SOLUTIONS

PROBLEM SET 3

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1. Exercise 7C.1b

A coulomb potential has the form:

$$V(r) = \frac{q_1 q_2}{4\pi \varepsilon_0 r}$$

where q_1 and q_2 are charges of two interacting particles, ε_0 is the permittivity of a vacuum, and r is the distance between the particles. If we let q_1 be the charge of the reference particle & let it be at the origin, and q_2 be the charge of the particle in question and r its distance from the origin, the operator is simply:

$$\hat{V}(r) = \frac{q_1 q_2}{4\pi \varepsilon_0 r} \cdot$$

where $\cdot$ represents the multiplication operation.

2. Exercises 7C.3b and 7C.4b

7C.3b To show: $\displaystyle\int_0^L \underbrace{\cos\left(\frac{n\pi x}{L}\right)}_{\psi_1^*} \underbrace{\cos\left(\frac{m\pi x}{L}\right)}_{\psi_2} dx = 0 \quad m \neq n$

From table of integrals: $\displaystyle\int \cos mx \cos nx \, dx = \frac{\sin(m-n)x}{2(m-n)} + \frac{\sin(m+n)x}{2(m+n)}$

$(m^2 \neq n^2)$

$$\int_0^L \cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right) dx = \frac{\sin\left(\frac{m\pi}{L} - \frac{n\pi}{L}\right)x}{2(m-n)\pi/L} + \frac{\sin\left(\frac{m\pi}{L} + \frac{n\pi}{L}\right)x}{2(m+n)\pi/L}\Bigg|_0^L$$

$$= \left(\frac{\sin(m-n)\pi}{2(m-n)\pi/L} + \frac{\sin(m+n)\pi}{2(m+n)\pi/L}\right) - 0$$

$= 0$ because $\sin(m-n)\pi = \sin(m+n)\pi = 0$ for m, n integers

7C.4b To show: $\displaystyle\int_0^{2\pi} \psi_1^* \psi_2 \, d\phi = 0$ where $\begin{cases} \psi_1 = e^{+i\phi} \\ \psi_2 = e^{-i\phi} \end{cases}$

$$\int_0^{2\pi} \psi_1^* \psi_2 \, d\phi = \int_0^{2\pi} (e^{+i\phi})^* (e^{-i\phi}) \, d\phi = \int_0^{2\pi} e^{-i\phi} \cdot e^{-i\phi} \, d\phi$$

$$= \int_0^{2\pi} e^{-2i\phi} \, d\phi = -\frac{1}{2i} e^{-2i\phi}\Big|_0^{2\pi}$$

$$= -\frac{1}{2i}\left(\underset{\substack{\uparrow \\ 1}}{e^{-4\pi i}} - \underset{\substack{\uparrow \\ 1}}{e^{0}}\right) = 0$$

3. Exercise 7C.5b

$$\langle E_K \rangle = \int_0^L \psi^* \hat{E}_K \psi \, dx \qquad \hat{E}_K = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad \psi = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

$$= \int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right) dx$$

$$= \left(\frac{2}{L}\right)\left(-\frac{\hbar^2}{2m}\right)\int_0^L \sin\left(\frac{\pi x}{L}\right)\cdot\left(\frac{\pi}{L}\right)^2\cdot\sin\left(\frac{\pi x}{L}\right)(-1)\, dx$$

$$= \left(\frac{\pi}{L}\right)^2\left(\frac{2}{L}\right)\left(\frac{\hbar^2}{2m}\right)\int_0^L \sin^2\left(\frac{\pi x}{L}\right) dx$$

$$= \frac{\pi^2\hbar^2}{mL^3}\left[\frac{x}{2} - \frac{\sin\frac{2\pi x}{L}}{4\pi/L}\right]_0^L$$

$$= \frac{\pi^2\hbar^2}{mL^3}\left[\left(\frac{L}{2}-0\right)-(0-0)\right]$$

$$= \frac{\pi^2\hbar^2}{2mL^2}$$ where m is mass of electron and L is length of tube

Units check $\hbar \rightarrow J\,s = kg\,m^2\,s^{-1}$

$m \rightarrow kg$

$L \rightarrow m$

$$\frac{\pi^2\hbar^2}{2mL^2} \rightarrow \frac{kg^2\,m^4\,s^{-2}}{kg\,m^2} \rightarrow kg\,m^2\,s^{-2} \rightarrow J \checkmark$$

4. In general, if the eigenfunctions of an operator are $f_1(x)$, $f_2(x)$ (with corresponding eigenvalues $w_1, w_2 \dots$), the wavefunction can be expanded in terms of $f_1(x), f_2(x) \dots$:

$$\psi = c_1 f_1(x) + c_2 f_2(x) + \dots$$

In our case, the operator is $\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$, the eigenfunctions are e^{+ikx} and e^{-ikx}, and the corresponding eigenvalues are $+k\hbar$ and $-k\hbar$.

