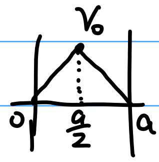
Zhi Chen HW# 18

1) know unperturbed solution in potential well of $0<x<a$:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}x\right) \qquad E_n^{(0)} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2$$

a) $V(x) = \frac{V_0}{a}\left(a - |2x-a|\right)$:



← even in $\frac{a}{2}$.

$$E_n^{(1)} = \langle n^{(0)} | V(x) | n^{(0)} \rangle$$

$$= \int_0^a \frac{2}{a} \underbrace{\sin^2\left(\frac{\pi n}{a}x\right)}_{\text{even}} \underbrace{\frac{V_0}{a}\left(a - |2x-a|\right)}_{\text{even about } a/2} dx$$

total even func about $a/2$

$$= \frac{2V_0}{a^2}\, 2\int_0^{a/2} \sin^2\left(\frac{\pi n}{a}x\right) 2x \; dx$$

$$= \frac{4V_0}{\cancel{a^2}}\left(-\frac{\cancel{a^2}\left(\cancel{2\pi n \sin(\pi n)} + 2\cos(\pi n) - \pi^2 n^2 - 2\right)}{8\pi^2 n^2}\right)$$

$$E_n^{(1)} = V_0\left(\frac{2\left(1-\cos(\pi n)\right) + (\pi n)^2}{2\pi^2 n^2}\right)$$

$$\boxed{\begin{array}{l} \text{If } n = \text{even},\ 1-\cos(\pi n) = 0, \text{ then } E_n^{(1)} = \frac{V_0}{2} \\ \text{If } n = \text{odd},\ 1-\cos(\pi n) = 2, \text{ then } E_n^{(1)} = V_0\,\frac{4+(\pi n)^2}{2(\pi n)^2} = V_0\left(\frac{1}{(\pi n)^2} + \frac{1}{2}\right) \end{array}}$$

It is valid when perturbation is small between energy level difference.

$$\hookrightarrow |V_{nk}| < |E_n^{(0)} - E_k^{(0)}| = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 |n^2 - k^2|$$

but on the order of magnitude, simply require

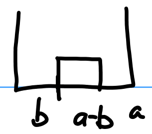
$$|E_n^{(1)}| \ll |E_n^{(0)}|$$

$$E_{n=1}^{(1)} = V_0\left(\frac{1}{\pi^2} + \frac{1}{2}\right) \approx \frac{V_0}{2}$$

$$E_{n=1}^{(0)} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

then want $\frac{V_0}{2} \ll \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$

or $\boxed{V_0 \ll \frac{\hbar^2}{m}\left(\frac{\pi}{a}\right)^2}$



1(b)

$$E_n^{(1)} = \int_0^a V_0\, \Theta_{b<x<a-b} \frac{2}{a} \sin^2\left(\frac{\pi n}{a}x\right) dx$$

$$= \int_b^{a-b} V_0 \frac{2}{a} \sin^2\left(\frac{\pi n}{a}x\right) dx$$

$$= \frac{2\pi a n - 4\pi b n + a\sin\left(\frac{2\pi n(b-a)}{a}\right) + a\sin\left(\frac{2\pi n\, b}{a}\right)}{4\pi n} V_0$$

$$= \left(\frac{a}{2} - b + a\left(\frac{\sin\left(\frac{2\pi n}{a}(b-a)\right) + \sin\left(\frac{2\pi n}{a}b\right)}{4\pi n}\right)\right) V_0$$

Valid when $|V_{nk}| < |E_n^{(0)} - E_k^{(0)}|$, or approximately $E_n^{(1)} \ll E_n^{(0)}$

$$\max\{E_{n=1}^{(1)}\} \sim V_0\left(\frac{a}{2} - b\right)$$

$$E^{(0)} \sim \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

then $E^{(1)} \ll E^{(0)}$

$$V_0\left(\frac{a}{2} - b\right) \ll \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

or $\boxed{V_0 \ll \frac{1}{\left(\frac{a}{2} - b\right)} \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2}$

