Graduate QM

HW # 6- Solution

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① $\psi(x) = c\left(1 - \frac{|x|}{a}\right)$ ; $|x| \leq a$

this can be written as $\psi(x) = \begin{cases} c\left(1+\frac{x}{a}\right) ; & x<0 \\ c\left(1-\frac{x}{a}\right) ; & x>0 \end{cases}$

Notice that this trial wavefunction contains $|x|$ which has a discontinuity in its first derivative.

let us first normalize $\psi(x)$ to find $\underline{\underline{C}}$

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow c^2 \int_{-\infty}^{\infty} \left(1 - \frac{|x|}{a}\right)^2 dx = 1 \quad ; -a \leq x \leq a$$

$$\Rightarrow c^2\left[\int_{-a}^{0} \left(1+\frac{x}{a}\right)^2 dx + \int_{0}^{a} \left(1-\frac{x}{a}\right)^2 dx\right] = 1 \quad \Rightarrow c = \sqrt{\frac{3}{2a}}$$

now need to calculate $\langle H \rangle = \langle T \rangle + \langle V \rangle$

but the kinetic energy term $\langle T \rangle$ is tricky as it contains derivatives which are discontineous at $x=0$.

so when the first derivative of the wave function is discontineous, the correct way to calculate the kinetic energy term is

$$\langle T \rangle = \langle \psi | T | \psi \rangle = \langle \psi | \frac{p^2}{2m} | \psi \rangle = \frac{1}{2m} \langle \psi | p p | \psi \rangle \quad \text{with } p = -i\hbar \frac{d}{dx}$$

$$= \frac{1}{2m} \langle p\psi | p\psi \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\frac{d\psi}{dx}\right)^* \left(\frac{d\psi}{dx}\right) dx \quad \begin{array}{c} p = p^\dagger \\ \text{hermitian} \end{array}$$

in 3D $\langle T \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} (\vec{\nabla} \psi^*(\vec{r})) \cdot (\vec{\nabla} \psi(\vec{r}))\, d^3r$

for our problem

$$\frac{d\psi}{dx} = \begin{cases} \frac{c}{a} & ; \; x<0 \\ -\frac{c}{a} & ; \; x>0 \end{cases}$$

$$\Rightarrow \langle T \rangle = \frac{\hbar^2}{2m} \left[ \int_{-a}^{0} \left(\frac{c}{a}\right)^2 dx + \int_{0}^{a} \left(-\frac{c}{a}\right)^2 dx \right] = \frac{\hbar^2 c^2}{ma} = \frac{\hbar^2}{ma} \frac{3}{2a}$$

$$= \frac{3\hbar^2}{2ma^2}$$

for the potential energy term, there is no problem as it has no derivatives

$$\langle V \rangle = \int_{-\infty}^{\infty} V \psi^* \psi \, dx \quad ; \quad V \text{ is real } = \tfrac{1}{2} m \omega^2 x^2 \; (H.O)$$

$$= c^2 \underbrace{\int_{-a}^{a} \tfrac{1}{2} m \omega^2 x^2 \left(1 - \frac{|x|}{a}\right)^2 dx}_{\text{even}}$$

$$= 2c^2 \frac{1}{2} m \omega^2 \underbrace{\int_{0}^{a} x^2 \left(1 - \frac{x}{a}\right)^2 dx}_{\frac{a^3}{30}}$$

$$= \frac{3}{2a} m \omega^2 \frac{a^3}{30} = \frac{1}{20} m \omega^2 a^2$$

$$\Rightarrow \langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{3\hbar^2}{2ma^2} + \frac{1}{20} m \omega^2 a^2$$

to minimize $\langle H \rangle$, take $\frac{\partial \langle H \rangle}{\partial a} = 0$

$$\frac{\partial}{\partial a}\langle H\rangle = \frac{3}{2}\frac{\hbar^2}{m}\left(\frac{-2}{a^3}\right) + \frac{1}{10} m\omega^2 a = 0$$

$$\Rightarrow a^4 = \frac{30\hbar^2}{m^2\omega^2}$$

$$\Rightarrow a^2 = \sqrt{30}\,\frac{\hbar}{m\omega}$$

$$\Rightarrow E_{g.s} = \frac{3\hbar^2}{2ma^2} + \frac{1}{20} m\omega^2 a^2$$

$$= \frac{3\hbar^2}{2m\left(\sqrt{30}\frac{\hbar}{m\omega}\right)} + \frac{1}{20} m\omega^2\left(\sqrt{30}\frac{\hbar}{m\omega}\right)$$

$$= \left(\frac{3}{2\sqrt{30}} + \frac{\sqrt{30}}{20}\right)\hbar\omega = \frac{3}{\sqrt{30}}\hbar\omega = \underbrace{0.548\,\hbar\omega}$$