The probability of observing a particular eigenvalue w_i is given by:

$$\frac{|c_i|^2}{\sum_i |c_i|^2}$$

In our case, $c_1 = \cos\chi$ and $c_2 = \sin\chi$.
Thus the probability of observing the values are:

$$+k\hbar: \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} = \frac{\cos^2\chi}{\cos^2\chi + \sin^2\chi} = \cos^2\chi$$

$$-k\hbar: \frac{\sin^2\chi}{\cos^2\chi + \sin^2\chi} = \sin^2\chi$$

If the probability of observing $+k\hbar$ is to be 0.9,

$$\cos^2\chi = 0.9 \Rightarrow \cos\chi = \sqrt{0.9} = 0.95$$

$$\sin^2\chi = 0.1 \Rightarrow \sin\chi = \sqrt{0.1} = 0.32$$

$$\Rightarrow \psi = 0.95e^{+ikx} \pm 0.32e^{-ikx}$$

5. a) $P(0, 0.2L) = \int_0^{0.2L} \psi^* \psi \, dx = \frac{2}{L} \int_0^{0.2L} \sin^2 \frac{3\pi x}{L} \, dx$

$= \frac{2}{L} \frac{L}{3\pi} \left[\frac{1}{2} \frac{3\pi x}{L} - \frac{1}{4} \sin \frac{6\pi x}{L} \right]_0^{0.2L}$

$= \frac{2}{3\pi} \left(\left(\frac{0.6\pi}{2} - \frac{1}{4} \sin 1.2\pi \right) - (0 - 0) \right)$

$= 0.2 - \frac{1}{6\pi} (-0.588)$

$= 0.203$

b) $\langle x \rangle = \int_0^L \psi^* \hat{x} \psi \, dx = \int_0^L \psi^* x \psi \, dx = \frac{2}{L} \int_0^L x \sin^2 \frac{3\pi x}{L} \, dx$

$= \frac{2}{L} \left(\frac{L}{3\pi} \right)^2 \int_{x=0}^{x=L} u \sin^2 u \, du \quad \left(u = \frac{3\pi x}{L} \right)$

$= \frac{2L}{9\pi^2} \left[\frac{u^2}{4} - \frac{u \sin 2u}{4} - \frac{\cos 2u}{8} \right]_{x=0}^{x=L}$

$= \frac{2L}{9\pi^2} \left[\frac{9\pi^2 x^2}{4L^2} - \frac{3\pi x}{4L} \sin \frac{6\pi x}{L} - \frac{1}{8} \cos \frac{6\pi x}{L} \right]_0^L$

$= \frac{2L}{9\pi^2} \left[\left(\frac{9\pi^2}{4} - \frac{3\pi}{4} \underbrace{\sin 6\pi}_{0} - \frac{1}{8} \underbrace{\cos 6\pi}_{1} \right) - \left(0 - 0 - \frac{1}{8} \right) \right]$

$= \frac{L}{2}$

$\langle x^2 \rangle = \int_0^L \psi^* \hat{x}^2 \psi \, dx = \int_0^L \psi^* x^2 \psi \, dx = \frac{2}{L} \int_0^L x^2 \sin^2 \frac{3\pi x}{L} \, dx$

$= \frac{2}{L} \left(\frac{L}{3\pi} \right)^3 \int_{x=0}^{x=L} u^2 \sin^2 u \, du \quad \left(u = \frac{3\pi x}{L} \right)$

$= \frac{2L^2}{27\pi^3} \left[\frac{u^3}{6} - \left(\frac{u^2}{4} - \frac{1}{8} \right) \sin 2u - \frac{u \cos 2u}{4} \right]_{x=0}^{x=L}$

$= \frac{2L^2}{27\pi^3} \left[\frac{27\pi^3 x^3}{6L^3} - \left(\frac{9\pi^2 x^2}{4L^2} - \frac{1}{8} \right) \sin \frac{6\pi x}{L} - \frac{3\pi x}{4L} \cos \frac{6\pi x}{L} \right]_0^L$

$$= \frac{2L^2}{27\pi^3}\left[\left(\frac{27\pi^3}{6} - \left(\frac{9\pi^2}{4} - \frac{1}{8}\right)\underbrace{\sin 6\pi}_{0} - \frac{3\pi}{4}\underbrace{\cos 6\pi}_{1}\right) - \left(0 - 0 - 0\right)\right]$$

$$\langle x^2\rangle = \frac{L^2}{3} - \frac{L^2}{18\pi^2}$$

$$\langle p_x\rangle = \int_0^L \psi^* \hat{p}_x \psi\, dx = \int_0^L \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{3\pi x}{L}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{3\pi x}{L}\right)\right)dx$$

$$= \frac{2}{L}\frac{\hbar}{i}\frac{3\pi}{L}\int_0^L \sin\frac{3\pi x}{L}\cos\frac{3\pi x}{L}\, dx$$

$$= \frac{6\pi\hbar}{iL^2}\frac{L}{3\pi}\int_{x=0}^{x=L} \sin u \cos u\, du \qquad \left(u = \frac{3\pi x}{L}\right)$$

$$= \frac{2\hbar}{iL}\left[\frac{1}{2}\sin^2 u\right]_{x=0}^{x=L} = \frac{2\hbar}{iL}\left[\frac{1}{2}\sin^2\frac{3\pi x}{L}\right]_0^L$$

$$= \frac{2\hbar}{iL}\left(\frac{1}{2}\sin^2 3\pi - \frac{1}{2}\sin^2 0\right)$$

$= 0$ We could have predicted this: particle has equal probability of moving to right & to left, so average is zero.

