}}$$

So our integral becomes

$$E_1^{(1)} = \frac{2V_0}{\pi} \int dy \quad \cos^3(y)$$

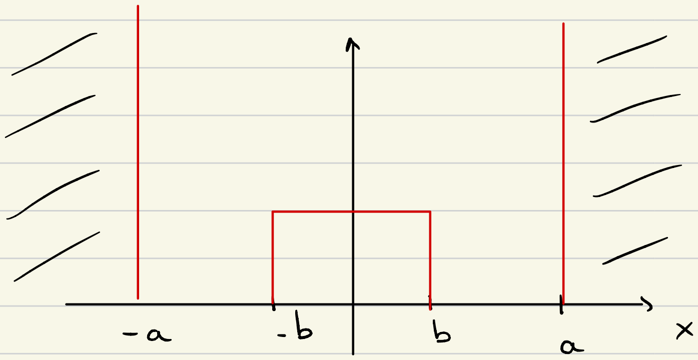
$$= \frac{2V_0}{\pi} \left[2 \sin\frac{\pi}{2} - \frac{2\sin^3\frac{\pi}{2}}{3} \right]$$

$$= \frac{2V_0}{\pi} \left[2 - \frac{2}{3} \right] = \frac{8}{3} \frac{V_0}{\pi}$$

Remember that $E_1^{(1)}$ is a CORRECTION to $E_1^{(0)} = \frac{\hbar^2\pi^2}{8ma^2}$

3) After watching the first exercise, do question 3 from the Exercises for Week 10.

$$V = \begin{cases} V_0 , & -b \leq x \leq +b \\ 0 , & b < |x| \leq a \\ \infty , & |x| > a \end{cases}$$



We treat this potential as an infinite square well with a perturbation at the centre.
The perturbation is described by H',

$$H' = \begin{cases} V_0 , & -b \leq x \leq b \\ 0 , & \text{elsewhere} \end{cases}$$

The ground state eigenfunction of the INFINITE square well is :

$$u_1^{(0)} = \frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a} x \right)$$

As we have done before, the correction to its energy is,

$$E_1^{(1)} = \int_{-a}^{a} u_1^{(0)*} \, H' \, u_1^{(0)} \, dx$$

$$= \int_{-b}^{b} \frac{V_0}{a} \cos^2\left(\frac{\pi}{2a} x\right) dx$$

Using $\cos^2(x) = \dfrac{1 + \cos(2x)}{2}$,

$$= \frac{V_0}{2a} \int_{-b}^{b} \left(1 + \cos\left(\frac{\pi}{a} x\right)\right) dx$$

$$= \frac{V_0}{2a} \left(x + \frac{a}{\pi} \sin\left(\frac{\pi}{a} x\right)\right) \Big|_{-b}^{b}$$

$$E_1^{(1)} = \frac{V_0}{2a} \left(2b + \frac{2a}{\pi} \sin\left(\pi \frac{b}{a}\right)\right)$$

<u>NB</u>

if $b = a \Rightarrow E_1^{(1)} = V_0$,

we have a constant shift of the energies.

4) Check that the normalization factor C_1 in the solution of degenerate perturbation theory problem (question 8 from the Exercises for Week 10), (about 35 minutes in) is $2^{-½}$.

Now, we look at DEGENERATE perturbation theory.

Consider a system w/ normalised wave functions Ψ_1, Ψ_2, Ψ_3.

Consider a perturbation H'

$$H' = \begin{pmatrix} 0 & 0 & V_1 e^{i\varphi} \\ 0 & V_0 & 0 \\ V_1 e^{-i\varphi} & 0 & 0 \end{pmatrix}$$

w/ $V_0, V_1 > 0$ & $V_0 \neq V_1$

We write the wave function of the perturbed system as a linear combination of the Ψ's.

$$\nu = c_1 \Psi_1 + c_2 \Psi_2 + c_3 \Psi_3$$

Putting back the "corrections" in the equations of the perturbation, we have the system

$$\begin{pmatrix} -E & 0 & V_1 e^{i\varphi} \\ 0 & V_0 - E & 0 \\ V_1 e^{-i\varphi} & 0 & -E \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0$$

$(H' - E)\,\underline{c} = 0$

$H'\underline{c} = E\,\underline{c}$

To find non-trivial solutions we need det = 0

$$\begin{vmatrix} -E & 0 & V_1 e^{i\varphi} \\ 0 & V_0 - E & 0 \\ V_1 e^{-i\varphi} & 0 & -E \end{vmatrix} = 0$$

$$(V_0 - E)(E^2 - V_1^2) = 0$$

So the sol. are $E = V_0$ & $E = \pm V_1$

As usual, we now find the eigenvectors' coefficients. Therefore we substitute the solution into the matrix.

- $E = V_0$, $\begin{pmatrix} -V_0 & 0 & V_1 e^{i\varphi} \\ 0 & 0 & 0 \\ V_1 e^{-i\varphi} & 0 & -V_0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$

$$\begin{cases} c_1 = \dfrac{V_1}{V_0} e^{i\varphi} c_3 \\[2ex] c_1 = \dfrac{V_0}{V_1} e^{i\varphi} c_3 \end{cases} \Rightarrow \begin{array}{l} c_1 = c_3 = 0 \\ c_2 \text{ is free} \end{array}$$

$$\Rightarrow \quad u_2 = \Psi_2$$

• $E = V_1$,
$$\begin{pmatrix} -V_1 & 0 & V_1 e^{i\varphi} \\ 0 & V_0 - V_1 & 0 \\ V_1 e^{-i\varphi} & 0 & -V_1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

$$\begin{cases} -V_1 c_1 + V_1 e^{i\varphi} c_3 = 0 \\ (V_0 - V_1) c_2 = 0 \\ V_1 e^{-i\varphi} c_1 - V_1 c_3 = 0 \end{cases}$$

$$\begin{cases} c_3 = e^{-i\varphi} c_1 \\ c_2 = 0 \end{cases}$$

$$\Rightarrow \quad u_1 = \Psi_1 + e^{-i\varphi} \Psi_3$$

Since Ψ_i are normalised, the normalisation factor is $\frac{1}{\sqrt{2}}$

$$u_1 = \frac{1}{\sqrt{2}} \left(\Psi_1 + e^{-i\varphi} \Psi_3 \right)$$

- $E = -V_1$, $\begin{pmatrix} V_1 & 0 & V_1 e^{i\varphi} \\ 0 & V_0+V_1 & 0 \\ V_1 e^{-i\varphi} & 0 & V_1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$

$$\begin{cases} V_1 c_1 + V_1 e^{i\varphi} c_3 = 0 \\ (V_0 + V_1) c_2 = 0 \\ V_1 e^{-i\varphi} c_1 + V_1 c_3 = 0 \end{cases}$$

$$\begin{cases} c_3 = -e^{-i\varphi} c_1 \\ c_2 = 0 \end{cases}$$

$$(c_1, c_2, c_3) = (1 \quad 0 \quad -e^{-i\varphi})$$

normalisation $\frac{1}{\sqrt{2}} \longrightarrow \left(\frac{1}{\sqrt{2}} \quad 0 \quad -\frac{1}{\sqrt{2}} e^{-i\varphi}\right)$

$$\Rightarrow \qquad u_3 = \frac{1}{\sqrt{2}} \left(\Psi_1 - e^{-i\varphi} \Psi_3 \right)$$

NB missing point 5. Will update solutions asap.