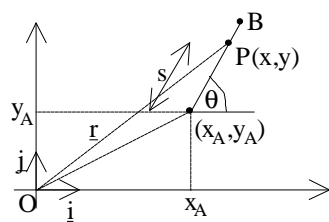
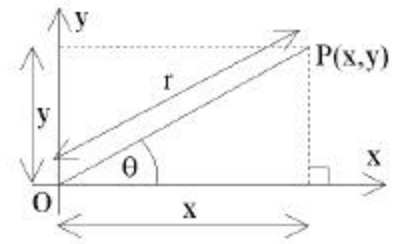


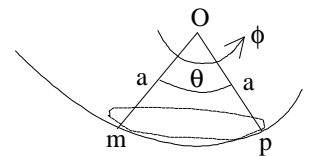
## Section 1: Classical Mechanics

### 1.1: Summarising Lagrangian Mechanics for Conservative Holonomic Systems

A *holonomic dynamical system* of  $n$  degrees of freedom is one where the position of configuration of the system can be specified by  $n$  generalised co-ordinates,  $q_1, q_2, \dots, q_n$ , which may be varied *arbitrarily* and *independently* without breaking the constraints on the system. Examples: (i) A particle constrained to move in a plane. **Possible** generalised co-ordinates are: (a) Rectangular Cartesian co-ordinates,  $(x, y)$ , with  $-\infty < x, y < \infty$ ; and (b) Polar co-ordinates,  $(r, \theta)$ , with  $0 \leq \theta \leq 2\pi$ , and  $0 \leq r < \infty$ . Note that in *both* cases,  $n = 2$ .



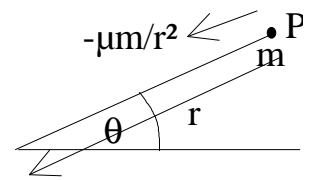
(ii) A particle constrained to move on a **sphere** of radius  $a$ . We have generalised co-ordinates  $(\theta, \phi)$ , with  $n = 2$  again. With respect to an **origin**  $O$ , the position vector  $\underline{r} = \overrightarrow{OP}$  of any point  $P$  of the system can be expressed as a *function* of the generalised co-ordinates:  $\underline{r} = \underline{r}(q_1, q_2, \dots, q_n)$  (---(1)). (iii) A *rod in a plane*. Here,  $n = 3$ , and the generalised co-ordinates are  $(x_A, y_A, \theta)$ . **Therefore**,  $x = x_A + s \cos \theta$ ;  $y = y_A + s \sin \theta$ ; and  $\underline{r} = x_i + y_j = \underline{r}(x_A, y_A, \theta)$ .



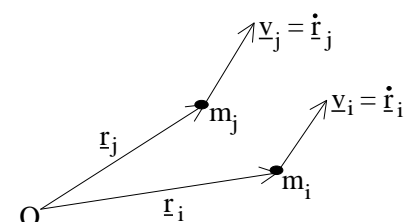
A *conservative force* is one which depends on position only, and which does no work when its point of application moves around any **closed** curve in space. A conservative dynamical system is one in which the forces acting on the system are all conservative. These conservative forces may be derived from a *potential* function or potential energy denoted by  $V$ , where  $V = V(q_1, q_2, \dots, q_n)$ . (---(2)). The expression for  $V$  for a *given* system is found by calculating the work done by the external forces when the system is **displaced** from an arbitrary configuration denoted by  $(q_1, \dots, q_n)$  to some *fixed standard configuration* denoted by  $(q_1, \dots, q_n)$ . The *generalised force*  $Q_\sigma$  (for  $\sigma = 1, 2, \dots, n$ ) corresponding to the *general* co-ordinates  $q_\sigma$  is defined by  $Q_\sigma = -\partial V / \partial q_\sigma$ , where  $\sigma = 1, 2, \dots, n$  (---(3)).

**Example:** “The Inverse Square law of attraction”. In the diagram,  $\mu$  ( $> 0$ ) and  $m$  are constants.  $q_1 = r, q_2 = \theta; q_1 = \infty, q_2 = \theta$ .  $V(q_1, q_2) = V(r, \theta)$   

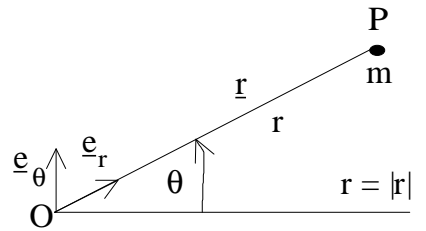
$$= \int_{r'=r}^{r'=\infty} \frac{-\mu m}{(r')^2} dr' = \left[ \frac{\mu m}{r'} \right]_{r'=r}^{r'=\infty} = \mu m / \infty - \mu m / r = -\mu m / r$$
 (independent of  $\theta$ ).  $V(r, \theta) = -\mu m / r$   
 (---(4)) (independent of  $\theta$ ).  $V(x, y) = -\mu m / \sqrt{x^2 + y^2}$ . Note that **both**  $x$  and  $y$  occur in *Cartesian* co-ordinates.



The *kinetic energy*  $T$  is defined by  $T = \sum_{i=1}^N \frac{1}{2} m_i \dot{r}_i^2$  (---(5)), where  $m_i$  and  $\underline{r}_i$  are the *mass* and *position vector* of the  $i^{\text{th}}$  particle of the system (which contains  $N$  particles in all). Using (1) in (5), where  $q_\sigma = q_\sigma(t)$  for  $\sigma = 1, 2, \dots, n$ ; we have  $\underline{v}_i = \frac{d\underline{r}_i}{dt} = \frac{\partial \underline{r}_i}{\partial q_1} \dot{q}_1 + \dots + \frac{\partial \underline{r}_i}{\partial q_n} \dot{q}_n = \underline{v}_i(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$  (---(6)), where the  $\dot{q}_\sigma$  are known as *generalised velocities*.



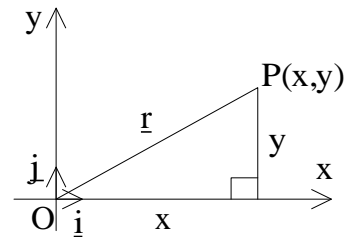
**Example:**  $\frac{d}{d\theta}(\underline{e}_r) = \underline{e}_\theta$ ;  $\frac{d}{d\theta}(\underline{e}_\theta) = -\underline{e}_r$ .  $|\underline{e}_r| = |\underline{e}_\theta| = 1$ .  $\underline{r} = \overrightarrow{OP} = r\underline{e}_r$ .  
 $\underline{v} = \dot{\underline{r}} = \frac{d}{dt}(r\underline{e}_r) = \dot{r}\underline{e}_r + r\frac{d}{dt}(\underline{e}_r) = \dot{r}\underline{e}_r + r\frac{d}{d\theta}(\underline{e}_r)\cdot\dot{\theta}$ . **So**  $\underline{v} = \dot{r}\underline{e}_r + r\dot{\theta}\underline{e}_\theta$ .  
 [Cartesian:  $\underline{r} = x\underline{i} + y\underline{j}$ , where  $\underline{i}$  and  $\underline{j}$  are fixed; and  $\dot{\underline{r}} = \frac{dx}{dt}\underline{i} + \frac{dy}{dt}\underline{j} = \dot{x}\underline{i} + \dot{y}\underline{j}$ ]. **Therefore**, we have  $T = \frac{1}{2}m\underline{v}^2 = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2)$  (---(7)). The Lagrangian function  $L$  is defined by  $L = T - V$  (---(8)). (2) and (6)  $\Rightarrow L = L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$  (we have  $2n$  independent variables) (---(9)).



**Example:** (4) and (7)  $\Rightarrow L = T - V = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - (-\frac{\mu m}{r}) = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}$  (---(10)).  
 The equations of motion for the system are obtained from  $L$  by  $\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}_\sigma}) - \frac{\partial L}{\partial q_\sigma} = 0$  (---(11)). We have  $n$  2nd order ordinary differential equations w.r.t. time  $t$ . **Exercise:** (10)  $\Rightarrow (\sigma = 1, q_1 = r) \frac{\partial L}{\partial q_1} = \frac{\partial L}{\partial r} = \frac{\partial}{\partial r}[\frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}] = (\frac{1}{2}m(0 + 2r\dot{\theta}^2) - \frac{\mu m}{r^2}) = m r \dot{\theta}^2 - \frac{\mu m}{r^2}$  (---(12)). And  $\frac{\partial L}{\partial \dot{q}_1} = \frac{\partial L}{\partial \dot{r}} = \frac{\partial}{\partial \dot{r}}[\frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}] = \frac{1}{2}m(2\dot{r} + 0) + 0 = m\dot{r}$  (---(13)). (13)  $\Rightarrow \frac{d}{dt}(\frac{\partial L}{\partial \dot{r}}) = \frac{d}{dt}(m\dot{r}) = m\ddot{r}$  (---(14)). (12) and (14) in (11)  $\Rightarrow m\ddot{r} - (m r \dot{\theta}^2 - \frac{\mu m}{r^2}) = 0$ , or  $m(\ddot{r} - r\dot{\theta}^2) = -\frac{\mu m}{r^2}$  (---(15)).

**Now take**  $\sigma = 2$ , so that we have  $\frac{\partial L}{\partial q_2} = \frac{\partial}{\partial \theta}[\frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}] = 0$  (---(16)).  $\frac{\partial L}{\partial \dot{q}_2} = \frac{\partial L}{\partial \dot{\theta}} = \frac{\partial}{\partial \dot{\theta}}[\frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}] = m r^2 \dot{\theta}$  (---(17)). **Now**  $\frac{d}{dt}(\frac{\partial L}{\partial \dot{\theta}}) = \frac{d}{dt}(m r^2 \dot{\theta}) = m(2r\dot{\theta}) + m r^2 \ddot{\theta}$  (---(18)). (16) and (18) in (11)  $\Rightarrow m(2r\dot{\theta} + r^2\ddot{\theta}) = 0$  (---(19)). So  $\frac{d}{dt}(m r^2 \dot{\theta}) = 0 \Rightarrow m r^2 \dot{\theta} = h$  (constant) (---(20)). **Notice** that in (10),  $L$  is independent of  $\theta$ , so that  $\frac{\partial L}{\partial \theta} = 0$  (---(21)). (21) in (11)  $\Rightarrow$  (with  $q = \theta$ )  $\frac{d}{dt}(\frac{\partial L}{\partial \dot{\theta}}) = 0 \Rightarrow \frac{\partial L}{\partial \dot{\theta}} = \text{constant}$  (---(22)).

**A Free Particle in a plane:**  $\underline{F} = \underline{0} \Rightarrow V(x, y) = \text{constant} = 0$ .  $\underline{i}$  and  $\underline{j}$  are fixed vectors.  $\underline{r} = x\underline{i} + y\underline{j}$ ;  $\underline{v} = \dot{\underline{r}} = \dot{x}\underline{i} + \dot{y}\underline{j}$ .  $L = T - V = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) = 0$ . If  $x$  and  $y$  are absent from  $L$ , then  $\frac{\partial L}{\partial \dot{x}} = \text{constant} = m\dot{x}$  (linear momentum in the  $x$  direction); and  $\frac{\partial L}{\partial \dot{y}} = \text{constant} = m\dot{y}$ . The generalised momentum  $p_\sigma$  corresponding to  $q_\sigma$  is defined (for  $\sigma = 1, 2, \dots, n$ ) by  $p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}$  (---(23)).