this result is close to the exact value which is

$\frac{1}{2}\hbar\omega = 0.5\,\hbar\omega$

$$\%\ \text{diff} = \frac{0.548 - 0.500}{0.500} \times 100\% = 9.6\%$$

which lies within less than 10 percent of the exact value

Q. E. D

② $V(x) = g\,|x|$

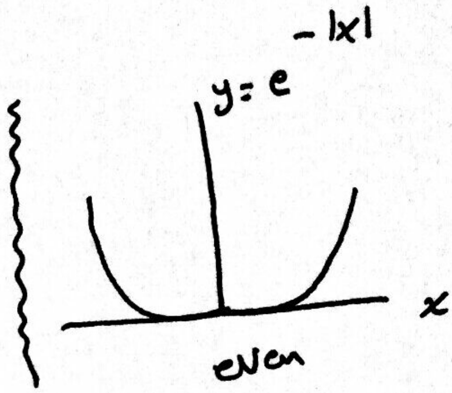
$\psi(x) = Ae^{-\alpha|x|}$ even  where $|x| = \begin{cases} -x \; ; & x<0 \\ x \; ; & x>0 \end{cases}$

normalize to find A  $\frac{d}{dx}|x| = \begin{cases} -1 \; ; & x<0 \\ 1 \; ; & x>0 \end{cases}$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$2A^2 \int_0^{\infty} e^{-2\alpha x} dx = 2A^2 \frac{1}{(2\alpha)^1} = 1 \Rightarrow A = \sqrt{\alpha}$$

$$\therefore \quad \psi(x) = Ae^{-\alpha|x|} = \begin{cases} Ae^{\alpha x} \; ; & x<0 \\ Ae^{-\alpha x} \; ; & x>0 \end{cases}$$




$$\frac{d\psi}{dx} = \begin{cases} \alpha Ae^{\alpha x} \; ; & x<0 \\ -\alpha Ae^{-\alpha x} \; ; & x>0 \end{cases}$$

$$\langle T \rangle = \frac{\hbar^2}{2m}\left[\int_{-\infty}^{0} \alpha^2 A^2 e^{2\alpha x} dx + \int_0^{\infty} \alpha^2 A^2 e^{-2\alpha x} dx\right]$$

$$= \frac{\hbar^2\alpha^2 A^2}{2m}\left[2\int_0^{\infty} e^{-2\alpha x} dx\right] = \frac{\hbar^2 \alpha^2 A^2}{m}\left[\frac{1}{2\alpha}\right] = \frac{\hbar^2 A^2}{2m}\alpha$$

$$= \frac{\hbar^2\alpha^2}{2m} \; ; \text{ when } A^2 = \alpha$$

Now

$$\langle V \rangle = \int_{-\infty}^{\infty} V\psi^*\psi\, dx = A^2 \underbrace{\int_{-\infty}^{\infty} g\,|x|\, e^{-\alpha|x|} e^{-\alpha|x|} dx}_{\text{even}}$$

$$= A^2 g\, 2\int_0^{\infty} x e^{-2\alpha x} dx = 2A^2 \frac{1\,g}{(2\alpha)^2}$$

$$= \frac{gA^2}{2\alpha^2} = \frac{g}{2\alpha}$$

$$\therefore \langle H \rangle = \frac{\hbar^2 \alpha^2}{2m} + \frac{g}{2\alpha}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 \quad \Rightarrow \quad \frac{\hbar^2 \alpha}{m} - \frac{g}{2\alpha^2} = 0$$

$$\Rightarrow \quad \alpha = \left( \frac{mg}{2\hbar^2} \right)^{1/3}$$

$$\Rightarrow E_{g.s} = \langle H \rangle \Big|_{\alpha = \left(\frac{mg}{2\hbar^2}\right)^{1/3}}$$

$$= \frac{\hbar^2}{2m} \left( \frac{m^2 g^2}{4\hbar^4} \right)^{1/3} + \frac{g}{2} \left( \frac{2\hbar^2}{mg} \right)^{1/3}$$

$$= \left[ \frac{1}{2} \left( \frac{1}{4} \right)^{1/3} + \frac{1}{2} (2)^{1/3} \right] \left( \frac{g^2 \hbar^2}{m} \right)^{1/3}$$

$$= 0.945 \left( \frac{g^2 \hbar^2}{m} \right)^{1/3}$$

which is somehow close to the exact value $0.809 \left( \frac{g^2\hbar^2}{m} \right)^{1/3}$.

we see that if we compare this result with that evaluated in the class for Gaussian wave function $\psi(x) = A e^{-bx^2}$ ; we Notice that the Gaussian is beter to represent the wave function as it gives much closer value to the exact value.

