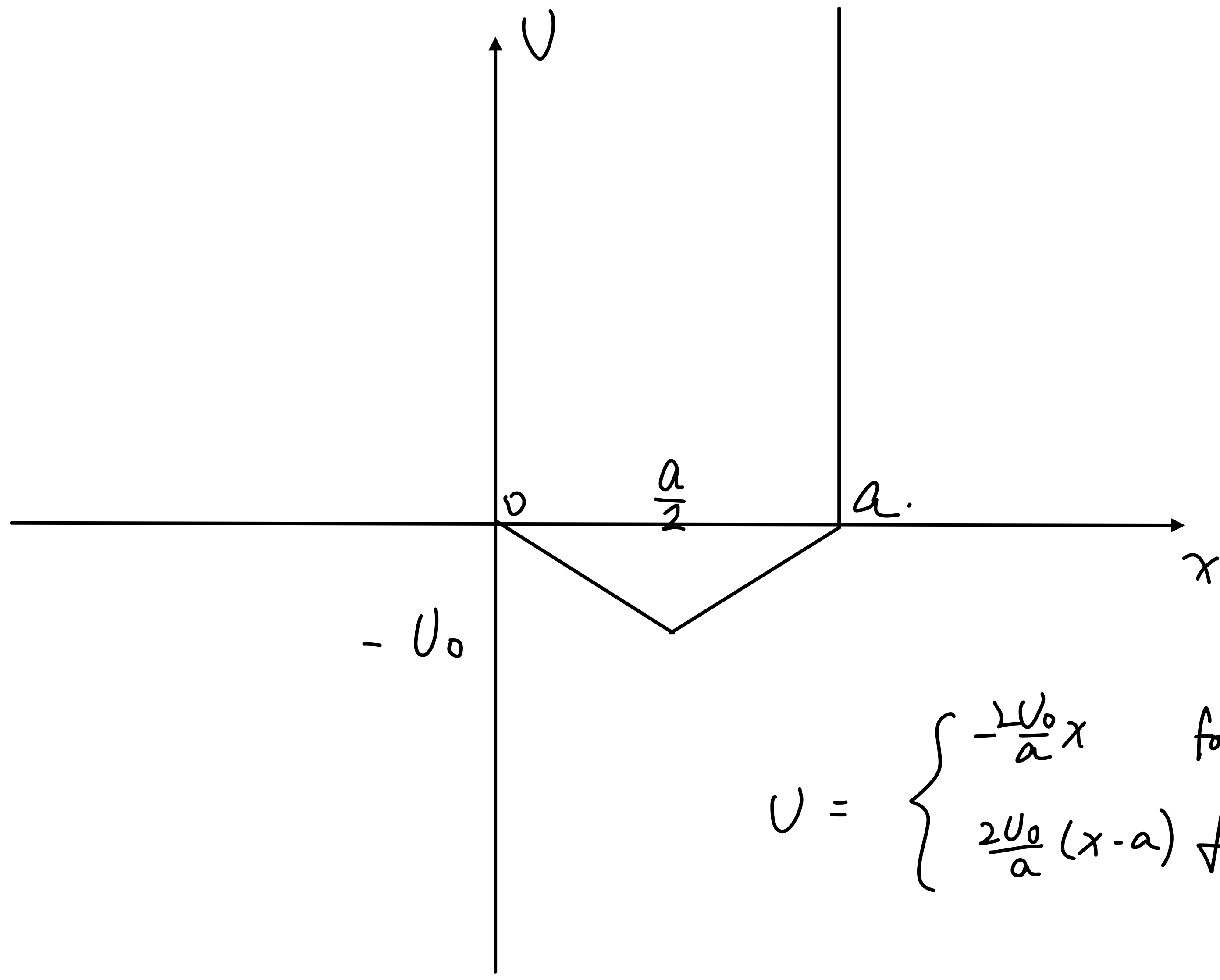
SQ4



$$U = \begin{cases} -\frac{2U_0}{a}x & \text{for } 0<x<\frac{a}{2} \\ \frac{2U_0}{a}(x-a) & \text{for } \frac{a}{2}<x<a \end{cases}$$

Since the potential $U(x)$ is symmetric about $x=\frac{a}{2}$, the probability density $|\psi|^2$ of the particle inside is also symmetric about $x=\frac{a}{2}$.

