4

2/ #10, pg 1208 CDL

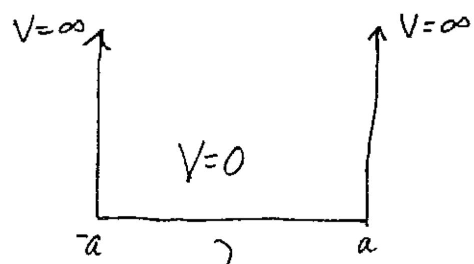
20/

$$\langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

=5

10

5



$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2$

a) $\psi(x) = \begin{cases} a^2 - x^2 & -a \le x \le a \\ 0 & \text{elsewhere} \end{cases}$

FIRST FIND $\langle \psi | \psi \rangle = \int_{-a}^{a} (a^2 - x^2)^2 \, dx$

$$= \int_{-a}^{a} (a^4 - 2a^2x^2 + x^4)\, dx$$

$$= 2\int_0^a (a^4 - 2a^2x^2 + x^4)\, dx$$

$$= 2a^5 - 2\left(\tfrac{2}{3}a^5\right) + \tfrac{2}{5}a^5$$

$$= a^5\left(2 - \tfrac{4}{3} + \tfrac{2}{5}\right)$$

$$= \underline{\underline{\tfrac{16}{15}a^5}}$$

$$\langle \psi(x) | -\tfrac{\hbar^2}{2m}\nabla^2 | \psi(x) \rangle = -\tfrac{\hbar^2}{2m}\int_{-a}^{a} (a^2 - x^2)\frac{d^2}{dx^2}(a^2 - x^2)\, dx$$

$$= \frac{-\hbar^2}{2m}\int_{-a}^{a} (a^2 - x^2)\,{-2}\, dx$$

$$= \tfrac{\hbar^2}{m} \times 2\int_0^a (a^2 - x^2)\, dx$$

$$= \tfrac{\hbar^2}{m}\left(2a^3 - \tfrac{2}{3}a^3\right)$$

$$= \frac{4\hbar^2 a^3}{3m}$$

$$\langle H \rangle = \frac{4\hbar^2 a^3}{3m}\,\frac{15}{16a^5} = \underline{\underline{\frac{5}{4}\frac{\hbar^2}{ma^2}}}$$

TRUE VALUE IS $\frac{\pi^2\hbar^2}{8ma^2}$ $\Rightarrow$ 1.3% error

$$\psi(x) = \begin{cases} (a^2 - x^2)(a^2 - \alpha x^2) & -a \le x \le a \\ 0 & \text{elsewhere} \end{cases}$$

Evaluate the integrals (optional):

$$\langle\psi|\psi\rangle = \int_{-a}^{a} (a^2-x^2)^2(a^2-\alpha x^2)^2\, dx$$

$$= \int_{-a}^{a} (a^4 - 2a^2x^2 + x^4)(a^4 - 2\alpha a^2 x^2 + \alpha^2 x^4)\, dx$$

$$= \int_{-a}^{a} (a^8 - 2a^6x^2\alpha + a^4\alpha^2x^4 - 2a^6x^2 + 4\alpha a^4 x^4 - 2a^2\alpha^2 x^6$$
$$+ a^4x^4 - 2\alpha a^2 x^6 + \alpha^2 x^8)\, dx$$

$$= 2\int_0^a (\qquad\qquad)\, dx$$

$$= 2\Big[\, a^9 - \tfrac{2}{3}a^9\alpha + \tfrac{1}{5}a^9\alpha^2 - \tfrac{2}{3}a^9 + \tfrac{4}{5}\alpha a^9 - \tfrac{2}{7}a^9\alpha^2$$
$$+ \tfrac{1}{5}a^9 - \tfrac{2}{7}\alpha a^9 + \tfrac{\alpha^2}{9}a^9 \,)$$

$$= a^9\Big[\left(\tfrac{2}{5} - \tfrac{4}{7} + \tfrac{2}{9}\right)\alpha^2 + \left(-\tfrac{4}{3} + \tfrac{8}{5} - \tfrac{4}{7}\right)\alpha$$
$$+ \left(2 - \tfrac{4}{3} + \tfrac{2}{5}\right)\Big]$$

$$= a^9\left[\frac{16}{315}\alpha^2 + \frac{-32}{105}\alpha + \frac{16}{15}\right]$$

$$H|\psi\rangle = -\hbar^2/2m \; d^2/dx^2 \left(a^4 - (\alpha+1)a^2x^2 + \alpha x^4 \right)$$

$$= -\hbar^2/2m \; \left(-2(\alpha+1)a^2 + 12\alpha x^2 \right)$$

$$\langle\psi|H|\psi\rangle = -\frac{\hbar^2}{2m} \int_{-a}^{a} (a^4 - (\alpha+1)a^2x^2 + \alpha x^4)(12\alpha x^2 - 2(\alpha+1)a^2)\, dx$$

$$= -\frac{\hbar^2}{m} \int_0^a dx\, (12a^4x^2\alpha - 12\alpha(\alpha+1)a^2x^4 + 12\alpha^2 x^6$$
$$- 2(\alpha+1)a^6 + 2(\alpha+1)^2 a^4 x^2 + -2\alpha(\alpha+1)a^2x$$

$$\langle \psi | H | \psi \rangle = +\frac{\hbar^2 a^7}{m}\left[\left(-\frac{2}{3}+\frac{12}{5}+\frac{2}{5}-\frac{12}{7}\right)\alpha^2 + \left(2-4-\frac{4}{3}+\frac{12}{5}+\frac{2}{5}\right)\alpha + \left(2-\frac{2}{3}\right)\right]$$