2) $E^{(1)} = \langle n^{(0)} | V(x) | n^{(0)} \rangle$

$$= \int_0^a \frac{2}{a} \sin^2\left(\frac{\pi n}{a}\right) V(x)\, dx$$

Use integration by parts, let $u = V(x)$ $dv = \sin^2\left(\frac{\pi n}{a}\right) dx$

integrale $\int \sin^2\left(\frac{\pi n}{a}\right) dx = \frac{2\pi n x}{4\pi n} - \frac{a \sin\left(\frac{2\pi n x}{a}\right)}{4\pi n}$

$$= \frac{x}{2} - \frac{a \sin\left(\frac{2\pi n x}{a}\right)}{4\pi n}$$

if n is sufficiently large such that $4\pi n \gg a$

then $\frac{a \sin\left(\frac{2\pi n x}{a}\right)}{4\pi n} \to 0$

then the integral becomes

$$E^{(1)} = \left(\frac{x}{2} V(x)\right)\Big|_0^a - \int_0^a \frac{x}{2} \frac{dV}{dx}\, dx$$

which is <u>independent of n.</u>

3) $H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + \frac{1}{2}\alpha x^2$

First find exact answer: let $H = \frac{p^2}{2m} + \frac{1}{2}(k+\alpha)x^2$

let $\frac{1}{2}m\omega^2 x^2 = \frac{1}{2}(k+\alpha)x^2$ or $\omega^2 = \left(\frac{k+\alpha}{m}\right)$

then we know Harmonic Oscillator has energy

$$E = \hbar\omega(n+\tfrac{1}{2}) = \hbar\sqrt{\frac{k+\alpha}{m}}(n+\tfrac{1}{2})$$

$$= \hbar\sqrt{\frac{k}{m}}\sqrt{1+\frac{\alpha}{k}}(n+\tfrac{1}{2})$$

do binomial expansion, which requires $\frac{\alpha}{k} < 1$

$$= \hbar\omega_0(n+\tfrac{1}{2})\left(1+\tfrac{1}{2}\frac{\alpha}{k} + \frac{\frac{1}{2}(\frac{1}{2}-1)}{2}\left(\frac{\alpha}{k}\right)^2 + \mathcal{O}\left(\frac{\alpha}{k}\right)^3\right)$$

or $\boxed{\alpha < k}$

$$\boxed{E = \hbar\omega_0(n+\tfrac{1}{2})\left(1+\tfrac{1}{2}\frac{\alpha}{k} - \tfrac{1}{8}\left(\frac{\alpha}{k}\right)^2 + \cdots\right)}$$

$$\boxed{\begin{aligned} \text{where } E_n^{(1)} &= \hbar\omega_0(n+\tfrac{1}{2})\left(\tfrac{1}{2}\frac{\alpha}{k}\right) \\ E_n^{(2)} &= \frac{-1}{8}\left(\frac{\alpha}{k}\right)^2\hbar\omega_0(n+\tfrac{1}{2}) \end{aligned}}$$

Now use perturbation theory:

$$E^{(1)} = \langle n^{(0)} | \tfrac{1}{2}\alpha x^2 | n^{(0)} \rangle$$

use $x = \sqrt{\frac{\hbar}{2m\omega_0}}(a_+ + a_-)$

then $x^2 = \frac{\hbar}{2m\omega_0}(a_+^2 + a_+a_- + a_-a_+ + a_-^2)$

$$\tfrac{1}{2}\alpha\frac{\hbar}{2m\omega_0}\langle n^{(0)} | a_+^2 + a_+a_- + a_-a_+ + a_-^2 | n^{(0)} \rangle$$

$$\hookrightarrow = \tfrac{1}{2}\alpha\frac{\hbar}{2m\omega_0}\left(\cancel{\sqrt{n+1}\sqrt{n+2}\,\delta_{n,n+2}} + (\sqrt{n}\sqrt{n} + \sqrt{n+1}\sqrt{n+1})\delta_{n,n} + \cancel{\sqrt{n-1}\sqrt{n}\,\delta_{n,n-2}}\right)$$

$$E^{(1)} \stackrel{!}{=} \tfrac{1}{2}\alpha\frac{\hbar}{2m\omega_0}(2n+1)$$

Now since $k = m\omega_0^2$

then $E^{(1)} = \frac{1}{2}\frac{\alpha}{k}\cancel{m\omega_0^2}\frac{\hbar}{2\cancel{m\omega_0}}(2n+1)$

$$\boxed{E_n^{(1)} = \hbar\omega_0\left(n+\frac{1}{2}\right)\left(\frac{1}{2}\frac{\alpha}{k}\right)}$$

$$E_n^{(2)} = \frac{\left|\langle k^{(0)}|\frac{1}{2}\alpha x^2|n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$\langle k^{(0)}|\frac{1}{2}\alpha x^2|n^{(0)}\rangle = \frac{1}{2}\alpha\frac{\hbar}{2m\omega_0}\langle k^{(0)}|a_+^2 + a_+a_- + a_-a_+ + a_-a_-|n^{(0)}\rangle$$