Thus wavefunction $\psi(x)$ of the particle is either symmetric or antisymmetric about $x=\frac{a}{2}$.

For ground state, the wave function should have no node, thus the ground state wavefunction should be symmetric about $x=\frac{a}{2}$.

Since we know the potential is symmetric, we should also use symmetric trial wavefunction.

Thus $\psi_1(x)$ and $\psi_3(x)$ would be appropriate for constructing wavefunction when using variational principle.

If we insist on adding anti symmetric wavefunction, e.g $\psi_2(x)$

$$\phi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3$$

$$H_{11} = E_1 + \int U\psi_1^2 dx.$$

$$H_{22} = E_2 + \int U\psi_2^2 dx$$

$$H_{33} = E_3 + \int U\psi_3^2 dx$$

$H_{12} = \int_0^a \psi_1 U \psi_2 \, dx.$

$\because$ $\psi_1 U \psi_2$ is antisymmetric about $x = \frac{a}{2}$, the integral is also antisymmetric.

Thus $H_{12} = 0$, same goes for H_{21}, H_{13} and H_{31}

$$H_{12} = H_{21} = H_{23} = H_{32} = 0$$

$$H_{13} = H_{31} = \int \psi_3 U \psi_1 \, dx = \int U\psi_1\psi_3 \, dx$$

$S_{11} = S_{22} = S_{33} = 1$ $\quad\because$ ψ_n forms orthonormal set.

$s_{ij} = 0$ otherwise.

$$H = \begin{pmatrix} E_1 + \int U\psi_1^2 dx & 0 & \int U\psi_1\psi_3 \, dx \\ 0 & E_2 + \int U\psi_2^2 dx & 0 \\ \int U\psi_1\psi_3 \, dx & 0 & E_3 + \int U\psi_3^2 dx \end{pmatrix}$$

Either: $E_2 + \int U\psi_2^2 dx = E \Rightarrow$ only ψ_2 is involved

or $c_2 = 0 \Rightarrow \psi_2$ is not involved in the trial wavefunction, both cases are undesirable.

For $\phi = c_1\psi_1 + c_3\psi_3$

$$\hat{H} = \begin{pmatrix} E_1 + \int U\psi_1^2 dx & \int U\psi_1\psi_3 dx \\ \int U\psi_1\psi_3\, dx & E_3 + \int U\psi_3^2 dx \end{pmatrix}$$

$$\int U\psi_1^2 dx$$

$\because U\psi_1^2$ is symmetric about $x = \frac{a}{2}$.

$$= 2\int_0^{\frac{a}{2}} -\frac{4U_0}{a^2}\, x\sin^2\left(\frac{\pi x}{a}\right) dx$$

$$= -\frac{8U_0}{a^2}\left(\frac{x^2}{4} - \frac{x\sin\frac{2\pi x}{a}}{4\frac{\pi}{a}} - \frac{\cos\frac{2\pi x}{a}}{8\frac{\pi^2}{a^2}}\right)\Bigg|_0^{\frac{a}{2}}$$

$$= -\frac{2U_0}{a^2}\left(\frac{a^2}{4} - \frac{a^2}{2\pi^2} - \frac{a^2}{2\pi^2}\right)$$

$$= -U_0\left(\frac{1}{2} + \frac{2}{\pi^2}\right)$$

$$\boxed{\begin{aligned} &\int y\sin^2(by)\,dy \\ &= \frac{1}{b^2}\int x\sin^2 x\, dx. \\ &= \frac{1}{b^2}\int \frac{x}{2}(1-\cos 2x)\,dx \\ &= \frac{1}{b^2}\left(\frac{x^2}{4} - \frac{x\sin 2x}{4} - \frac{\cos 2x}{8}\right) \\ &= \frac{y^2}{4} - \frac{y\sin 2by}{4b} - \frac{\cos 2by}{8b^2} \end{aligned}}$$

$$\int U\psi_3^2 dx$$

$$= -\frac{8U_0}{a^2}\left(\frac{x^2}{4} - \frac{x\sin\frac{6\pi x}{a}}{4\frac{3\pi}{a}} - \frac{\cos\frac{6\pi x}{a}}{8\frac{9\pi^2}{a^2}}\right)\Bigg|_0^{\frac{a}{2}}$$

