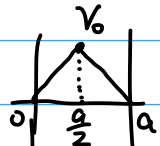


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HW#18

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

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

a) $V(x) = \frac{V_0}{a}(a - |2x - a|)$:  ← even in $\frac{a}{2}$.

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

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

total even func about $a/2$

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

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

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

If $n = \text{even}$, $1 - \cos(\pi n) = 0$, then $E_n^{(1)} = \frac{V_0}{2}$

If $n = \text{odd}$, $1 - \cos(\pi n) = 2$, then $E_n^{(1)} = V_0 \frac{4 + (\pi n)^2}{2(\pi n)^2} = V_0 \left(\frac{1}{(\pi n)^2} + \frac{1}{2} \right)$

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

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

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

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

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

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

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

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

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

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 independent of n .

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

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

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

then we know Harmonic Oscillator has energy

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

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

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

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

or $\boxed{\alpha < k}$

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

Now use perturbation theory:

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

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

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

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

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

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

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

Now since $k = m\omega_0^2$

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

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

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

$$\begin{aligned} \langle k^{(0)} | \frac{1}{2} \alpha x^2 | n^{(0)} \rangle &= \frac{1}{2} \alpha \frac{\hbar}{2m\omega_0} \langle k^{(0)} | a_f^2 + a_+ a_- + a_- a_+ + a_- a_- | n^{(0)} \rangle \\ &= \frac{1}{2} \alpha \frac{\hbar}{2m\omega_0} \left(\sqrt{n+1} \sqrt{n+2} \delta_{k,n+2} + (\sqrt{n} \sqrt{n+1} + \sqrt{n+1} \sqrt{n+1}) \cancel{\delta_{k,n}} + \sqrt{n} \sqrt{n-1} \delta_{k,n-2} \right) \\ &= \frac{1}{2} \alpha \frac{\hbar}{2m\omega_0} \left(\sqrt{n+1} \sqrt{n+2} \delta_{k,n+2} + \sqrt{n} \sqrt{n-1} \delta_{k,n-2} \right) \end{aligned}$$

$$\begin{aligned} \text{then } \left| \langle k^{(0)} | \frac{1}{2} \alpha x^2 | n^{(0)} \rangle \right|^2 &= \left(\frac{1}{2} \alpha \frac{\hbar}{2m\omega_0} \right)^2 \left((n+1)(n+2) \delta_{k,n+2} + 2\sqrt{n+1} \sqrt{n+2} \sqrt{n} \sqrt{n-1} \cancel{\delta_{k,n}} + n(n-1) \delta_{k,n-2} \right) \\ &= \frac{\alpha^2 \hbar^2}{16m^2 \omega_0^2} \left((n+1)(n+2) \delta_{k,n+2} + n(n-1) \delta_{k,n-2} \right) \end{aligned}$$

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

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

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

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

$$= \frac{-\alpha^2 \hbar}{32 m^2 \omega_0^3} [n^2 + 3n + 2 - n^2 + n]$$

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

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

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

→ 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:

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

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

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

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

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

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

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

← First order correction.

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

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

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

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

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

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

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

$$\begin{aligned} \text{For } \sum_{\substack{k=\text{odd} \\ k \neq n \\ n=\text{odd}}} \left(\frac{1}{k+n} - \frac{1}{k-n} \right) &= \left\{ \frac{1}{1+n} + \frac{1}{3+n} + \dots + \frac{1}{(n-2)+n} + \frac{1}{(n+2)+n} + \dots \right\} \\ &\quad - \left\{ \frac{1}{1-n} + \frac{1}{3-n} + \dots + \frac{1}{(n-2)-n} + \frac{1}{(n+2)-n} + \frac{1}{(n+4)-n} + \dots \right\} \\ &= \left(\cancel{\frac{1}{1+n}} + \cancel{\frac{1}{3+n}} + \dots + \cancel{\frac{1}{2n-2}} + \cancel{\frac{1}{2n+2}} + \dots \right) \\ &\quad - \left(\cancel{\frac{1}{1-n}} + \cancel{\frac{1}{3-n}} + \dots + \cancel{\frac{1}{2-n}} + \cancel{\frac{1}{2}} + \dots + \cancel{\frac{1}{n-3}} + \cancel{\frac{1}{n-1}} + \frac{1}{1+n} + \frac{1}{3+n} + \dots + \cancel{\frac{1}{2n-2}} + \frac{1}{2n} + \cancel{\frac{1}{2n+2}} + \dots \right) \\ \hookrightarrow &= -\frac{1}{2n} \quad \leftarrow \text{we basically expect all terms to cancel except the } -\frac{1}{2n} \text{ term in } \sum_k \left(\frac{1}{k-n} \right). \end{aligned}$$

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

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

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

expect applicability when

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

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

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

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