

Some sample Quantum Mechanics problems from Atkins

9. Size of quantum $\Rightarrow E = h\nu$ $\nu = c/\lambda$
 $h = 6.627 \times 10^{-34} \text{ J} \cdot \text{S}$ $= 1/\tau$
10. Watts = J/second photon/second = $h\nu/\text{sec}$
 $10^7 \text{ photon}/10 \mu \text{ second} = 10^7/10 \cdot 10^{-6} = 10^{12} \text{ photon/second}$
11. de Broglie problem $p = h/\lambda = \nu$
 recall $J = \text{kg m}^2/\text{s}^2$
 $1\text{g} \times 1 \text{ m s}^{-2} = 10^{-3} \text{ kg m s}^{-1}$
 $= 10^{-3} \text{ J} \cdot \text{S} \cdot \text{m}^{-1}$
 $\lambda = 6.6 \times 10^{-34} \text{ J} \cdot \text{S}/10^{-3} \text{ J} \cdot \text{S m}^{-1} = 6.6 \times 10^{-31} \text{ m}$
14. Photon pressure momentum problem \rightarrow photon absorbed
 can view as energy $h\nu \rightarrow 1/2 m v^2$ (heating / lack \rightarrow)
 or momentum $\mathbf{p} = h/\lambda = m\mathbf{v}$ (photon \mathbf{k} property)
 $F = m_a = dp/dt \Rightarrow (h/\lambda)$ (note photon)
 (Problem 14 incomplete) – assume 10^{15} photon/second laser
 – assume all hit sail
 $(6.6 \times 10^{-34} \text{ J} \cdot \text{S}/650 \times 10^{-7} \text{ m}) (10^{15} \text{ s}^{-1}) \sim 10^{-8} \text{ N}$
 \rightarrow if even on sail can calculate
- Pressure = F/A
 $A = 1 \text{ km}^2 = 10^6 \text{ m}^2$ $p \sim 10^{-14} \text{ N/m}^2$
 1 kg space craft \rightarrow what is sail? At km^2 !!
 $v = a \cdot t = (F/m) t$
15. Uncertainty $\Delta p \Delta x > \hbar/2$ $\Delta p = 10^{-4} \cdot p$; $\Delta x \geq (\Delta p)^{-1} (\hbar/2) \sim$

Topics of use in Quantum Mechanics:

Electrostatics

Interaction electron-proton $-e^2/r$ $r = a_0 = 0.53 \text{ \AA}$
 problem here is units $e = 1.6 \times 10^{-19} \text{ C}$
 in MKS $U = q_1 q_2 / 4\pi \epsilon_0 r$ $r = 0.53 \times 10^{-10} \text{ m}$
 $q - \text{C}$, $r - \text{m}$
 $\epsilon = 8.85 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}$

$$(1.6 \times 10^{-19} \text{ C})^2 / 4\pi (8.85 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}) (0.53 \times 10^{-10} \text{ m})$$

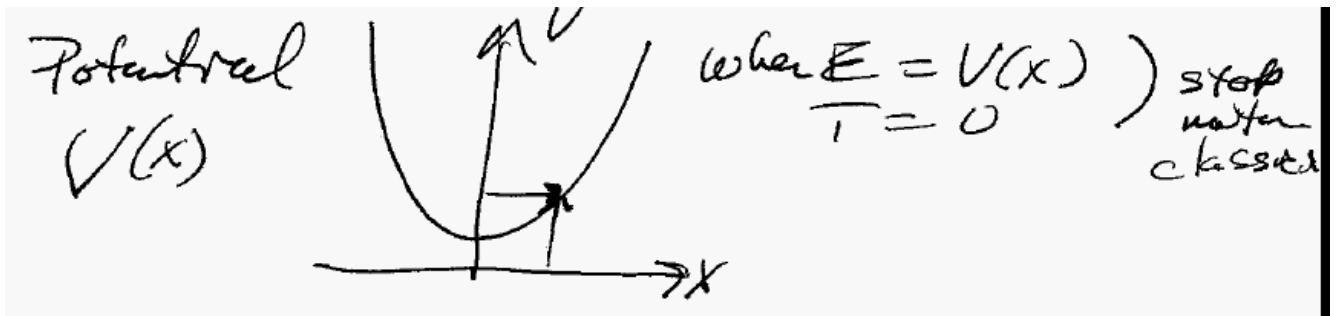
$$\sim 3 \times 10^{-38} / (4\pi \times 0.5) \left(\begin{matrix} \sim 6 \\ \sim 9 \end{matrix} \right) 10^{-22} \sim 0.5 \times 10^{-15} \text{ J}$$