③ Again $V(x) = g|x|$

ⓐ
$$\psi(x) = c(a^2 - |x|^2) = \begin{cases} c(a^2 - x^2) \,; & x < 0 \\ c(a^2 - x^2) \,; & x > 0 \end{cases}$$

Normalize $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

$$c^2 \int_{-a}^{a} (a^2 - x^2)^2 dx = 1 \implies 2c^2 \int_0^a (a^2 - x^2)^2 dx = 1$$

$$\implies c = \sqrt{\frac{15}{16} \frac{1}{a^5}}$$

$$\langle T \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\frac{d\psi}{dx}\right)^* \left(\frac{d\psi}{dx}\right) dx \;; \quad \psi'(x) = \begin{cases} -2cx \,; & x < 0 \\ -2cx \,; & x > 0 \end{cases}$$

$$= \frac{\hbar^2}{2m} \left[ \int_{-a}^{0} (-2cx)^2 dx + \int_0^a (-2cx)^2 dx \right\}$$

$$= \frac{\hbar^2}{2m} 2 \int_0^a (-2cx)^2 dx = \frac{4}{3} \frac{\hbar^2 a^3}{m} c^2 = \frac{5}{4} \frac{\hbar^2}{ma^2}$$

Now $$\langle V \rangle = \int_{-a}^{a} V \psi^* \psi = c^2 g \int_{-a}^{a} |x| (a^2 - |x|^2)^2$$

$$= c^2 g \; 2 \int_0^a x (a^2 - x^2)^2 dx = c^2 g \frac{a^6}{3}$$

$$= \frac{5}{16} g a$$

$$\implies \langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{5}{4} \frac{\hbar^2}{m} \frac{1}{a^2} + \frac{5}{16} g a$$

$$\frac{\partial \langle H \rangle}{\partial a} = 0 = \frac{5}{4} \frac{\hbar^2}{m} \left(-\frac{2}{a^3}\right) + \frac{5}{16} g \implies a = \left(\frac{8\hbar^2}{mg}\right)^{1/3}$$

$$\implies E_{g.s} = \frac{5}{4} \frac{\hbar^2}{m} \left(\frac{m^2 g^2}{64 \hbar^4}\right)^{1/3} + \frac{5}{16} g \left(\frac{8\hbar^2}{mg}\right)^{1/3}$$

$$= \left[\frac{5}{4}\left(\frac{1}{64}\right)^{1/3} + \frac{5}{16}(8)^{1/3}\right] \left(\frac{g^2 \hbar^2}{m}\right)^{1/3} = 0.9\cancel{3}4 \left(\frac{g^2 \hbar^2}{m}\right)^{1/3}$$

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which is somehow close to the exact value of $0.809 \left(\frac{g^2 \hbar^2}{m}\right)^{1/3}$

(b) $\psi(x) = Ax(a-|x|)$ ; $|x| \leq a$

normalize $A^2 \int_{-a}^{a} x^2(a-|x|)^2 dx = 1$

$$2A^2 \int_0^a x^2(a-x)^2 dx = 1 \quad \Rightarrow \quad A = \sqrt{\frac{15}{a^5}}$$

$$\psi(x) = Ax(a-|x|) = \begin{cases} Ax(a+x) ; & x<0 \\ Ax(a-x) ; & x>0 \end{cases}$$

$$\psi'(x) = \begin{cases} A(a+2x) ; & x<0 \\ A(a-2x) ; & x>0 \end{cases}$$

$$\langle T \rangle = \int_{-\infty}^{\infty} \frac{\hbar^2}{2m}\left(\frac{d\psi^*}{dx}\right)\left(\frac{d\psi}{dx}\right) dx = \frac{\hbar^2}{2m}\, 2\int_0^a A^2(a-2x)^2 dx$$

$$= \frac{4}{3}\frac{\hbar^2}{m} a^3 A^2 = \frac{20\hbar^2}{ma^2}$$

$$\langle V \rangle = \int_{-a}^{a} V\psi^*\psi = \int_{-a}^{a} g|x|\,\psi^*\psi$$

$$= gA^2\left[\int_{-a}^{0} -x(ax+x^2)^2 dx + \int_0^a x(ax-x^2)^2 dx\right]$$

$$= gA^2\, 2\int_0^a x(ax-x^2)^2 dx = gA^2\frac{a^6}{30} = \frac{1}{2}ga$$

$$\Rightarrow \langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{20\hbar^2}{ma^2} + 1/2\, ga$$

$$\frac{\partial\langle H \rangle}{\partial a} = 0 = \frac{20\hbar^2}{m}\left(\frac{-2}{a^3}\right) + \frac{1}{2}g \quad \Rightarrow \quad a = \left(\frac{80\hbar^2}{mg}\right)^{1/3}$$

$$\Rightarrow E_{1st} = \frac{20\hbar^2}{m}\left(\frac{m^2g^2}{80^2\hbar^4}\right)^{1/3} + \frac{1}{2}g\left(\frac{80\hbar^2}{mg}\right)^{1/3}$$

$$= \left[20\left(\frac{1}{6400}\right)^{1/3} + \frac{1}{2}(80)^{1/3}\right]\left(\frac{g^2\hbar^2}{m}\right)^{1/3}$$

$$= 3.23\left(\frac{g^2\hbar^2}{m}\right)^{1/3}$$ $\approx$ double the exact value $1.855\left(\frac{g^2\hbar^2}{m}\right)^{1/3}$