$$= \frac{\hbar^2}{m} a^7 \left(\frac{44}{105}\alpha^2 - \frac{8}{15}\alpha + \frac{4}{3}\right)$$

b)

$$\therefore \langle H \rangle = \frac{\frac{\hbar^2}{m} a^7 \left(\frac{44}{105}\alpha^2 - \frac{8}{15}\alpha + \frac{4}{3}\right)}{a^9 \left(\frac{16}{315}\alpha^2 - \frac{32}{105}\alpha + \frac{16}{15}\right)}$$

$$= \frac{\hbar^2}{ma^2}\left[\frac{(44\alpha^2 - 56\alpha + 140)}{(16\alpha^2 - 96\alpha + 336)} \times \frac{\overset{33}{\cancel{315}}}{\cancel{105}}\right]$$

$$= \frac{\hbar^2}{ma^2}\left[\frac{132\alpha^2 - 168\alpha + 420}{16\alpha^2 - 96\alpha + 336}\right]$$

$$= \frac{\hbar^2}{ma^2}\left[\frac{4}{8}\left(\frac{33\alpha^2 - 42\alpha + 105}{2\alpha^2 - 12\alpha + 42}\right)\right]$$

$$= \frac{\hbar^2}{2ma^2}\left(\frac{33\alpha^2 - 42\alpha + 105}{2\alpha^2 - 12\alpha + 42}\right)$$

c)

To minimize $d\langle H \rangle / d\alpha = 0$

$$\frac{d\langle H \rangle}{d\alpha} = \frac{\hbar^2}{2ma^2}\left[\frac{66\alpha - 42}{2\alpha^2 - 12\alpha + 42} - \frac{1\,(4\alpha - 12)(33\alpha^2 - 42\alpha + 105)}{(2\alpha^2 - 12\alpha + 42)^2}\right]$$

$$= 0 \quad \Rightarrow \quad 66\alpha - 42 = \frac{(4\alpha - 12)(33\alpha^2 - 42\alpha + 105)}{2\alpha^2 - 12\alpha + 42}$$

$$(66\alpha-42)(2\alpha^2-12\alpha+42) = 4(\alpha-3)(33\alpha^2-42\alpha+105)$$

$$12(11\alpha-7)(\alpha^2-6\alpha+21) = 12(\alpha-3)(11\alpha^2-14\alpha+35)$$

$$11\alpha^3-73\alpha^2+273\alpha-147 = 11\alpha^3-47\alpha^2+77\alpha-105.$$

$$\Downarrow$$

$$-26\alpha^2+196\alpha-42=0$$

$$\Downarrow$$

$$13\alpha^2-98\alpha+21=0$$

The roots will be $\dfrac{98 \pm \sqrt{98^2-4(13)(21)}}{26}.$

$$\alpha_+ = 7.318$$

$$\alpha_- = 0.221$$

$$\langle H \rangle_{\alpha_+} \approx 25.53 \frac{\hbar^2}{2ma^2} \qquad \langle H \rangle_{\alpha_-} = 2.46743 \frac{\hbar^2}{2ma^2}$$

$$E_{0_{TRUE}} = \frac{\pi^2\hbar^2}{8ma^2} = \frac{\pi^2}{4}\frac{\hbar^2}{2ma} \qquad \text{fantastic agreement!}$$

$$= 2.46740 \frac{\hbar^2}{2ma}$$

The other solution $\langle H \rangle_{\alpha+}$ is an estimate of the energy of the next higher state with even symmetry, $n=3$, which has $n^2=9$ times higher energy: $E_{n=3} = 22.2\,\hbar^2/2ma^2$. So that estimate is off by 13%.

f) The 1st excited state wave f'n is odd (grnd st. is even). ∴ simplest would be $x(a^2-x^2)$.
This makes 1st excited state orthogonal to the ground state.

Evaluate energy of first excited state (optional).

$$\langle \psi_x | \psi_x \rangle = \int_{-a}^{a} x^2(a^2-x^2)^2\,dx$$

$$= \int_{-a}^{a} a^4x^2 - 2a^2x^4 + x^6\,dx$$

$$= 2\left[\tfrac{1}{3}a^7 - \tfrac{2}{5}a^7 + \tfrac{1}{7}a^7\right]$$

$$= \frac{16}{105}a^7$$

$$\langle \psi | H | \psi \rangle = \frac{\hbar^2}{2m}\int_{-a}^{a} x(a^2-x^2)\; d^2/dx^2 \; x(a^2-x^2)\,dx$$

$$= -\frac{\hbar^2}{2m}\int_{-a}^{a} x(a^2-x^2)(-6x)\,dx$$

$$= \frac{6\hbar^2}{2m}\int_{-a}^{a} x^2a^2 - x^4 \quad dx$$

$$= \frac{6\hbar^2}{2m} \times 2\left[\tfrac{1}{3}a^5 - \tfrac{1}{5}a^5\right]$$

$$= \frac{4}{5}\frac{\hbar^2 a^5}{m}$$

$$\therefore \quad \langle H \rangle = \underline{\underline{\frac{21}{4}\frac{\hbar^2}{ma^2}}}$$

$\left(\text{TRUE } E_0 = \frac{\pi^2}{2}\frac{\hbar^2}{ma^2}\right)$.