A cyclic (or ignorable) co-ordinate is one that is **absent** from the Lagrangian function (like  $\theta$  in equation (10)). So equation (11) and definition (23) implies that the **generalised momentum**  $p_\sigma$  corresponding to (or is CONJUGATE to) a cyclic co-ordinate  $q_\sigma$  is constant.

## 1.2: Hamiltonian Mechanics

The **Hamiltonian function**  $H$  is defined by  $H = \sum_{\sigma=1}^n (\dot{q}_\sigma p_\sigma) - L$  (---(1)), where the  $p_\sigma$  are given by 1.1.23, and  $\sigma = 1, 2, \dots, n$ .  $L$  depends on the  $q_\sigma$  and the  $\dot{q}_\sigma$ , i.e. on  $2n$  variables. Also, we have the  $p_\sigma$ , so that we have  $3n$  variables in total. Not all of these variables are *independent* — see 1.1.23:  $p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}$  ( $\sigma = 1, 2, \dots, n$ ):  $n$  simultaneous equations. The  $n$  simultaneous equations are **solved** for the  $\dot{q}_\sigma$  ( $\sigma = 1, 2, \dots, n$ ) in terms of the  $q_\sigma$  and the  $p_\sigma$ ; and are then substituted into (1), so that  $H$  becomes a *function* of the  $q_\sigma$  and the  $p_\sigma$  only:  $H = H(q_1, \dots, q_n, p_1, \dots, p_n)$  (---(2)).

From (1.1.10),  $L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}$ . From (1.1.23),  $p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}$  (---(3)); and  $p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m r^2 \dot{\theta}$  (---(4)). (3) and (4)  $\Rightarrow \dot{r} = p_r/m$  (---(5)); and  $\dot{\theta} = p_\theta/mr^2$  (---(6)). (1.1.10), (5) and (6) in (1)  $\Rightarrow H = \dot{r}p_r + \dot{\theta}p_\theta - (\frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + \frac{\mu m}{r}) = (\frac{p_r}{m})p_r + (\frac{p_\theta}{mr^2})p_\theta - (\frac{1}{2}m((\frac{p_r}{m})^2 + r^2(\frac{p_\theta}{mr^2})^2) + \frac{\mu m}{r})$ ;  $H = (\frac{p_r^2}{2m}) + (\frac{p_\theta^2}{2mr^2}) - \frac{\mu m}{r}$  (---(7)). Here,  $H = H(r, p_r, p_\theta)$  — not in this case  $\theta$ .

**Recall:** (1):  $H = (\sum_{\sigma=1}^n \dot{q}_\sigma p_\sigma) - L$ , where  $p_\sigma = \partial L / \partial \dot{q}_\sigma$ ; and  $H = H(q_1, \dots, q_n, p_1, \dots, p_n)$ . (1)  $\Rightarrow \delta H = \sum_{\sigma=1}^n [(\delta \dot{q}_\sigma) p_\sigma + \dot{q}_\sigma (\delta p_\sigma)] - \sum_{\sigma=1}^n [(\partial L / \partial q_\sigma) \delta q_\sigma + (\partial L / \partial \dot{q}_\sigma) \delta \dot{q}_\sigma] = \sum_{\sigma=1}^n (p_\sigma - (\partial L / \partial \dot{q}_\sigma)) \delta \dot{q}_\sigma + \sum_{\sigma=1}^n [(-\partial L / \partial q_\sigma) \delta q_\sigma + \dot{q}_\sigma \delta p_\sigma]$  (---(8)), where  $( ) = 0$  by 1.1.23; and the blue bit is  $\dot{p}_\sigma$ . **Notes:**  $-\partial L / \partial q_\sigma = -\dot{p}_\sigma$ ; and Lagrange's equations say that  $d/dt(\partial L / \partial \dot{q}_\sigma) - \partial L / \partial q_\sigma = 0 \Leftrightarrow \dot{p}_\sigma = \partial L / \partial q_\sigma$ .

**Therefore,**  $\delta H = \sum_{\sigma=1}^n [(-\dot{p}_\sigma) \delta q_\sigma + \dot{q}_\sigma \delta p_\sigma]$  (---(9)), where in (9),  $\delta q_\sigma$  and  $\delta p_\sigma$  are arbitrary independent increments. (9)  $\Rightarrow \partial H / \partial q_\sigma = -\dot{p}_\sigma$ , and  $\partial H / \partial p_\sigma = \dot{q}_\sigma$ ; or  $\dot{q}_\sigma = \partial H / \partial p_\sigma$  (---(10a)), and  $\dot{p}_\sigma = -\partial H / \partial q_\sigma$  (---(10b)). We have 2n first order D.E.'s in time t; and 10a and 10b are known as Hamilton's canonical equations of motion (Lagrange's Equations  $\Rightarrow$  Hamilton's Equations).

**Converse.** Assume (10a, 10b), with  $p_\sigma = \partial L / \partial \dot{q}_\sigma$ . Now  $H = \sum_{\sigma=1}^n (\dot{q}_\sigma p_\sigma) - L$ , so that  $\delta H = \sum_{\sigma=1}^n [(\delta \dot{q}_\sigma) p_\sigma + \dot{q}_\sigma \delta p_\sigma] - \sum_{\sigma=1}^n [(\partial L / \partial q_\sigma) \delta q_\sigma + (\partial L / \partial \dot{q}_\sigma) \delta \dot{q}_\sigma] = \sum_{\sigma=1}^n \{ (p_\sigma - (\partial L / \partial \dot{q}_\sigma)) \delta \dot{q}_\sigma + (\partial H / \partial p_\sigma) \delta p_\sigma - (\partial L / \partial q_\sigma) \delta q_\sigma \}$ . Note that  $( )$  is again 0. Therefore,  $\partial H / \partial p_\sigma = \partial H / \partial p_\sigma$ , and, more importantly,  $\partial H / \partial q_\sigma = -\partial L / \partial q_\sigma$ ; (by 10b)  $\dot{p}_\sigma = \partial L / \partial q_\sigma$ , or  $d/dt(\partial L / \partial \dot{q}_\sigma) - (\partial L / \partial q_\sigma) = 0$ , Lagrange's equations. So the **Lagrangian** and **Hamiltonian** equations are equivalent.

**Example:** (7) in (10a, 10b)  $\Rightarrow$  (with  $\sigma = 1$ :  $q_1 = r$ ,  $p_1 = p_r$ ;  $\sigma = 2$ :  $q_2 = \theta$ ,  $p_2 = p_\theta$ )  $\dot{r} = (10a) = \partial H / \partial p_r = (7) = \partial / \partial p_r [(p_r^2 / 2m) + (p_\theta^2 / 2mr^2) - (\mu m / r)] = 1/2m \cdot 2p_r = (p_r / m)$  (---(11)). And  $\dot{\theta} = (10a) = \partial H / \partial p_\theta = \partial / \partial p_\theta [(p_r^2 / 2m) + (p_\theta^2 / 2mr^2) - (\mu m / r)] = (p_\theta / mr^2)$  (---(12)). Now  $\dot{p}_r = -\partial H / \partial r = -\partial / \partial r [(p_r^2 / 2m) + (p_\theta^2 / 2mr^2) - (\mu m / r)] = -(p_\theta^2 / 2m)(-2r^{-3}) - \mu m / r^2 = (p_\theta^2 / mr^3) - \mu m / r^2$  (---(13)); and  $\dot{p}_\theta = -\partial H / \partial \theta = 0$  (---(14))  $\Rightarrow p_\theta = \text{constant}$ . **Eliminating**  $p_r$  and  $p_\theta$  from equations (11) to (14) implies that  $m(\ddot{r} - r\dot{\theta}^2) = -\mu m / r^2$  (1.1.5); and that  $m(r\ddot{\theta} + 2\dot{r}\dot{\theta}) = 0$  (1.1.19).

## The Interpretation of H

Now  $\underline{r}_i = \underline{r}_i(q_1, \dots, q_n)$  (1.1.1)  $\Rightarrow \dot{\underline{r}}_i = d\underline{r}_i / dt = (\partial \underline{r}_i / \partial q_1) \dot{q}_1 + (\partial \underline{r}_i / \partial q_2) \dot{q}_2 + \dots + (\partial \underline{r}_i / \partial q_n) \dot{q}_n$  (---(15)). (15)  $\Rightarrow 1/2 m_i \dot{\underline{r}}_i^2 = 1/2 m_i \sum_{\sigma=1}^n (\partial \underline{r}_i / \partial q_\sigma) \cdot (\partial \underline{r}_i / \partial q_\rho) \dot{q}_\sigma \dot{q}_\rho$  (---(16)). So (16) is a homogeneous quadratic form (in the  $\dot{q}_1, \dots, \dot{q}_n$ ). By Euler's theorem for homogeneous functions, we obtain  $\sum_{\sigma=1}^n \dot{q}_\sigma (\partial T / \partial \dot{q}_\sigma) = 2T$  (---(17)).

10th October 2000

**Example** of Euler's Theorem: consider  $f(x, y) = ax^2 + 2hxy + by^2$ . Now  $f(\lambda x, \lambda y) = a(\lambda x)^2 + 2h(\lambda x)(\lambda y) + b(\lambda y)^2 = \lambda^2(ax^2 + 2hxy + by^2) = \lambda^2 f$ . If  $f(x_1, \dots, x_n)$  is homogeneous in  $x_1, \dots, x_n$  of  $n^{\text{th}}$  degree, then  $f(\lambda x_1, \dots, \lambda x_n) = \lambda^n f(x_1, \dots, x_n)$ . Euler:  $\sum_{\sigma=1}^n x_\sigma (\partial f / \partial x_\sigma) = nf$ . **Example:**  $f(x, y) = ax^2 + 2hxy + by^2$ . Now  $\partial f / \partial x = 2ax + 2hy + 0$ , and  $\partial f / \partial y = 0 + 2hx + 2by$ , so that  $x \partial f / \partial x + y \partial f / \partial y = x(2ax + 2hy) + y(2hx + 2by) = 2[ax^2 + 2hxy + by^2] = 2f$ .

Now, by the definition of H in equation (1),  $H = \sum_{\sigma=1}^n \dot{q}_\sigma (\partial L / \partial \dot{q}_\sigma) - L$  (---(18)). From 1.1.8,  $L = T - V$ . From 1.1.2, V is only a function of the  $(q_1, \dots, q_n)$ , and not also a function of the  $\dot{q}_1, \dots, \dot{q}_n$ . Therefore,  $\partial L / \partial \dot{q}_\sigma = \partial / \partial \dot{q}_\sigma (T - V) = (\partial T / \partial \dot{q}_\sigma) + 0$  (---(19)). Using (19) and (17) in (18)  $\Rightarrow H = \sum_{\sigma=1}^n \dot{q}_\sigma (\partial T / \partial \dot{q}_\sigma) - (T - V) = 2T - (T - V)$ ;  $H = T + V$  (---(20)). So the Hamilton function is the sum of the **kinetic and potential** energies of the system.