$$\langle p_x^2\rangle = \int_0^L \psi^* \hat{p}_x^2 \psi\, dx = \frac{2}{L}\int_0^L \sin\left(\frac{3\pi x}{L}\right)\left[\left(\frac{\hbar}{i}\right)^2 \frac{d^2}{dx^2}\sin\left(\frac{3\pi x}{L}\right)\right]dx$$

$$= -\frac{2\hbar^2}{L}(-1)\left(\frac{3\pi}{L}\right)^2 \int_0^L \sin^2\left(\frac{3\pi x}{L}\right) dx$$

$$= \frac{18\pi^2\hbar^2}{L^3}\frac{L}{3\pi}\left[\frac{1}{2}\frac{3\pi x}{L} - \frac{1}{4}\sin\frac{6\pi x}{L}\right]_0^L$$

$$= \frac{6\pi\hbar^2}{L^2}\left[\left(\frac{3\pi}{2} - 0\right) - \left(0 - 0\right)\right]$$

$$= \frac{9\pi^2\hbar^2}{L^2}$$

$$\Delta x = (\langle x^2\rangle - \langle x\rangle^2)^{1/2}$$

$$= \left(\frac{L^2}{3} - \frac{L^2}{18\pi^2} - \left(\frac{L}{2}\right)^2\right)^{1/2} = 0.21\,L$$

$$\Delta p = (\langle p^2\rangle - \langle p\rangle^2)^{1/2}$$

$$= \left(\frac{9\pi^2\hbar^2}{L^2} - 0\right)^{1/2} = \frac{3\pi\hbar}{L}$$

$$\Delta x \Delta p = 0.21L\left(\frac{3\pi\hbar}{L}\right) = 1.98\,\hbar > \frac{\hbar}{2}$$

As we discussed in class, $(\langle x^2\rangle - \langle x\rangle^2)^{1/2}$ is the standard deviation in x, a measure of the uncertainty in x. Likewise for p. Therefore we have tested the uncertainty principle. Note that $\Delta x \Delta p > \frac{\hbar}{2}$, in accord with the uncertainty principle.

6. Exercise 8A.3b

$$E_n = \frac{n^2h^2}{8mL^2}$$

i) $\Delta E(1 \rightarrow 3) = (3^2 - 1^2)\frac{h^2}{8mL^2} = \frac{h^2}{mL^2}$

$h = 6.626 \times 10^{-34}$ Js $\quad m = m_e = 9.109 \times 10^{-31}$ kg $\quad L = 1.50 \times 10^{-9}$ m

$\Delta E = 2.14 \times 10^{-19}$ J $= 129$ kJ/mol $= 1.34$ eV $= 1.08 \times 10^{4}$ cm^{-1}

ii) $\Delta E(6 \rightarrow 7) = (7^2 - 6^2)\frac{h^2}{8mL^2} = \frac{13h^2}{8mL^2}$

$\Delta E = 3.48 \times 10^{-19}$ J $= 209$ kJ/mol $= 2.17$ eV $= 1.75 \times 10^{4}$ cm^{-1}

7. Exercise 8A.9b

$$E^{(L)} = \frac{(n_1^2+n_2^2+n_3^2)h^2}{8mL^2} \quad \text{(eq. 8A.16 b, let } L_1 = L_2 = L_3 = L\text{)}$$

$$E^{(0.9L)} = \frac{(n_1^2+n_2^2+n_3^2)h^2}{8m(0.9L)^2}$$

$$\%\ \text{change} = \frac{E^{(0.9L)} - E^{(L)}}{E^{(L)}} \cdot 100\,\% = \frac{\frac{1}{0.9^2} - \frac{1}{1^2}}{\frac{1}{1^2}} \cdot 100\,\%$$

$$= 23\,\%$$

8. $E_n = \frac{n^2 h^2}{8mL^2}$ $n = 1, 2, \ldots$

$E_2 - E_1 = \frac{3h^2}{8mL^2} = \boxed{1.24 \times 10^{-39}\ J}$ TINY

$32\ amu = 32 \cdot 1.661 \times 10^{-27}\ kg$

$L = 5.0\ cm = 0.05\ m$

$h = 6.626 \times 10^{-34}\ J\ s$

At $T = 300\ K$, $\frac{1}{2} kT = 2.07 \times 10^{-21}\ J$ = ave. kin. en. in 1-D

Separation $= \Delta E = (2n+1) \frac{h^2}{8mL^2} = 2.02 \times 10^{-24}\ J$

$\frac{n^2 h^2}{8mL^2} = 2.07 \times 10^{-21}\ J \Rightarrow \boxed{n = 2.2 \times 10^9}$

HUGE