$$= -\frac{2U_0}{a^2}\left(\frac{a^2}{4} + \frac{a^2}{18\pi^2} + \frac{a^2}{18\pi^2}\right)$$

$$\therefore -U_0\left(\frac{1}{2} + \frac{2}{9\pi^2}\right)$$

$$\int U \psi_1 \psi_3 \, dx.$$

$$= 2\int_0^{\frac{a}{2}} \frac{4U_0}{a^2} x \sin\frac{\pi x}{a} \sin\frac{3\pi x}{a} \, dx$$

$$= 2\int_0^{\frac{a}{2}} \frac{4U_0}{a^2} \frac{x}{2}\left(\cos\frac{2\pi x}{a} - \cos\frac{4\pi x}{a}\right) dx$$

$$= \frac{4U_0}{a^2}\left(\frac{x\sin\frac{2\pi}{a}x}{\frac{2\pi}{a}} - \frac{\cos\frac{2\pi}{a}x}{\frac{4\pi^2}{a^2}} + \frac{x\sin\frac{4\pi x}{a}}{\frac{4\pi}{a}} - \frac{\cos\frac{4\pi}{a}x}{\frac{16\pi^2}{a^2}} \right)\Bigg|_0^{\frac{a}{2}}$$

$$= \frac{4U_0}{a^2}\left(\frac{a^2}{2\pi^2}\right)$$

$$= \frac{2U_0}{\pi^2}$$

$$\int y \cos by \, dy$$

$$= \frac{1}{b^2}\int x\cos x \, dx$$

$$= \frac{1}{b^2}(x\sin x - \cos x)$$

$$= \frac{y\sin by}{b} - \frac{\cos by}{b^2}$$

For $\begin{pmatrix} a & c \\ d & b \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \lambda\begin{pmatrix} x \\ y \end{pmatrix}$

$$(\lambda - a)(\lambda - b) - cd = 0$$

$$\lambda^2 - (a+b)\lambda + ab - cd$$

$$\lambda = \frac{a+b \pm \sqrt{(a-b)^2 + 4cd}}{2}$$

$$a+b = 10E_1 - U_0\left(1 + \frac{20}{9\pi^2}\right)$$

$$a-b = -8E_1 - U_0\frac{16}{9\pi^2}$$

$$E = \frac{10E_1 - U_0\left(1+\frac{20}{9\pi^2}\right) \pm \sqrt{8^2\left(E_1 + \frac{2U_0}{9\pi^2}\right)^2 + 4\left(\frac{2U_0}{\pi^2}\right)^2}}{2}$$

$$= \frac{10E_1 - U_0\left(1+\frac{20}{9\pi^2}\right) \pm 8E_1\sqrt{\left(1+\frac{2U_0}{9\pi^2 E_1}\right)^2 + \left(\frac{U_0}{2\pi^2 E_1}\right)^2}}{2}$$

$$= \frac{10E_1 - U_0\left(1+\frac{20}{9\pi^2}\right) \pm 8E_1\left(1 + \frac{2}{9\pi^2}\frac{U_0}{E_1} + \frac{U_0^2}{8\pi^4 E_1^2}\right)}{2}$$

$\left(\text{For } \frac{U_0}{E_1} \ll 1\right)$

$$E_{min} = E_1 - U_0\left(\frac{1}{2} + \frac{2}{\pi^2} + \frac{U_0}{2\pi^4 E_1}\right)$$

$$\frac{c_3}{c_1} = \frac{\frac{U_0^2}{2\pi^4 E_1}}{\frac{2U_0}{\pi^2}}$$

$$= \frac{U_0}{4\pi^4 E_1} \approx 0.00257\frac{U_0}{E_1} \quad \text{very small!}$$

SQ5

a) $E_1^{(1)} = \langle \psi_1^{(0)} | U | \psi_1^{(0)} \rangle$

$= -U_0 \left(\frac{1}{2} + \frac{2}{\pi^2} \right)$ $\Longleftrightarrow$ consistent with variational method

$E_1^{(2)} = \sum_{n=2}^{\infty} \frac{|\langle \psi_n^{(0)} | U | \psi_1^{(0)} \rangle|^2}{E_1^{(0)} - E_n^{(0)}}$

$= \sum_{n=1}^{\infty} -\frac{1}{((2n+1)^2-1)E_1} \left(U_0 \frac{((2n^2+2n+1)(-1)^n - 2n - 1)}{\pi^2 n^2 (n+1)^2} \right)^2$

Contribution from ψ_3:

$E_1^{(2)} = -\frac{1}{8E_1} \left(\frac{U_0(-5-3)}{\pi^2 4} \right)^2$

$= -\frac{U_0^2}{2\pi^4 E_1}$ (also consistent with variational method)

Since all higher terms are negative, perturbation theory gives a lower (thus better) estimation on ground state energy.