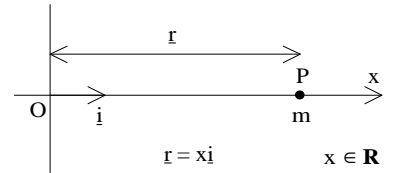
Equations (3), (4) and (7)  $\Rightarrow H = (p_r^2/2m) + (p_\theta^2/2mr^2) + (-\mu m/r) = (3), (4) = ((\dot{r})^2/2m) + (mr^2\dot{\theta})^2/2mr^2 + (-\mu m/r) = \frac{1}{2}m(\dot{r}^2 + (r\dot{\theta})^2) + (-\mu m/r) \text{ ---(21)} = T + V$ . Now *differentiating* the Hamiltonian function w.r.t. **time** gives  $\frac{dH}{dt} = \frac{dH}{dt}(q_1, \dots, q_n, p_1, \dots, p_n) = (\partial H/\partial q_1)\dot{q}_1 + (\partial H/\partial q_2)\dot{q}_2 + \dots + (\partial H/\partial q_n)\dot{q}_n + (\partial H/\partial p_1)\dot{p}_1 + \dots + (\partial H/\partial p_n)\dot{p}_n \text{ ---(22)}$ . The *canonical* equations are  $\dot{q}_\sigma = \partial H/\partial p_\sigma$ , and  $\dot{p}_\sigma = -\partial H/\partial q_\sigma$ . Therefore,  $\frac{dH}{dt} = (-\dot{p}_1\dot{q}_1) + \dots + (-\dot{p}_n\dot{q}_n) + (\dot{q}_1\dot{p}_1) + \dots + (\dot{q}_n\dot{p}_n)$ ;  $\frac{dH}{dt} = 0 \text{ ---(23)}$ . Thus  $H$  is a **constant** of the motion.

## Examples

**Q:** Consider a particle  $P$  of mass  $m$  moving along the **x-axis** subject to a force  $\mathbf{F} = -kx\mathbf{i}$ , where  $k > 0$ , and  $\mathbf{i}$  is along the  $x$ -axis. Show that the system is *holonomic*, and find the number of *degrees of freedom*. Show that the force is **conservative**, and find the potential energy,  $V(x)$ , subject to  $V(0) = 0$ . Show that the *Lagrangian*,  $L$ , is given by  $L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$ , and that the *generalised* momentum corresponding to the *generalised* co-ordinate  $x$  is  $p_x$ , where  $p_x = m\dot{x}$ .

Show that the *Hamiltonian*  $H$  is given by  $H = \frac{1}{2m}p_x^2 + \frac{1}{2}kx^2$ . Obtain the *Lagrangian* equation of motion,  $m\ddot{x} + kx = 0$ , and the **canonical** equations of motion:  $\dot{x} = p_x/m$ , and  $\dot{p}_x = -kx$ . Finally, show that the **Lagrangian** and the **canonical** equations are *equivalent*.

**A:** In the *diagram*,  $x =$  **an arbitrary** real variable:  $q_1 = x$ , a *holonomic* system; and  $n =$  the number of degrees of freedom, 1.  $\mathbf{F} = -kx\mathbf{i}$  ( $k > 0$ ). Is there a  $V(x)$  s.t.  $-\frac{dV}{dx}\mathbf{i} = \mathbf{F}$ ? The work done by  $\mathbf{F}$  in moving its point of application from  $P$  to  $O$  is given by  $W_{P \rightarrow O} = \int_P^O \mathbf{F} \cdot d\mathbf{r} = \int_x^0 (-kx\mathbf{i}) \cdot (dx)\mathbf{i} = -k \int_x^0 x dx = [-\frac{kx^2}{2}]_x^0 = \frac{kx^2}{2}$ . Therefore,  $W_{P \rightarrow O} = V(x) = \frac{1}{2}kx^2$ . Alternatively, find  $V(x)$  s.t.  $\mathbf{F} = -\frac{dV}{dx}\mathbf{i}$  ( $\mathbf{F} = -kx\mathbf{i}$ ). Therefore,  $-kx\mathbf{i} = -\frac{dV}{dx}\mathbf{i} \Rightarrow \frac{dV}{dx} = kx \Rightarrow V = \int kx dx = \frac{1}{2}kx^2 + c$ . But  $V(0) = 0 \Rightarrow c = 0$ , so that  $V = \frac{1}{2}kx^2$ .



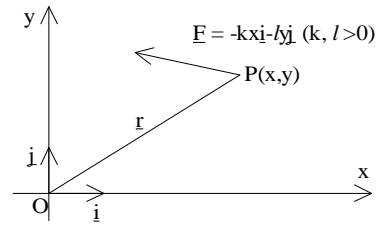
**Now**  $L = T - V$ , where  $T$ , the KE, is *defined* by  $T = \sum_{i=1}^N \frac{1}{2}m\dot{\mathbf{r}}_i^2$ . Here, we have *one* particle of mass  $m$  and position vector  $x$ , so that  $T = \frac{1}{2}m\dot{x}^2$ . Therefore,  $L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$ . **QED**. Now we have *generalised* co-ordinate  $q_1 = x$ ; and the *generalised momentum*  $p_1$  is given by  $p_1 = \partial L/\partial \dot{q}_1 = \partial/\partial \dot{x}[\frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2] = \frac{1}{2}(2m\dot{x}) = m\dot{x}$ . **QED**.

The **Hamiltonian** is defined by  $H = \sum_{\sigma=1}^n (\dot{q}_\sigma p_\sigma) - L = \dot{q}_1 p_1 - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = \frac{d}{dt}(x)m\dot{x} - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = m\dot{x}^2 - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2$ ;  $H = p_x^2/2m + \frac{1}{2}kx^2$ . **QED**. Now 1.1.11 says that the *equations of motion* for the system are obtained from  $L$  by using  $\frac{d}{dt}(\partial L/\partial \dot{q}_\sigma) - (\partial L/\partial q_\sigma) = 0$ . Therefore,  $\partial L/\partial \dot{q}_1 = \partial/\partial \dot{q}_1(L) = m\dot{x}$ , as before.

So  $\frac{d}{dt}(\partial L/\partial \dot{q}_1) = m\ddot{x}$ . **Now**  $\partial L/\partial q_1 = \partial/\partial x(\frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2) = -kx$ . So we have  $m\ddot{x} - (-kx) = 0$ . **QED**. We now **want to obtain** the canonical equations of motion.  $10a \Rightarrow \dot{q}_\sigma = \partial H/\partial p_\sigma$ . So  $\dot{q}_1 = \partial/\partial p_1(\frac{1}{2m}p_x^2 + \frac{1}{2}kx^2)$ ;  $\dot{x} = \partial/\partial p_x(\frac{1}{2m}p_x^2 + \frac{1}{2}kx^2)$ ;  $\dot{x} = p_x/m$ . **QED**. And  $(10b) \Rightarrow \dot{p}_\sigma = -\partial H/\partial q_\sigma$ , so that  $\dot{p}_x = -\partial/\partial x(\frac{1}{2m}p_x^2 + \frac{1}{2}kx^2) = -(\frac{1}{2})k(2x) = -kx$ . **QED**.

Are the equations *equivalent*? The *Lagrangian* equation  $\Rightarrow m\ddot{x} = -kx$ ; and the *canonical* equations  $\Rightarrow \dot{p}_x = -kx$ . Equating for  $-kx$ ,  $\dot{p}_x = m\ddot{x}$ . But as  $p_x = m\dot{x}$ , then  $\dot{p}_x = m\ddot{x}$ . Equivalence! Similarly, we *equate* for  $m$  for the **other** equation.

Q: A particle P of mass  $m$  moves in the  $xy$ -plane subject to a force  $\mathbf{F} = -kx\mathbf{i} - ly\mathbf{j}$ , where  $k$  and  $l$  are positive constants. Repeat the above question for this system. A:  $q_1 = x$ ,  $q_2 = y$ : a *holonomic* system with two d.o.f. Use the curl( $\mathbf{F}$ )  $\equiv 0$  test, or  $W_{P \rightarrow O} = V(P) = \int_P^O \mathbf{F} \cdot d\mathbf{r} = \int_P^O (-kx\mathbf{i} - ly\mathbf{j}) \cdot dx\mathbf{i} + dy\mathbf{j} = \int_P^O -kxdx - lydy = \int_P^O -kxdx + \int_P^O -lydy = \int_x^0 -kxdx + \int_y^0 -lydy = [-\frac{1}{2}kx^2]_x^0 + [-\frac{1}{2}ly^2]_y^0$ ;  $V = \frac{1}{2}kx^2 + \frac{1}{2}ly^2$ .

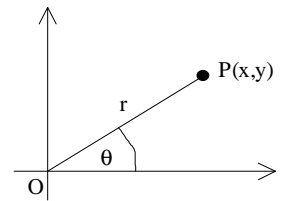


Now  $T = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2$ , so that  $L = T - V = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2 - \frac{1}{2}kx^2 - \frac{1}{2}ly^2$ . Now  $p_1 = \frac{\partial L}{\partial \dot{q}_1} = \frac{\partial L}{\partial \dot{x}} = m\dot{x}$ . Similarly,  $p_2 = m\dot{y}$ . Therefore,  $H = \dot{q}_1 p_1 + \dot{q}_2 p_2 - L = m\dot{x}^2 + m\dot{y}^2 - \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\dot{y}^2 + \frac{1}{2}kx^2 + \frac{1}{2}ly^2 = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2 + \frac{1}{2}kx^2 + \frac{1}{2}ly^2 = \frac{1}{2m}p_x^2 + \frac{1}{2m}p_y^2 + \frac{1}{2}kx^2 + \frac{1}{2}ly^2$ . Now for the *Lagrangian* equations of motion:  $\frac{\partial L}{\partial \dot{q}_1} = m\dot{x}$ , as before, so that  $\frac{d}{dt}(\frac{\partial L}{\partial \dot{x}}) = m\ddot{x}$ . And  $\frac{\partial L}{\partial q_1} = \frac{\partial L}{\partial x} = -kx$ , so that  $m\ddot{x} - (-kx) = 0$ . Similarly,  $m\ddot{y} + ly = 0$ .

Now for the *canonical* equations of motion:  $10a \Rightarrow \dot{q}_1 = \frac{\partial}{\partial p_1}(H)$ ;  $\dot{x} = \frac{\partial}{\partial p_x}(H) = p_x/m$ . Similarly,  $\dot{y} = p_y/m$ . And  $10b \Rightarrow \dot{p}_x = -\frac{\partial}{\partial x}(H) = -kx$ ; and  $\dot{p}_y = -ly$ . We have **already** shown that the two sets of equations of motion are *equivalent*.

Q: A particle P of mass  $m$  moves in space, subject to a force  $\mathbf{F} = -kx\mathbf{i} - ly\mathbf{j} - nz\mathbf{k}$ , where  $k$ ,  $l$  and  $n$  are positive constants. Repeat the above question for this system. A: Just include third terms in the above answers.