$$\text{macro: } U = 1389 q_1 q_2 / r \quad (\text{kJ/mol})$$

Classical box – spacing order kT

$$\text{He in } 1\mu \text{ value } 25^\circ \text{ C and } 1^\circ \text{ K}$$

$$E = \hbar^2 \pi^2 n^2 / 2ma^2 = \hbar^2 n^2 / 8ma^2 \quad 1 - 0 \quad \Delta E_{3D} = \Delta E_{1D} \quad n = 1 \rightarrow n = 2$$



Acceptable w/f \rightarrow integrable / finite

e^{ax} $(-\infty < x < \infty)$ – nope – blows up

$e^{im\phi}$ $(0 < \phi < 2\pi)$ – yes m integer (continuous)
 – no – non continuous

x $(0 < x < 10)$ – no – discontinuity (tricky, needs be zero)

$|x - 10|$ $(-10 < x < 10)$ – okay, but not good (1st derivative not continuous at $x = 0$)

$\sin ax$ $(-\pi/a < x < \pi/a)$ – yes

$\cos ax$ – same

Operator Linear / Hermitian $\int \psi_j^* \alpha \psi_i d\tau = \int \psi_i \alpha^* \psi_j d\tau$

Note $\alpha \psi_i = \alpha_i \psi_i$

$\alpha^* \psi_i^* = \alpha_i^* \psi_i^*$

$\int \psi_i^* \alpha \psi_i = \int \psi_i \alpha^* \psi_i^*$

$a_i \int \psi_i^* \psi_i = a_i^* \int \psi_i \psi_i^*$

$a_i = a_i^*$

a_i – real

Derive 3D KE KE 1D = $-\hbar^2/2m d^2/dx^2$
 $= p^2/2m = \hbar^2/2m (d/dx \cdot d/dx)$

3D momentum

$(\hbar/i) (d/dx \hat{i} + d/dy \hat{j} + d/dz \hat{k}) = \hbar/i \nabla$

$p^2/2m = -\hbar^2/2m (\nabla \cdot \nabla) = -\hbar^2/2m (d^2/dx^2 + d^2/dy^2 + d^2/dz^2)$

Any momentum: $\mathbf{L} = \mathbf{n} \times \mathbf{p}$ review cross product

$$\mathbf{r} \times \mathbf{p} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \mathbf{i} (y p_z - p_y z) + \mathbf{j} (z p_x - p_z x) + \mathbf{k} (x p_y - p_x y)$$

$$= L_x \mathbf{i} + L_y \mathbf{j} + L_z \mathbf{k}$$

keep order in case commutivity is important

$$L_x = y p_z - p_y z = y (\hbar/i) \partial/\partial z - (\hbar/i) \partial/\partial y z$$

$$= (\hbar/i) (y \partial/\partial z - z \partial/\partial y)$$

$\partial/\partial y$ rotation z

Free particle:

$$H\psi = E\psi = (T + U) \psi$$

$$= (-\hbar^2/2m) \partial^2/\partial x^2 \psi = E\psi$$

Solution: $e^{ikx} \quad (-\hbar^2/2m) (ik)^2 \psi = E\psi$
 $E = \hbar^2 k^2 / 2m$

all energies are possible no restrictions k
 \rightarrow propagation vector

$$\hbar k = \sqrt{E/2m} = p = \hbar/\lambda$$

$$k = 2\pi/\lambda$$

Constrain particle

classically bounce back from wall
 Quantum Mechanics – slight penetration
 due to wave continuous at $x = 0$