If we only consider contribution from ψ_1 and ψ_3, both method yield consistent result.

$\psi_1^{(1)} = \sum_{n=2}^{\infty} \frac{\langle \psi_n^{(0)} | U | \psi_1^{(0)} \rangle}{E_1^{(0)} - E_n^{(0)}} \psi_n^{(0)}$

$= \sum_{n=1}^{\infty} -\frac{1}{((2n+1)^2-1)E_1^{(0)}} \frac{U_0((2n^2+2n+1)(-1)^n - 2n - 1)}{\pi^2 n^2 (n+1)^2} \psi_n^{(0)}$

$= \sum_{n=1}^{\infty} -\frac{U_0}{4E_1^{(0)}} \frac{(2n^2+2n+1)(-1)^n - 2n - 1}{\pi^2 n^3 (n+1)^3} \psi_n^{(0)}$

Consider $\psi_3^{(0)}$ term only:

$\psi_1^{(1)} = -\frac{U_0}{4E_1^{(0)}} \frac{-5-3}{\pi^2 8}$

$= \frac{U_0}{4\pi^2 E_1^{(0)}} \psi_3^{(0)}$ (also consistent with variational method)

(See Appendix for detailed calculation of $\langle \psi_m | U | \psi_n \rangle$)

Consider 1st excited state

$$E_2^{(1)} = \langle \psi_2 | U | \psi_2 \rangle$$

$$= -U_0 \left(\frac{1}{2} + \frac{1}{2\pi^2} \right)$$

$$E_2^{(2)} = \sum_{n \neq 2}^{\infty} \frac{|\langle \psi_n | U | \psi_2 \rangle|^2}{E_2^{(0)} - E_n^{(0)}}$$

$$= \sum_{m=2}^{\infty} -\frac{1}{((2m)^2 - 4)E_1^{(0)}} \left(\frac{8U_0 (16m \cos^3 (\frac{m\pi}{2}))}{\pi^2 ((2m)^2 - 4)^2} \right)^2$$

$$= \sum_{m=2}^{\infty} -\frac{1}{4(m+1)(m-1)E_1^{(0)}} \left(\frac{128 U_0 m \cos^2 (\frac{m\pi}{2})}{4\pi^2 (m+1)(m-1)} \right)^2$$

$$= \sum_{l=1}^{\infty} -\frac{1}{(4(2l+1)(2l-1))^3 E_1^{(0)}} (128 U_0)^2$$

$$= \sum_{l=1}^{\infty} -\frac{256 U_0^2}{\pi^4 (2l+1)^3 (2l-1)^3 E_1^{(0)}} \approx 0.0981 \frac{U_0^2}{E_1^{(0)}}$$

Only $\psi_{n=4l+2}$ would contribute to $E_2^{(2)}$ for positive integer l

Appendix

$$\int \psi_m U \psi_n \, dx.$$

$$= \int \frac{2}{a} U \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi x}{a}\right) dx.$$

$$= \frac{2}{a}\left(\int_0^{\frac{a}{2}} -\frac{2U_0}{a} x \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)dx + \int_{\frac{a}{2}}^{a} \frac{2U_0}{a}(x-a)\sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)dx\right.$$

$$= \frac{4U_0}{a^2}\left(\int_0^{\frac{a}{2}} -x\sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)dx + \int_{\frac{a}{2}}^{a} x\sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)dx\right) - \int_{\frac{a}{2}}^{a} a \sin\frac{m\pi x}{a}\sin\frac{n\pi x}{a} dx\Big)$$