Q: Consider question 2 in the **special** case when  $k = l (= \omega^2)$ . Repeat question 1 using **plane** polar co-ordinates,  $(r, \phi)$ , instead of *rectangular* Cartesian co-ordinates,  $(x, y)$ . A: If  $k = l$ , then  $\mathbf{F} = -kx\mathbf{i} - ky\mathbf{j} = -k(x\mathbf{i} + y\mathbf{j}) = -k\mathbf{r} = -\omega^2\mathbf{r} = -\omega^2 r\mathbf{e}_r$ . Here,  $q_1 = r$ , and  $q_2 = \theta$ .  $W_{P \rightarrow O} = V(P) = \int_P^O \mathbf{F} \cdot d\mathbf{r} = \int_P^O (-\omega^2\mathbf{r}) \cdot dr\mathbf{e}_r + d\theta\mathbf{e}_\theta = \int_P^O -\omega^2 r dr = [-\frac{\omega^2 r^2}{2}]_r^0 = \frac{\omega^2 r^2}{2}$ . Now  $T = \frac{1}{2}m\dot{\mathbf{r}}^2$ . As  $\dot{\mathbf{r}} = \dot{r}\mathbf{e}_r + (r\dot{\theta})\mathbf{e}_\theta$ , we have  $\dot{\mathbf{r}}^2 = \dot{r}^2 + (r\dot{\theta})^2$ . **Therefore**,  $T = \frac{1}{2}m(\dot{r}^2 + (r\dot{\theta})^2)$ , so that  $L = T - V = \frac{1}{2}m(\dot{r}^2 + (r\dot{\theta})^2) - \frac{1}{2}\omega^2 r^2 = \frac{1}{2}(m\dot{r}^2 + r^2\dot{\theta}^2 - \omega^2 r^2)$ .



Now  $H = \dot{q}_1 p_1 + \dot{q}_2 p_2 - L$ , where  $p_1 = \frac{\partial L}{\partial \dot{r}} = \frac{1}{2}(2r\dot{\theta}^2 - 2r\omega^2) = r\dot{\theta}^2 - r\omega^2 = p_r$ ; and  $p_2 = \frac{\partial L}{\partial \dot{\theta}} = 0 = p_\theta$ . So  $H = \dot{r}(r\dot{\theta}^2 - r\omega^2) + \dot{\theta}(0) - \frac{1}{2}(m\dot{r}^2 + r^2\dot{\theta}^2 - \omega^2 r^2) = \dot{r}(r\dot{\theta}^2 - r\omega^2) - \frac{1}{2}(m\dot{r}^2 + r^2\dot{\theta}^2 - \omega^2 r^2) = \dot{r}(p_r) - \frac{1}{2}m\dot{r}^2 - \frac{1}{2}r(r\dot{\theta}^2 - r\omega^2) = p_r(\dot{r} - \frac{1}{2}r) - \frac{1}{2}m\dot{r}^2$ . Now for the *Lagrangian* equations of motion:  $\frac{\partial L}{\partial \dot{r}} = m\dot{r}$ , so that  $\frac{d}{dt}(\frac{\partial L}{\partial \dot{r}}) = m\ddot{r}$ . And  $\frac{\partial L}{\partial r} = r\dot{\theta}^2 - r\omega^2$ . So the first equation is  $m\ddot{r} + r\omega^2 - r\dot{\theta}^2 = 0$ . Now  $\frac{\partial L}{\partial \dot{\theta}} = r\dot{\theta}$ , so that  $\frac{d}{dt}(\frac{\partial L}{\partial \dot{\theta}}) = r\ddot{\theta}$ . Further,  $\frac{\partial L}{\partial \theta} = 0$ , so that our second equation is  $r\ddot{\theta} = 0$ . Now for the *canonical* equations of motion:  $10a \Rightarrow \dot{r} = \frac{\partial}{\partial p_r}(H) = \dot{r} - \frac{1}{2}r$ ;  $\dot{\theta} = \frac{\partial}{\partial p_\theta}(H) = 0$ . And  $10b \Rightarrow \dot{p}_r = -\frac{\partial}{\partial r}(H) = p_r/2$ ;  $\dot{p}_\theta = -\frac{\partial}{\partial \theta}(H) = 0$ .

Q: Consider question 3 in the special case where  $k = l = n (= \omega^2)$ . Repeat question 1 using spherical polar co-ordinates,  $(r, \theta, \phi)$ , instead of *rectangular* Cartesian co-ordinates,  $(x, y, z)$ . A: Please refer to the *solution sheet given out in the lectures*.

Q: A particle moves in *space* with the Lagrangian  $L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V + \dot{x}A + \dot{y}B + \dot{z}C$ , where  $V$ ,  $A$ ,  $B$  and  $C$  are given *functions* of  $x$ ,  $y$  and  $z$ . Show that the **equations of motion** consist of  $m\ddot{x} = -\frac{\partial V}{\partial x} + \dot{y}(\frac{\partial B}{\partial x} - \frac{\partial A}{\partial y}) - \dot{z}(\frac{\partial A}{\partial z} - \frac{\partial C}{\partial x})$ , with two *similar* equations. Find the Hamiltonian  $H$ , and obtain the **canonical** equations of motion.

**A:**  $\partial L/\partial \dot{x} = m\dot{x} + A$ , so that  $d/dt(\partial L/\partial \dot{x}) = m\ddot{x} + \partial A/\partial t = m\ddot{x} + \dot{x} \partial A/\partial x + \dot{y} \partial A/\partial y + \dot{z} \partial A/\partial z$ . **And**  $\partial L/\partial x = -\partial V/\partial x + \dot{x} \partial A/\partial x + \dot{y} \partial B/\partial x + \dot{z} \partial C/\partial x$ , so that  $m\dot{x} + \partial A/\partial t - (\partial L/\partial x) = 0$ ;  $m\ddot{x} = -\partial V/\partial x + \dot{x} \partial A/\partial x + \dot{y} \partial B/\partial x + \dot{z} \partial C/\partial x - (\dot{x} \partial A/\partial x + \dot{y} \partial A/\partial y + \dot{z} \partial A/\partial z) = -\partial V/\partial x + \dot{y}(\partial B/\partial x - \partial A/\partial y) - \dot{z}(\partial A/\partial z - \partial C/\partial x)$ . **QED**, with two *similar* equations. Now  $H = \dot{x}p_x + \dot{y}p_y + \dot{z}p_z - L$ , where  $p_x = \partial L/\partial \dot{x} = m\dot{x} + A$ ;  $p_y = m\dot{y} + B$ ; and  $p_z = m\dot{z} + C$ . Therefore,  $H = m\dot{x}^2 + A\dot{x} + m\dot{y}^2 + B\dot{y} + m\dot{z}^2 + C\dot{z} - L = \dots = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + V$ .

Now get *rid* of  $\dot{x}$ ,  $\dot{y}$  and  $\dot{z}$ :  $\dot{x} = p_x - A/m$ ;  $\dot{y} = p_y - B/m$ ; and  $\dot{z} = p_z - C/m$ , so that  $H = \frac{1}{2}m((p_x - A/m)^2 + (p_y - B/m)^2 + (p_z - C/m)^2) + V = \frac{1}{2m}((p_x - A)^2 + (p_y - B)^2 + (p_z - C)^2) + V$ . Let us now obtain the *canonical equations*.  $10a \Rightarrow \dot{x} = \partial H/\partial p_x = \frac{1}{2m}2(p_x - A) = p_x - A/m$ . *Similarly*,  $\dot{y} = p_y - B/m$ ; and  $\dot{z} = p_z - C/m$ . **Now**  $10b \Rightarrow \dot{p}_x = -\partial H/\partial x = -[\frac{1}{2m}[2(p_x - A)(-\partial A/\partial x)] + 2(p_y - B)(-\partial B/\partial x) + 2(p_z - C)(-\partial C/\partial x)] + \partial V/\partial x = \frac{1}{m}[(p_x - A)\partial A/\partial x + (p_y - B)\partial B/\partial x + (p_z - C)\partial C/\partial x] - \partial V/\partial x$ . We get similar expressions for  $\dot{p}_y$  and  $\dot{p}_z$ .

**Q:** The *Lagrangian* of the one-dimensional anharmonic oscillator is given by  $L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2 - \alpha x^3 + \beta x\dot{x}^2$ , where  $\omega$ ,  $\alpha$  and  $\beta$  are real *constants*. Find the **HAMILTONIAN** function, and write down the *canonical* equations of motion. If initially  $x = 0$  and  $\dot{x} = u$ , **deduce** that  $\frac{1}{2}\dot{x}^2(1 + 2\beta x) + \frac{1}{2}\omega^2 x^2 + \alpha x^3 = \frac{1}{2}u^2$ .

**A:**  $H = \dot{x}p_x - L$ , where  $p_x = \partial L/\partial \dot{x} = \dot{x} + 2\beta x\dot{x}$ . So  $H = \dot{x}p_x - L = (p_x/1 + 2\beta x)p_x - \{\frac{1}{2}(p_x/1 + 2\beta x)^2 - \frac{1}{2}\omega^2 x^2 - \alpha x^3 + \beta x(p_x/1 + 2\beta x)^2\} = p_x^2/(1 + 2\beta x) - p_x^2/2(1 + 2\beta x) + \frac{1}{2}\omega^2 x^2 + \alpha x^3 = \frac{1}{2}p_x^2/(1 + 2\beta x) + \frac{1}{2}\omega^2 x^2 + \alpha x^3$ . **Now**  $\partial H/\partial p_x = \dot{p}_x \Rightarrow \frac{1}{2}p_x^{2(-1)(2\beta)/(1+2\beta x)^2} + \omega^2 x + 3\alpha x^2 = \dot{p}_x$ . *Therefore*,  $\dot{p}_x = \beta p_x^2/(1 + 2\beta x)^2 - \omega^2 x - 3\alpha x^2$ ; **and**  $\partial H/\partial p_x = \dot{x} \Rightarrow p_x/(1 + 2\beta x) = \dot{x}$ .

**Since**  $\partial H/\partial t = 0$ , then  $H = \text{constant} = E$ , say. At  $t = 0$ ,  $x = 0$  and  $\dot{x} = u$ . So we **have**  $p_x = u$  at  $t = 0$ . *Substituting*,  $E = \frac{1}{2}u^2 \Rightarrow \frac{1}{2}p_x^2/(1 + 2\beta x) + \frac{1}{2}\omega^2 x^2 + \alpha x^3 = \frac{1}{2}u^2$ . *Substituting for*  $p_x$ , we have  $\frac{1}{2}\dot{x}^2(1 + 2\beta x) + \frac{1}{2}\omega^2 x^2 + \alpha x^3 = \frac{1}{2}u^2$  as **required**.

### 1.3: Generalised Potential Functions

In the *previous* sections, the potential function  $V$  is only a function of the **generalised** co-ordinates (see 1.1.2). It is possible to generalise the previous work to include velocity dependent and time dependent potentials. The main motivation for this is to obtain the *Lagrangian* and *Hamiltonian* functions for a **charged** particle moving in an **electro-magnetic field**.

11th October 2000

From 1.1.3, the *generalised* forces  $Q_\sigma$  in the case of *ordinary* potential functions are given by  $Q_\sigma = -\partial V/\partial q_\sigma$ , where  $\sigma = 1, 2, \dots, n$ . Now let  $U$  be a *generalised* potential function, so that  $U = U(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n, t)$  (---(1)). Provided that the *generalised* forces  $Q_\sigma$  are now given by the expression  $Q_\sigma = -(\partial U/\partial q_\sigma) + d/dt(\partial U/\partial \dot{q}_\sigma)$  (---(2)), then *Lagrangian* and *Hamiltonian* functions can be defined in the usual way, such that the **motion** of the system is given by the Lagrangian or Hamiltonian equations respectively.