$$= \frac{1}{2}\alpha\frac{\hbar}{2m\omega_0}\left(\sqrt{n+1}\sqrt{n+2}\,\delta_{k,n+2} + \cancel{(\sqrt{n}\sqrt{n}+\sqrt{n+1}\sqrt{n+1})\delta_{k,n}}^{0} + \sqrt{n}\sqrt{n-1}\,\delta_{k,n-2}\right)$$

$$= \frac{1}{2}\alpha\frac{\hbar}{2m\omega_0}\left(\sqrt{n+1}\sqrt{n+2}\,\delta_{k,n+2} + \sqrt{n}\sqrt{n-1}\,\delta_{k,n-2}\right)$$

then $$\left|\langle k^{(0)}|\frac{1}{2}\alpha x^2|n^{(0)}\rangle\right|^2 = \left(\frac{1}{2}\alpha\frac{\hbar}{2m\omega_0}\right)^2\left((n+1)(n+2)\,\delta_{k,n+2} + 2\sqrt{n+1}\sqrt{n+2}\sqrt{n}\sqrt{n-1}\,\cancel{\delta_{k,n+2}\delta_{k,n-2}}^{0}\right.$$
$$\left. + n(n-1)\,\delta_{k,n-2}\right)$$

$$= \frac{\alpha^2\hbar^2}{16m^2\omega_0^2}\left((n+1)(n+2)\,\delta_{k,n+2} + n(n-1)\,\delta_{k,n-2}\right)$$

then $$E_n^{(2)} = \sum_{k\neq n}\frac{\left|\langle k^0|\frac{1}{2}\alpha x^2|n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} = \frac{\frac{\alpha^2\hbar^2}{16m^2\omega_0^2}\left((n+1)(n+2)\,\delta_{k,n+2} + n(n-1)\,\delta_{k,n-2}\right)}{\hbar\omega_0(n-k)}$$

$$\Rightarrow = \frac{\alpha^2\hbar^{\cancel{2}}}{16m^2\omega_0^2}\frac{1}{\cancel{\hbar}\omega_0}\frac{(n+1)(n+2)\,\delta_{k,n+2}}{n-k} + \frac{n(n-1)\,\delta_{k,n-2}}{n-k}$$

$$\Rightarrow = \frac{\alpha^2\hbar}{16m^2\omega_0^3}\left[\frac{(n+1)(n+2)}{n-(n+2)} + \frac{n(n-1)}{n-(n-2)}\right]$$

$$= \frac{\alpha^2\hbar}{16m^2\omega_0^3} \left[\frac{(n+1)(n+2)}{-2} + \frac{n(n-1)}{2} \right]$$

$$\stackrel{!}{=} \frac{-\alpha^2\hbar}{32m^2\omega_0^3} \left[\cancel{n^2} + 3n + 2 - \cancel{n^2} + n \right]$$

$$\stackrel{!}{=} \frac{-\alpha^2\hbar}{8m^2\omega_0^3} \left(n + \frac{1}{2}\right)$$

$$\stackrel{!}{=} -\left(\frac{\alpha}{k}\right)^2 (m\omega_0^2)^2 \frac{\hbar}{8m^2\omega_0^3} \left(n+\frac{1}{2}\right)$$

$$\boxed{E_n^{(2)} \stackrel{!}{=} -\frac{1}{8}\left(\frac{\alpha}{k}\right)^2 \hbar\omega_0 \left(n+\frac{1}{2}\right)}$$

→ we see that perturbation theory results match with the results using expansion of the exact solution.

Condition of convergence when

$$|V_{kn}| \ll E_n - E_k$$

$$\frac{\alpha^2}{16} \frac{\hbar^2}{m^2\omega_0^2} \left[(n+1)(n+2)\,\delta_{k,n+2} + n(n-1)\,\delta_{k,n-2} \right] < \hbar\omega_0 (n-k)$$

then by order of magnitude:

$$\frac{\alpha^2}{16} \frac{\hbar^2}{m^2\omega_0^2} \ll \hbar\omega_0$$

$$\alpha^2 \ll \frac{16m^2\omega_0^3}{\hbar}$$

$$\boxed{\alpha \ll \sqrt{\frac{16\, m^2 \left(\frac{k}{m}\right)^{3/2}}{\hbar}}}$$