Math tools:

$$\sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right) = \cos\frac{(m-n)\pi x}{a} - \cos\frac{(m+n)\pi x}{a}$$

$$\int x\cos bx \, dx = \frac{x\sin bx}{b} + \frac{\cos bx}{b^2}.$$

Combining 2 equations,

$$\int x \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)dx$$

$$= \int\left(x\cos\left(\frac{m-n}{a}\pi x\right) - x\cos\left(\frac{m+n}{a}\pi x\right)\right)dx$$

$$= \frac{ax}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) + \frac{a^2}{(m-n)^2\pi^2}\cos\left(\frac{m-n}{a}\pi x\right) - \frac{ax}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right) - \frac{a^2}{(m+n)^2\pi^2}\cos\left(\frac{m+n}{a}\pi x\right) + C$$

$$S = \int_{\frac{a}{2}}^{a}\sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)dx$$

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

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

$$= \frac{a}{\pi}\left(-\frac{1}{m-n}\sin\left(\frac{m-n}{2}\pi\right) + \frac{1}{m+n}\sin\left(\frac{m+n}{2}\pi\right)\right)$$

Sub the upper limits and lower limits.

$$I(0) = \text{Sub } 0: \quad \frac{a^2}{(m-n)^2\pi^2} - \frac{a^2}{(m+n)^2\pi^2}.$$

$$I\left(\frac{a}{2}\right) = \text{Sub } \frac{a}{2}: \quad \frac{a^2}{2(m-n)\pi}\sin\left(\frac{m-n}{2}\pi\right) + \frac{a^2}{(m-n)^2\pi^2}\cos\left(\frac{m-n}{2}\pi\right) - \frac{a^2}{2(m+n)\pi}\sin\left(\frac{m+n}{2}\pi\right) - \frac{a^2}{(m+n)^2\pi^2}\cos\left(\frac{m+n}{2}\pi\right)$$

$$I(a): \text{Sub } a: \quad \frac{a^2}{(m-n)^2\pi^2}\cos((m-n)\pi) - \frac{a^2}{(m+n)^2\pi^2}\cos((m+n)\pi)$$

$$= \frac{a^2}{(m-n)^2\pi^2}(-1)^{m-n} - \frac{a^2}{(m+n)^2\pi^2}(-1)^{m+n}.$$

If m and n are of same parity (i.e. both odd or both even)

$$I\left(\frac{a}{2}\right) = \frac{a^2}{(m-n)^2\pi^2}(-1)^{\frac{m-n}{2}} - \frac{a^2}{(m+n)^2\pi^2}(-1)^{\frac{m+n}{2}}$$

$$I(a) = \frac{a^2}{(m-n)^2\pi^2} - \frac{a^2}{(m+n)^2\pi^2} = I(0)$$

$$S = 0$$

$\int \psi_m U \psi_n \, dx$ for m, n same parity.

$$= \frac{4U_0}{a^2}\left(-I\left(\frac{a}{2}\right) + I(0) + I(a) - I\left(\frac{a}{2}\right)\right)$$

$$= -\frac{8U_0}{a^2}\left(I\left(\frac{a}{2}\right) - I(0)\right)$$

$$= -\frac{8U_0}{a^2}\left(\frac{a^2}{(m-n)^2\pi^2}\left((-1)^{\frac{m-n}{2}}+1\right) - \frac{a^2}{(m+n)^2\pi^2}\left((-1)^{\frac{m+n}{2}}+1\right)\right)$$

$$= -\frac{8U_0}{\pi^2}\left(\frac{(-1)^{\frac{m-n}{2}}+1}{(m-n)^2\pi^2} - \frac{(-1)^{\frac{m+n}{2}}+1}{(m+n)^2\pi^2}\right)$$

For m and n of different parity.

$$I\left(\frac{a}{2}\right) = \frac{a^2}{2(m-n)\pi}(-1)^{\frac{m-n-1}{2}} - \frac{a^2}{2(m+n)\pi}(-1)^{\frac{m+n-1}{2}}$$

$$I(a) = -I(0)$$

$$S = \frac{a^2}{(m-n)\pi}(-1)^{\frac{m-n-1}{2}} - \frac{a^2}{2(m+n)\pi}(-1)^{\frac{m+n-1}{2}} = 2I\left(\frac{a}{2}\right)$$

$\therefore \int \psi_m V \psi_n$ for m, n opposite parity

$$= \frac{4V_0}{a}\left(2I\left(\frac{a}{2}\right) - S\right)$$

$$= 0$$