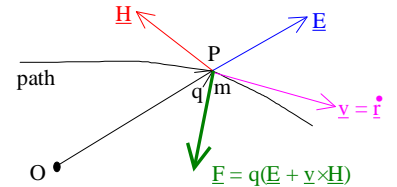
This is seen as follows: in terms of generalised forces  $Q_\sigma$ , Lagrange's equations are as follows:  $\frac{d}{dt}(\frac{\partial T}{\partial \dot{q}_\sigma}) - (\frac{\partial T}{\partial q_\sigma}) = Q_\sigma$  (---(3)), with  $\sigma = 1, 2, \dots, n$ . (2) in (3)  $\Rightarrow \frac{d}{dt}(\frac{\partial T}{\partial \dot{q}_\sigma}) - (\frac{\partial T}{\partial q_\sigma}) = -(\frac{\partial U}{\partial q_\sigma}) + \frac{d}{dt}(\frac{\partial U}{\partial \dot{q}_\sigma})$ ;  $\frac{d}{dt}(\frac{\partial}{\partial \dot{q}_\sigma}(T-U)) - (\frac{\partial}{\partial q_\sigma}(T-U)) = 0$  (---(4)). Now let  $L = T-U$  (---(5)). (4) and (5)  $\Rightarrow \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}_\sigma}) - (\frac{\partial L}{\partial q_\sigma}) = 0$  (---(6)), which are  $L$ 's equations — where the *Lagrangian* function now contains a **potential** function depending on the generalised *velocities* and *time*, as well as the generalised *co-ordinates*.

The **Hamiltonian** function,  $H$ , from (1.2.1), is  $H = (\sum_{\sigma=1}^n \dot{q}_\sigma p_\sigma) - L$ , where  $p_\sigma = (\frac{\partial L}{\partial \dot{q}_\sigma})$  (1.1.23), and  $L$  is as defined by (5) above. Now (1), (5) and (1.2.1)  $\Rightarrow L = L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n, t)$  (---(7);  $H = H(q_1, \dots, q_n, p_1, \dots, p_n, t)$  (---(8)); and the derivation of Hamiltonian's canonical equations (1.2.10a/10b) goes through as in section 1.2, but with the **additional** result that  $\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$  (---(9)).

(1.2.19) says that  $\frac{\partial L}{\partial \dot{q}_\sigma} = (\frac{\partial}{\partial \dot{q}_\sigma}(T-V)) = (\frac{\partial T}{\partial \dot{q}_\sigma}) - (\frac{\partial V}{\partial \dot{q}_\sigma})$ , where the red bit is 0. If  $L = T-U$ , then  $(\frac{\partial L}{\partial \dot{q}_\sigma}) = (\frac{\partial T}{\partial \dot{q}_\sigma}) - (\frac{\partial U}{\partial \dot{q}_\sigma}) \neq \frac{\partial T}{\partial \dot{q}_\sigma}$ , where the blue bit is  $\neq 0$ . However, 1.2.19 no longer holds (with  $V$  replaced by  $U$ ), so that  $L$  is not a **homogeneous** quadratic function of the generalised velocities. Therefore,  $H$  can not now be interpreted as the **sum** of the *kinetic* and the *potential* energies.

Also, we can easily see that  $\frac{dH}{dt} = \frac{\partial H}{\partial t}$  (---(10)), so that  $H$  is a *constant* of the motion if and only if  $H$  does not depend **explicitly** on  $t$ , i.e. iff  $\frac{\partial H}{\partial t} = 0$ . **Example:** The most important example of a system having a generalised potential function is that of a **charged** particle moving in an *electromagnetic field*.

Suppose that the particle has **mass**  $m$  and **charge**  $q$ . The force  $\underline{F}$  on the particle (in SI units) is given by  $\underline{F} = q(\underline{E} + \underline{v} \times \underline{H})$  (---(11)), where  $\underline{E}$  and  $\underline{H}$  are the *electric* and the *magnetic* field strengths respectively.  $\underline{E}$  and  $\underline{H}$  are given in terms of the *scalar* and the *vector* potentials  $\phi$  and  $\underline{A}$  respectively, by  $\underline{E} = -\text{grad}(\phi) - \frac{\partial \underline{A}}{\partial t}$  (---(12); and  $\underline{H} = \text{curl}(\underline{A})$  (---(13)), where  $\phi = \phi(\underline{r}, t)$  (---(14));  $\underline{A} = \underline{A}(\underline{r}, t)$  (---(15)); and  $\underline{v} = \dot{\underline{r}}$  is the *velocity* of the particle.



(11), (12) and (13)  $\Rightarrow F_x = -q(\frac{\partial \phi}{\partial x}) - q(\frac{\partial A_x}{\partial t}) + q[\dot{y}((\frac{\partial A_y}{\partial x}) - \frac{\partial}{\partial y} A_x) - \dot{z}((\frac{\partial A_x}{\partial z}) - \frac{\partial}{\partial x} A_z)]$  (---(16)), where  $(x, y, z) = \underline{r}$ ;  $(\dot{x}, \dot{y}, \dot{z}) = \dot{\underline{r}} = \underline{v}$ ;  $\underline{F} = (F_x, F_y, F_z)$ ; and  $\underline{A} = (A_x, A_y, A_z)$  (relative to *rectangular cartesian co-ordinates* at  $O$ ). Note that **similar** expressions can be written down for  $F_y$  and  $F_z$ ; and in (16),  $F_x$  is the *generalised force* corresponding to the **cartesian** general co-ordinate  $x$ .

13th October 2000

Consider the *general potential function*  $U(x, y, z, \dot{x}, \dot{y}, \dot{z}) = U(\underline{r}, \underline{v}, t) = q\phi(\underline{r}, t) - q(\underline{v} \cdot \underline{A}(\underline{r}, t))$  (---(17)). ( $= q\phi(x, y, z, t) - q(\dot{x}A_x(x, y, z, t) + \dot{y}A_y(\dots) + \dot{z}A_z(\dots))$ ). This is *verified* by substituting into equation (2),  $Q_\sigma = -\frac{\partial U}{\partial q_\sigma} + \frac{d}{dt}(\frac{\partial U}{\partial \dot{q}_\sigma})$ :  $\frac{\partial U}{\partial x} = q\frac{\partial \phi}{\partial x} - q(\dot{x}(\frac{\partial A_x}{\partial x}) + \dot{y}(\frac{\partial A_y}{\partial y}) + \dot{z}(\frac{\partial A_z}{\partial z}))$  (---(18));  $\frac{\partial U}{\partial \dot{x}} = -qA_x$ . (---(19)). So  $\frac{d}{dt}(\frac{\partial U}{\partial \dot{x}}) = -q((\frac{\partial A_x}{\partial x})\dot{x} + (\frac{\partial A_x}{\partial y})\dot{y} + (\frac{\partial A_x}{\partial z})\dot{z} + (\frac{\partial A_x}{\partial t}))$  (---(20)). Now (18) and (20) imply that we have  $F_x = \frac{d}{dt}(\frac{\partial U}{\partial \dot{x}}) - \frac{\partial U}{\partial x} = -q\frac{\partial \phi}{\partial x} - q(\frac{\partial A_x}{\partial t}) + q[\dot{y}((\frac{\partial A_y}{\partial x}) - (\frac{\partial A_x}{\partial y})) - \dot{z}((\frac{\partial A_x}{\partial z}) - (\frac{\partial A_z}{\partial x}))]$  (---(21)).

The **RHS** of (21) is *identical* to the **RHS** of (16). Similarly for  $F_y$  and  $F_z$ . Now (5) and (17)  $\Rightarrow L = T-U = \frac{1}{2}m\mathbf{v}^2 - q\phi + q\mathbf{v}\cdot\mathbf{A} = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - q\phi(x,y,z,t) + q(\dot{x}A_x(x,y,z,t) + \dot{y}A_y(\dots) + \dot{z}A_z(\dots))$  (---(22)). (1.1.23) and (22)  $\Rightarrow p_x = \partial L/\partial \dot{x} = m\dot{x} + qA_x$  (---(23a));  $p_y = \partial L/\partial \dot{y} = m\dot{y} + qA_y$  (---(23b)); and  $p_z = \partial L/\partial \dot{z} = m\dot{z} + qA_z$  (---(23c)).

Now a *reminder* that  $\mathbf{E} = -\nabla\phi - (\partial\mathbf{A}/\partial t)$  (---(12)); and that  $\mathbf{H} = \text{curl}(\mathbf{A})$  (---(13)). (1.2.1), (23a-c) and (22)  $\Rightarrow \mathbf{H} = (\dot{x}p_x + \dot{y}p_y + \dot{z}p_z) - L = \dot{x}(m\dot{x} + qA_x) + \dot{y}(m\dot{y} + qA_y) + \dot{z}(m\dot{z} + qA_z) - \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + q\phi - q(\dot{x}A_x + \dot{y}A_y + \dot{z}A_z) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + q\phi(x,y,z,t)$  (---(24)). So  $\mathbf{H} = T + q\phi$  (---(25)), *mechanical KE + scalar potential only*. In (25), the term involving the **vector** potential (i.e.  $-q(\mathbf{v}\cdot\mathbf{A})$ ) is *absent*. **Contrast** this with (1.2.22). Now (23a-c) in (24)  $\Rightarrow \mathbf{H} = \frac{1}{2}m((p_x - qA_x)^2 + (p_y - qA_y)^2 + (p_z - qA_z)^2) + q\phi = (\frac{1}{2}m)\mathbf{(p - qA)}^2 + q\phi$  (---(26)), where  $\mathbf{p} = (p_x, p_y, p_z)$ .

17th October 2000

## Essential Background to Quantum Mechanics

Newton conceived *light rays* as being a stream of tiny corpuscles, but Huygens, his contemporary, held that light had a *wave-like* form. Because of Newton's immense prestige in science, his view prevailed until Young at the beginning of the 19th century made his discovery that under certain circumstances, two beams of light can **cancel** each other out.

This phenomenon of *destructive interference* could only be explained by the **wave** theory. The latter theory thus displaced the **corpuscular** theory for the whole of the 19th century, until the phenomena of *Black Body Radiation* and the *Photoelectric Effect* failed to find explanation by the wave theory. Einstein (in 1905) gave a simple explanation of the latter by assuming that the energy of radiation is carried in small "*packets*" or "*quanta*", such that the energy  $E$  and the frequency  $\nu$  are related by  $E = h\nu$  (---(1)), where  $h$  is a *universal* constant called Planck's constant ( $h = 6.626 \times 10^{-34}\text{Js}$ ). These quanta (or photons) travel with the speed of **light**.

The corpuscular nature of radiation was further demonstrated by Compton (in 1923) in an experiment where X-rays were scattered by electrons. The mechanism was explained by using the theory of **elastic** collisions in classical mechanics, associating with rays of wavelength  $\lambda$  photons of momentum  $p = h/\lambda$  (---(2)). Therefore, radiation appears in *two* roles: the **wave** and the **corpuscle** roles.