4) $E^{(1)} = \int_0^a \frac{2}{a} \sin^2\left(\frac{\pi}{a} n x\right) \alpha\, \delta(x - a/2)\, dx$

$$\stackrel{!}{=} 2\frac{\alpha}{a} \sin^2\left(\frac{\pi n}{a} \frac{a}{2}\right)$$

$$E^{(1)} \stackrel{!}{=} 2\frac{\alpha}{a} \sin^2\left(\frac{\pi n}{2}\right)$$

For $n =$ odd	,	$E^{(1)} = 2\frac{\alpha}{a}$
$n =$ even	,	$E^{(1)} = 0$

← First order correction.

$$V_{kn} = \int_0^a \frac{2}{a} \sin\left(\frac{\pi n}{a} x\right) \sin\left(\frac{\pi k}{a} x\right) \alpha\, \delta(x - a/2)\, dx$$

$$\stackrel{!}{=} 2\frac{\alpha}{a} \sin\left(\frac{\pi n}{2}\right) \sin\left(\frac{\pi k}{2}\right)$$

→ If both n, k are odd, then $V_{kn} = \pm 2\frac{\alpha}{a}$

→ If one of them is even, then $V_{kn} = 0$

$$E^{(2)}_{n,odd} = \sum_k{}' \frac{|V_{kn}|^2}{E_n - E_k} = \sum_{\substack{k \neq n \\ k = odd}} \frac{\left(2\frac{\alpha}{a}\right)^2}{\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 (n^2 - k^2)}$$

$$E^{(2)}_{n,odd} \stackrel{!}{=} \frac{8\alpha^2 m}{\pi^2 \hbar^2} \sum_{\substack{k = odd \\ k \neq n}} \frac{1}{n^2 - k^2}$$

Find $\sum_{k=\text{odd},\, k\neq n} \frac{1}{n^2-k^2} = \sum_{k=\text{odd}} \frac{1}{2n}\left(\frac{1}{k+n} - \frac{1}{k-n}\right)$

For $\sum_{\substack{k=\text{odd}\\ k\neq n\\ n=\text{odd}}} \left(\frac{1}{k+n}-\frac{1}{k-n}\right) = \left\{\frac{1}{1+n}+\frac{1}{3+n}+\cdots+\frac{1}{(n-2)+n}+\frac{1}{(n+2)+n}+\cdots\right\}$

$- \left\{\frac{1}{1-n}+\frac{1}{3-n}+\cdots+\frac{1}{(n-2)-n}+\frac{1}{(n+2)-n}+\frac{1}{(n+4)-n}+\cdots\right\}$

$= \left(\cancel{\frac{1}{1+n}}+\cancel{\frac{1}{3+n}}+\cdots+\cancel{\frac{1}{2n-2}}+\cancel{\frac{1}{2n+2}}+\cdots\right)$

$-\left(\cancel{\frac{1}{1-n}}+\cancel{\frac{1}{3-n}}+\cdots+\cancel{\frac{-1}{2}}+\cancel{\frac{1}{2}}+\cdots+\cancel{\frac{1}{n-3}}+\cancel{\frac{1}{n-1}}+\cancel{\frac{1}{1+n}}+\cancel{\frac{1}{3+n}}+\cdots\cancel{\frac{1}{2n-2}}+\frac{1}{2n}+\cancel{\frac{1}{2n+2}}+\cdots\right)$

↳ $= -\frac{1}{2n}$ ← we basically expect all terms to cancel except the $-1/2n$ term in $\sum_k -\left(\frac{1}{k-n}\right)$.

So $\sum_k \frac{1}{n^2-k^2} = \frac{1}{2n}\sum_k\left(\frac{1}{k+n}-\frac{1}{k-n}\right) = \frac{1}{2n}\left(-\frac{1}{2n}\right) = -\frac{1}{4n^2}$

$\Rightarrow E_n^{(2)} = \frac{8\alpha^2 m}{\pi^2\hbar^2}\sum_{\substack{k=\text{odd}\\ k\neq n}}\frac{1}{n^2-k^2} = \sum_{n=\text{odd}}\frac{8\alpha^2 m}{\pi^2\hbar^2}\frac{1}{-4n^2}$ when both n, k are odd.

$\Rightarrow E_n^{(2)} = 0$ when one of them is even.

expect applicability when

$|V_{kn}| \ll |E_n^{(0)} - E_k^{(0)}|$

For a single level difference, i.e. let $n=1$, $k=2$.

$\frac{2\alpha}{a} \ll \left|\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2(1^2-2^2)\right|$

$$\boxed{\alpha \ll 3\frac{\hbar^2 a}{4m}\left(\frac{\pi}{a}\right)^2}$$