The corpuscular nature of matter is *obvious*, but what is surprising is that electrons, atoms and even molecules display effects which are typically wave like. In 1927, Davisson and Germer showed that electrons are diffracted by *crystals* to give five interference patterns. Similarly, Stern (in 1932) showed that the same situation is found for *Helium* atoms and *Hydrogen* molecules. Equation 2, connecting the **momentum** to the **wavelength**, was found to be true in all cases.

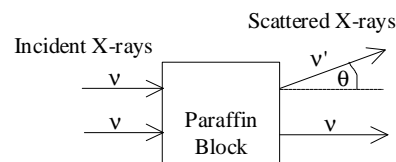
It was De Broigle (in 1925) who proposed that matter displayed the same *wave-corpuscle* duality as found in radiation. He said that a material particle has a matter wave associated with it, just as a light quantum has a light wave. Also, the relation between the two aspects is given by (1), where  $E$  is the energy of the **particle**, and  $\nu$  is the **frequency** of the matter wave.

Now, since in the *Theory of Relativity*, energy and momentum are not independent entities, but energy and the three spatial components of momentum are the four components of a relativistic “four-vector”, the energy being the “time” component, it is suggested that for consistency with equation (1), we have  $p = h\tau$ . Since  $\nu$  denotes the number of waves *per unit time*,  $\tau$  must signify the number of waves per unit *length*, i.e.  $1/\lambda$ , where  $\lambda$  is the wavelength. Thus de Broigle arrived at the relation (equation (2)) which has been completely confirmed by **experiment**.

Thus we see that *matter* and *radiation* sometime behave like waves, and sometimes behave like corpuscles. This dual behaviour is called the **wave-particle duality**. How are these two aspects to be reconciled? We are indebted to Born (1926) for the *Statistical Interpretation*. According to this, the intensity of the associated wave at a point of space is *proportional* to the probability of finding the corresponding particle at that point. This idea will be made more precise later as the **Quantum Theory** is developed.

## Section 2: Physical Background to Quantum Mechanics

**Compton Effect (1923)**. Compton found that when X-rays were passed through a block of paraffin, the *scattered* rays had a smaller frequency (or longer wavelength) than the incident rays. Some of the rays passed through the block without any *change*. It was known that the scattering was due to electrons, and on the basis of **classical** theory, the electrons would oscillate with the same frequency,  $\nu$ , as that of the incident radiation.

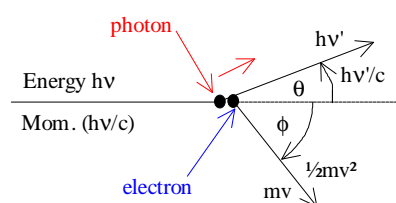


The oscillating electron would now behave as an *oscillating dipole*, and thus would radiate energy with the same frequency,  $\nu$ . However, from experiment, it was found that the actual frequency was less than the frequency of the actual radiation. So *classical* theory fails to explain the effect. Experiment  $\Rightarrow \delta\lambda = \lambda' - \lambda = \frac{c}{\nu'} - \frac{c}{\nu} = 2.4 \times 10^{-10}(1 - \cos\theta)$  in *c.g.s. units*, or  $2.4 \times 10^{-12}(1 - \cos\theta)$  in *SI units* (---(1)).

**Compton** explained the results as follows: assume that the X-rays consist of *photons of energy*  $h\nu$  ( $h = \text{planck's constant}$ ), and that the scattering is due to the **collision** with electrons. Consider the collision of a photon with an *electron* (which may be assumed to be at rest). From classical physics, the momentum of an electromagnetic wave of energy  $\epsilon$  is  $\frac{\epsilon}{c}$  (where  $c$  is the *speed of light*) and assume from this result that the **momentum** of the photon is  $\frac{h\nu}{c} = \frac{h}{\lambda}$ .

The result of the *collision* is determined by using the principles of the conservation of **energy** and **linear momentum** (e.g. elastic collision of *spheres*). In the diagram, we can formulate the following conservation of energy:  $h\nu = h\nu' + \frac{1}{2}mv^2$  (---(2)). Also, the conservation of linear momentum (**parallel** to the incident radiation)

is  $\frac{h\nu}{c} = \frac{h\nu'}{c}(\cos\theta) + mv\cos\phi$  (---(3)); and, **perpendicular** to the incident radiation, it is  $0 = \frac{h\nu'}{c}(\sin\theta) - mv\sin\phi$  (---(4)).



Eliminating  $\phi$ , (3) and (4)  $\Rightarrow \frac{h^2}{c^2}(v^2 - 2vv'\cos\theta + (v')^2) = (mv)^2$  (---(5)). (2) and (5)  $\Rightarrow$  (eliminating  $v^2$ )  $\frac{h^2}{c^2}(v^2 - 2vv'\cos\theta + (v')^2) = 2mh(v - v')$  (---(6)). But  $v \approx v'$ , so in the LHS of (6), we have  $\delta v = v' - v = -(\frac{h}{mc^2})(1 - \cos\theta)v^2$  (---(7)). But since  $v = \frac{c}{\lambda}$ , then  $\delta v = -\frac{c}{\lambda^2}\delta\lambda$  (---(8)). (7) and (8)  $\Rightarrow -\frac{c}{\lambda^2}\delta\lambda = -\frac{h}{mc^2}\frac{c^2}{h^2}(1 - \cos\theta)$ ;  $\delta\lambda = \frac{h}{mc}(1 - \cos\theta)$  (---(9)), where  $\frac{h}{mc}$  is “Compton’s wavelength”, and is given by  $\lambda_0 = 2.426 \times 10^{-12} \text{m}$ . A calculation using **relativistic** mechanics yields the same result (equation (9)) without having to make the approximation  $v' \approx v$ .

18th October 2000

## 2.2: The Wave Nature of Matter

In the *previous* section, we showed how radiation showed a **particle** like nature. The particle like nature of matter is obvious from everyday experience. Is it possible for matter to exhibit a *wave-like* nature? In 1924, de Broglie suggested just this. He postulated that the relations used in the Compton Effect:  $E = hv$  (---(1)), and  $p = h/\lambda$  (---(2)), which estimated a *connection* between the **wave** nature of radiation and its **particle-like** nature, should also be true for particles of *matter*.

In 1927, Davisson and Germer showed that a beam of electrons exhibits *diffraction effects* when passed through a crystal. The explanation of this is given by the de Broglie equations ((1) and (2)). An electron **accelerated** through 10,000 volts has a corresponding wavelength of  $0.122 \text{ \AA} = 0.122 \times 10^{-10} \text{m}$ . *Similarly*, scattering slow **neutrons** gives **diffraction** patterns. A thermal *neutron* corresponding to a temperature of  $300^\circ \text{K}$  has  $\lambda = 1.81 \text{ \AA} = 1.81 \times 10^{-10} \text{m}$ . Stern (1932): Molecular rays ( $\text{H}_2$ , He) give diffraction patterns as well.

## 2.3: The Wave Theory and Corpuscular Theory Reconciled: Born’s Interpretation

In preceding sections, we have seen how both *radiation* and *matter* appear in two contradictory roles: as waves and as particles (or corpuscles). Which is **right**? The answer is both are correct up to a point. Born’s Explanation (1926): To every particle, there corresponds a wave, and the amplitude of the wave at any point determines the probability of the particle being at that point. If the amplitude of the wave is **zero** at any point, then the probability of finding the particle at that point is **vanishingly** small.

## Section 3: Quantum Theory

### 3.1: The “Derivation” of Schrodinger’s Wave Equation

According to *de Broglie*, a particle with energy  $E$  and momentum  $p$  is *associated* with a wave of frequency  $\nu$  and wavelength  $\lambda$ , given by  $E = h\nu$  (---(1)), and  $p = h/\lambda$  (---(2)), where  $h$  is *Planck’s constant*,  $6.62618 \times 10^{-34} \text{Js}$ . Suppose that the particle is travelling **along** the x-axis under the action of no force (a *free particle*).

Using the **complex** representation of waves, the associated wave may be written as  $\psi(x,t) = A \exp[2\pi i(x/\lambda - vt)]$  (---(3)). (1) and (2) in (3)  $\Rightarrow \psi(x,t) = A \exp[2\pi i(px/\hbar - E/\hbar t)]$  (---(4)). Let  $\hbar = h/2\pi$  (---(5)), then (4) and (5)  $\Rightarrow \psi(x,t) = A \exp[(i/\hbar)(px - Et)]$  (---(6)). We shall now obtain a DE satisfied by  $\psi$ : (6)  $\Rightarrow \partial\psi/\partial x = A((ip/\hbar)\exp[...]) = (ip/\hbar)\psi$ ;  $\partial^2\psi/\partial x^2 = (ip/\hbar)^2\psi = -(p^2/\hbar^2)\psi$  (---(7)). Also,  $\partial\psi/\partial t = -(iE/\hbar)\psi$  (---(8)). Now, for a free particle,  $E = p^2/2m$  (---(9)). (7), (8) and (9)  $\Rightarrow \partial^2\psi/\partial x^2 = -(p^2/\hbar^2)\psi = -(2mE/\hbar^2)\psi = (8) = -(2mi/\hbar)\partial\psi/\partial t \Rightarrow -(\hbar^2/2m)\partial^2\psi/\partial x^2 = \hbar \partial\psi/\partial t$  (---(10)).

20th October 2000

We can generalise (10) to a wave travelling in any direction. Suppose that the momentum vector is  $\underline{p}$ , with components  $(p_x, p_y, p_z)$ , then (6) becomes  $\psi(\underline{r},t) = A \exp[(i/\hbar)(\underline{p}\cdot\underline{r} - Et)]$  (---(11)). (11)  $\Rightarrow \text{grad}\psi = \underline{i}\partial\psi/\partial x + \underline{j}\partial\psi/\partial y + \underline{k}\partial\psi/\partial z = (i\underline{p}/\hbar)\psi$ . Now  $\text{div}(\text{grad}\psi) = \text{div}((i\underline{p}/\hbar)\psi)$ . Recall:  $\text{div}(\mu\underline{a}) = \mu\text{div}(\underline{a}) + \underline{a}\cdot\text{grad}\mu$ . Therefore,  $\text{div}(\text{grad}\psi) = (i\psi/\hbar)\text{div}(\underline{p}) + \underline{p}\cdot\text{grad}(i\psi/\hbar)$ . Because the first part is zero ( $\underline{p}$  is a constant vector), then  $= \underline{p}\cdot(i/\hbar)^2\underline{p}\psi = -p^2/\hbar^2\psi = \nabla^2\psi$  (---(14)), where  $p^2 = \underline{p}^2 = \underline{p}\cdot\underline{p}$ . Now (11)  $\Rightarrow \partial\psi/\partial t = -(iE/\hbar)\psi$  (---(15)). Further, (9), (14) and (15)  $\Rightarrow (\hbar^2/2m)\nabla^2\psi(\underline{r},t) = \hbar \partial\psi/\partial t(\underline{r},t)$  (---(16)). This is correct for a freely moving particle.

If the particle is **not** free, but is moving under the influence of conservative forces (with a potential function  $V(\underline{r},t)$ ), the energy equation (9) becomes  $E = (\underline{p}^2/2m) + V(\underline{r},t)$  (---(17)). We assume that (14) and (15) (with some new  $\psi$  different from that in equation (11)) are true in this situation as well. Therefore,  $-(\hbar^2/2m)\nabla^2\psi = (\underline{p}^2/2m)\psi = (11) = (E - V(\underline{r},t))\psi = \hbar \partial\psi/\partial t - V(\underline{r},t)\psi$  (where the first part comes from (15)), i.e.  $(-\hbar^2/2m)\nabla^2\psi(\underline{r},t) + V(\underline{r},t)\psi(\underline{r},t) = \hbar \partial\psi/\partial t(\underline{r},t)$ . (---(18)).

The above is the famous **Schrödinger Equation** (the time-dependent version). The above "derivation" is bogus since it is assumed that the momentum  $\underline{p}$  and the corresponding wavelength  $\lambda$  are independent of position in the presence of external forces. However, its justification is that results deduced from it are in agreement with **experimental results**.

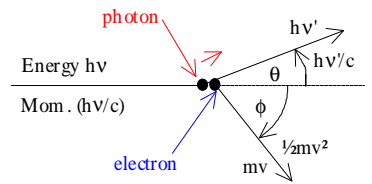
## Examples

**[Constants:**  $h = 6.62618 \times 10^{-34} \text{Js}$ ;  $h/2\pi = \hbar = 1.05459 \times 10^{-34} \text{Js}$ ;  $c = 2.99792 \times 10^8 \text{ms}^{-1}$ ;  $m_e$  (electron mass)  $= 9.10953 \times 10^{-31} \text{kg}$ ;  $e$  (absolute value of electron charge)  $= 1.60219 \times 10^{-19} \text{C}$ ;  $1 \text{eV}$  (electron volt)  $= 1.60219 \times 10^{-19} \text{J}$ ].

**Q:** The **maximum** energy of photoelectrons emitted from potassium is 2.1eV when illuminated by light of wavelength  $3 \times 10^{-7} \text{m}$ , and 0.5eV when illuminated by light of wavelength  $5 \times 10^{-7} \text{m}$ . Use these results to obtain values for **Planck's** constant, and the **minimum** energy to free an electron from potassium.

**A:** Use  $E_x = hv - \phi$ . Now  $(?)\text{eV} = h(c/\lambda) - \phi$ , so we have  $2.1\text{eV} = h(2.99792 \times 10^8 / 3 \times 10^{-7}) - \phi$  (---(1)); and  $0.5\text{eV} = h(2.99792 \times 10^8 / 5 \times 10^{-7}) - \phi$  (---(2)). Equating for  $\phi$ ,  $h(2.99792 \times 10^8 / 3 \times 10^{-7}) - 2.1\text{eV} = h(c/5 \times 10^{-7}) - 0.5\text{eV}$ ;  $-1.6\text{eV} = h(c/5 \times 10^{-7} - c/3 \times 10^{-7})$ ;  $-1.6\text{eV} = h(5.99584 \times 10^{14} - 9.993 \times 10^{14})$ ;  $-1.6\text{eV} = h(-3.997226 \times 10^{14})$ ;  $\underline{h = 6.4132 \times 10^{-34}}$ . Similarly, equating for  $\phi$ , we get  $\phi = 1.9\text{eV}$ .

Q: An X-ray photon of wavelength  $1.0 \times 10^{-12} \text{m}$  is incident on a stationary electron. Calculate the wavelength of the scattered photon, if it is detected at an angle of (i)  $60^\circ$ , (ii)  $90^\circ$ , and (iii)  $120^\circ$  to the incident radiation. A: We have the situation shown, and the equation  $\delta\lambda = \frac{h}{mc}(1-\cos\theta)$ , where  $\delta\lambda = \lambda' - \lambda = \lambda' - 1.0 \times 10^{-12}$ . (i)  $\theta = 60^\circ$ :



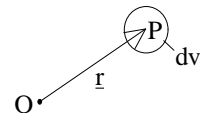
$\lambda' - 1.0 \times 10^{-12} = \frac{h}{mc}(1 - \cos 60^\circ)$ . **Because**  $\frac{h}{mc} = 6.62618 \times 10^{-34} / (9.10953 \times 10^{-31})(2.99792 \times 10^8) = 2.426 \times 10^{-12}$ , then  $\lambda' - 1.0 \times 10^{-12} = 2.426 \times 10^{-12}(1 - 1/2) = 1.213 \times 10^{-12}$ ;  $\lambda' = 1.0 \times 10^{-12} + 1.213 \times 10^{-12} = 2.213 \times 10^{-12}$ ; and the wavelength of the scattered photon is  $2.213 \times 10^{-12} \text{m}$ .

(ii)  $\theta = 90^\circ$ :  $\lambda' - 1.0 \times 10^{-12} = 2.426 \times 10^{-12}(1 - \cos 90^\circ)$ ;  $\lambda' = 2.426 \times 10^{-12} + 1.0 \times 10^{-12} = 3.426 \times 10^{-12} \text{m}$ . (iii)  $\theta = 120^\circ$ :  $\lambda' - 1.0 \times 10^{-12} = 2.426 \times 10^{-12}(1 - \cos 120^\circ)$ ;  $\lambda' = 1.0 \times 10^{-12} + 2.426 \times 10^{-12}(1.5) = 4.639 \times 10^{-12}$ . **Conclusion:** as the angle of detection of the scattered photon increases, so does the wavelength of the scattered photon.

24th October 2000

### 3.2: Interpretation of the Wave Function, $\psi$

According to **Born**, the  $|\psi|^2$  is proportional to the probability of the particle being "at" a given point. More precisely, if  $P(\underline{r}, t)dv$  is the probability of the particle being in a small volume  $dv$  about  $\underline{r}$  at time  $t$ , then the probability density  $P(\underline{r}, t)$  is given by  $P(\underline{r}, t) = \alpha |\psi(\underline{r}, t)|^2$ . Note:  $|w|^2 = u^2 + v^2 = (u + iv)(u + iv)^* = (u + iv)(u + iv)^* = (u + iv)(u - iv) = u^2 + v^2$ , where we use  $*$  to denote conjugate in Quantum Mechanics.



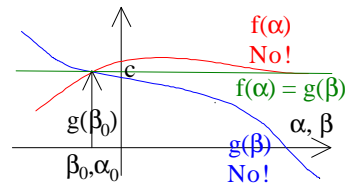
Therefore,  $P(\underline{r}, t) = \alpha \psi(\underline{r}, t) \psi^*(\underline{r}, t)$  (---(1)), where  $\alpha$  is a positive constant which is determined by the requirement that the particle must exist somewhere in space, i.e.  $\int_R P(\underline{r}, t) dv = 1$  (---(2)), where  $R$  denotes the region containing the particle. (1) into (2)  $\Rightarrow \alpha \int_R \psi \psi^* dv = 1$  (---(3)). So  $P(\underline{r}, t) = (\psi(\underline{r}, t) \psi^*(\underline{r}, t)) / (\int_R \psi \psi^* dv)$  (---(4)). If the wave function  $\psi$  is s.t.  $\alpha = 1$  in (3), i.e.  $\int_R \psi \psi^* dv = 1$  (---(5)), then  $\psi$  is said to be normalised.

So for normalised wave functions  $\psi$ ,  $|\psi|^2 = \psi \psi^*$  is the probability density function for the position of the particle in space. Provided that  $\int_R \psi \psi^* dv$  exists, then if we define  $\psi' = \frac{1}{\sqrt{k}} \psi$ , then  $\int_R \psi' \psi'^* = \frac{1}{k} \int_R \psi \psi^* dv = \frac{1}{k} (k) = 1$  — so  $\psi'$  is normalised. As the TDSE is linear, if  $\psi$  is a solution, then so is  $\psi' = \frac{1}{\sqrt{k}} \psi$ . So we can get a normalised wave function as a result.

### 3.3: The Time Independent Schrödinger Equation

Equation (3.1.18)  $\Rightarrow (-\hbar^2/2m)\nabla^2\psi(\underline{r}, t) + V(\underline{r}, t)\psi(\underline{r}, t) = \hbar \frac{\partial \psi}{\partial t}(\underline{r}, t)$  (---(1)). Suppose that  $V$  is now independent of time, and thus is a function of position only. We now use the separation of variables method to look for solutions of the form  $\psi(\underline{r}, t) = u(\underline{r})T(t)$ , i.e.  $(-\hbar^2/2m)\nabla^2[u(\underline{r})T(t)] + V(\underline{r})[u(\underline{r})T(t)] = i\hbar \frac{\partial}{\partial t}[u(\underline{r})T(t)] = i\hbar u(\underline{r}) \frac{d}{dt}(T(t))$ ;  $(-\hbar^2/2m)T(t)\nabla^2(u(\underline{r})) + V(\underline{r})u(\underline{r})T(t) = i\hbar u(\underline{r}) \frac{d}{dt}(T(t))$ . Now divide by  $u(\underline{r})T(t)$  to give  $(-\hbar^2/2m)(1/u(\underline{r}))\nabla^2(u(\underline{r})) + V(\underline{r}) = (i\hbar/T(t)) \frac{d}{dt}(T(t))$  (---(2)). The LHS depends on  $\underline{r}$  only (or on  $x, y, z$ ); while the RHS depends on  $t$  only.

Let  $\alpha$  and  $\beta$  be *two independent* variables, and let  $f(\alpha)$  and  $g(\beta)$  be 2 functions of these respective variables. Now **suppose** that  $f(\alpha) = g(\beta)$ , with  $-\infty < \alpha, \beta < \infty$ . Since  $x, y, z$  and  $t$  are *independent variables*, then (2)  $\Rightarrow$  both sides must equal the **same** constant —  $E$ , say, i.e.  $1/u(\underline{r})[(-\hbar^2/2m)\nabla^2(u(\underline{r})) + V(\underline{r})u(\underline{r})] = E$  (---(3)), and  $(\hbar/T(t))^{(d(T(t))/dt)} = L$  (---(4)). *Integration* of (4)  $\Rightarrow T(t) = \exp(-iEt/\hbar)$  (---(5)). Comparing with the plane wave solution for a free particle, equation 3.1.11  $\Rightarrow \psi(\underline{r},t) = A\exp[(i/\hbar)(\underline{p}\cdot\underline{r}-Et)] = A\exp[(i\hbar)\underline{p}\cdot\underline{r}]\exp[-iEt/\hbar]$ . Note that the **2nd exponential** is our equation (5).



25th October 2000

Now (3)  $\Rightarrow H u(\underline{r}) = E u(\underline{r})$  (---(6)), where  $H = (-\hbar^2/2m)\nabla^2 + V(\underline{r})$  (---(7)). Equation (6) is called the Schrödinger Time Independent Wave Equation, where  $E$  denotes the **constant** value of the energy of the particle. From (7),  $H$  is an operator *acting* on  $u(\underline{r})$  to yield a constant **multiple** of  $u(\underline{r})$ . This is of the form of an *eigenvalue* equation, where the constant  $E$  is known as the eigenvalue, and the corresponding function  $u(\underline{r})$  is known as the eigenfunction.

So a solution  $\psi_E(\underline{r},t)$  is given by  $\psi_E(\underline{r},t) = u_E(\underline{r})\exp(-iEt/\hbar)$  (---(8)), where  $E$  is a *constant value of the energy*. By **Born's** Interpretation (3.2.1),  $p(\underline{r},t) = \psi_E \psi_E^* / \int_R \psi_E \psi_E^* dv = (8) = u_E(\underline{r})u_E^*(\underline{r}) / \int_R u_E(\underline{r})u_E^*(\underline{r})dv$ , which shows that the *probability density function*  $p(\underline{r},t)$  is **independent** of  $t$  for these *special* solutions,  $\psi_E(\underline{r},t)$ . For **this** reason, these solutions are called stationary states. The *most general solution* is given by  $\psi(\underline{r},t) = \sum_E a_E \psi_E(\underline{r},t)$ , where  $a_E \in \mathbb{C}$  (*complex*) depending on  $E$ . (**Aside:** The TDSE is  $H\psi(\underline{r},t) = \hbar \partial\psi/\partial t$ ).

### 3.4: Conditions That $\psi$ Must Satisfy

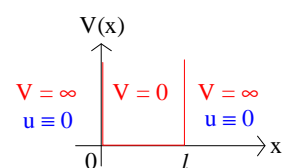
We're *interested* in “physically acceptable” solutions of the SE. Since  $\psi$  determines a *probability density function*, then it must be everywhere single-valued and finite. Further, except where  $V$  has *infinite discontinuities*,  $\psi$  and  $\text{grad}\psi$  are **everywhere** continuous. Finally, if the particle is confined to a *certain finite region*  $R$  of space, then the probability of finding the particle in  $R$  must be **unity**.

This implies that  $\psi$  must be *square integrable*:  $\int_R |\psi|^2 dv = \int_R \psi \psi^* dv = \text{constant} = \beta < \infty$  (---(1)). Writing  $\psi' = \psi/\sqrt{\beta}$ , then  $\psi'$  is *normalised*:  $\int_R |\psi'|^2 dv = 1$ . These *states* are called **bound** states. Note: a *plane wave* is **not** a bound state:  $\psi(\underline{r},t) = A\exp[(i/\hbar)(\underline{p}\cdot\underline{r}-Et)]$ ;  $|\psi|^2 = |A|^2$ .

27th October 2000

### 3.5: A Particle in an Infinitely Deep One-Dimensional Potential Well

The *1-dimensional time-independent SE* is given by (Section 3.3, 6 and 7)  $(-\hbar^2/2m)d^2u/dx^2 + V(x)u(x) = Eu(x)$  (---(1)). An *infinite discontinuity* in  $V(x)$  at  $x = 0, l \Rightarrow u(x) \equiv 0$  when  $x < 0$  and  $x > l$ . By the **continuity** of  $u(x)$ ,  $u(0) = 0 = u(l)$  (---(2)). So for  $0 < x < l$ , equation (1) **becomes**  $d^2u/dx^2 + k^2u = 0$  (---(3)), where  $k^2 = 2mE/\hbar^2$  (---(4)). **Solutions** of (3) are of the form  $u(x) = A\sin(kx) + B\cos(kx)$  (---(5)), where  $A$  and  $B$  are *arbitrary constants*.



(2) and (5)  $\Rightarrow 0 = u(0) = A\sin(0) + B\cos(0) = B$ . **Therefore,  $B = 0$  (---(6)).** Now (2) again  $\Rightarrow u(l) = 0 = (5)$ , (6)  $= A\sin(kl) \Rightarrow A = 0$  or  $\sin(kl) = 0$ . **But  $A = 0$** , with (6) in (5)  $\Rightarrow u(x) \equiv 0$  for all  $x$ . But this is *not physically acceptable* — we require  $|u(x)|^2$  to be **proportional** to a probability density function for the position of the particle.

A density function cannot vanish identically. **Therefore,  $\sin(kl) = 0$  (as  $A \neq 0$ )  $\Rightarrow kl = n\pi$** , where  $n \in \mathbf{Z}$  (---(7)). But  $n = 0 \Rightarrow u(x) \equiv 0$ , *not physically acceptable*. Now  $u(x)_{n=p}$ ,  $p \in \mathbf{N} = -u(x)_{n=p}$ , and so  $u_{n=p}$  is *linearly dependent* on the solution  $u_{n=p}$ . **Therefore, the set of linearly independent solutions are  $u_n(x) = A_n \sin(n\pi x/l)$  (---(8))**, where  $n = 1, 2, 3, \dots$  Now (4) and (7)  $\Rightarrow (n\pi/l)^2 = k^2 = 2mE/\hbar^2 \Rightarrow E_n = \frac{1}{2m}(\hbar\pi/l)^2 n^2$  (---(9)), where  $n = 1, 2, 3, \dots$

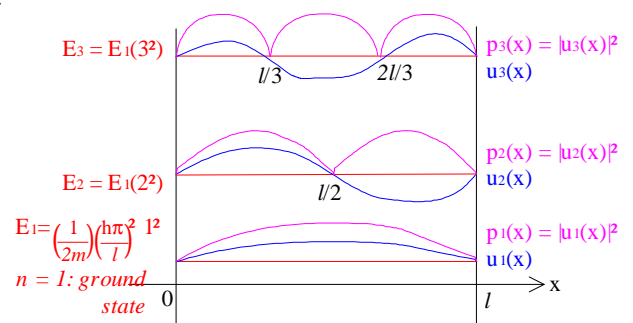
This is a *bound state problem* so that we can **normalise** the wave function. Therefore,  $\int_{-\infty}^{\infty} |u(x)|^2 dx = 1 \Rightarrow \int_0^l |A_n \sin(n\pi x/l)|^2 dx = 1 \Rightarrow |A_n|^2 \int_0^l \sin^2(n\pi x/l) dx = 1 \Rightarrow |A_n|^2 (l/2) = 1$ . So  $|A_n| = \sqrt{2/l}$  (this is the  $r$  in  $z = re^{i\theta}$  — **complex polar** notation);  $A_n = (\sqrt{2/l})e^{i\delta_n}$ , where  $0 \leq \delta_n < 2\pi$ .

*No loss of generality occurs* if we take  $\delta_n = 0$  for all  $n$ , i.e. the **measurable** quantities to do with  $u_n(x)$  (such as the *probability density function* for the position of the particle) are **not** dependent on  $\delta_n$ . So  $A_n = (\sqrt{2/l})$ ;  $u_n(x) = (\sqrt{2/l})\sin(n\pi x/l)$  for  $0 < x < l$ ; and  $A_n = 0$  for  $x \leq 0$  and for  $x \geq l$ , where  $E_n = \frac{1}{2m}(\hbar\pi/l)^2 n^2$  (---(9)). Note that  $n$  is called a **quantum number** for this problem.

31st October 2000

## Probability Distributions

For  $\underline{n} = 1$ ,  $|u_1(x)|^2 = (2/l)\sin^2(\pi x/l) = p_1(x)$ . For  $\underline{n} = 2$ ,  $|u_2(x)|^2 = (2/l)\sin^2(2\pi x/l) = p_2(x)$ . For  $\underline{n} = 3$ ,  $|u_3(x)|^2 = (2/l)\sin^2(3\pi x/l) = p_3(x)$ . **Exercise:** Consider a *macroscopic* particle:  $m = 10^{-4}$  grams, with  $l = 10^{-2}$  cm. Then  $E_1 = \frac{1}{2m}(\hbar\pi/l)^2 1^2 \approx 10^{-46}$  ergs  $\approx 10^{-53}$  J, which is so *small* that it **cannot** be detected experimentally. The speed of this particle is  $v$ , where  $\frac{1}{2}mv^2 = 10^{-53}$  J;  $v \approx 10^{-23}$  ms $^{-1}$ . How long will it take to *get across the well*? If  $v = \frac{1}{l}$ , then  $t = \frac{l}{v} = 1 \times 10^{-4} / 1 \times 10^{-23} = 1 \times 10^{19}$  s  $\approx 3.17 \times 10^{11}$  **years**. However, **consider** an electron, with  $m \approx 10^{-27}$  grams. Then  $E_1 \approx 5 \times 10^{-30}$  J, so that  $\frac{1}{2}mv^2 = 5 \times 10^{-30} \Rightarrow v \approx 3$  m/s.



**Q:** An *electron* is confined to a **one-dimensional potential well** of width  $3 \times 10^{-10}$  m which has *infinitely* high sides. Calculate (i) the three **lowest** allowed values of the electron energy; (ii) the wavelength of the electromagnetic wave that would cause the electron to be **excited** from the lowest to the highest of these three levels; and (iii) *all possible wavelengths* of the radiation emitted following the excitation in (ii).

**A:** (i) With  $l = 3 \times 10^{-10}$  m,  $E = \frac{1}{2m}(\hbar\pi/l)^2 = \frac{1}{2(9.10953 \times 10^{-31})(\pi \times (1.05459 \times 10^{-34}) / (3 \times 10^{-10}))^2} \approx 6.694 \times 10^{-19}$  J  $\approx 4.18$  eV. Further,  $E_2 = 4E_1$ , and  $E_3 = 9E_1$ . (ii) To go *from*  $E_1$  to  $E_3$  would take **energy**  $E_3 - E_1 = 5.3554 \times 10^{-18}$  J ( $8E_1$ ). Now *using*  $E = h\nu = hc/\lambda$ , so that  $5.3554 \times 10^{-18} = (6.62618 \times 10^{-34}) \times (2.99792 \times 10^8) / \lambda$ , we get  $\lambda = 3.709 \times 10^{-8}$  m. (iii) We have *3 possibilities*:  $\lambda_{31}$  ( $E_3 \rightarrow E_1$ ) =  $3.71 \times 10^{-8}$  m (as above);  $\lambda_{21}$  ( $E_2 \rightarrow E_1$ ) =  $9.90 \times 10^{-8}$  m; and  $\lambda_{32}$  ( $E_3 \rightarrow E_2$ ) =  $5.94 \times 10^{-8}$  m.

**Recap:**  $\psi_n(x,t) = u_n(x)\exp(-iE_n t/\hbar)$ , where  $u_n(x) = (\sqrt{2/l})\sin(n\pi x/l)$  for  $0 < x < l$ , and 0 for  $x \leq 0$  and  $x \geq l$ ; and  $E_n = \frac{1}{2m}(\hbar\pi/l)^2 n^2$  for  $n = 1, 2, \dots, \infty$ .  $\psi_n$  are *normalised*  $\Rightarrow \int_{-\infty}^{\infty} |\psi_n|^2 dx = 1$ . Consider the *average* value (or *expectation* value) of the x-coordinate of the particle,  $\bar{x} = \langle x \rangle = \int_{-\infty}^{\infty} x |\psi_n|^2 dx = (\frac{2}{l}) \int_0^l x \sin^2(n\pi x/l) dx = \frac{l}{2} = \langle x \rangle_q$ .

Classically, the probability of the particle being **anywhere** between 0 and  $l$  is constant, and the *probability density function* is  $1/l$ . So  $\langle x \rangle_{cl} = \int_0^l x \cdot \frac{1}{l} dx = [\frac{x^2}{2l}]_0^l = \frac{l}{2} = \langle x \rangle_q$ . Similarly,  $\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n|^2 dx = \int_{-\infty}^{\infty} \psi_n^* x^2 \psi_n dx$  (\* = complex conjugate)  $= (\frac{2}{l}) \int_0^l x^2 \sin^2(n\pi x/l) dx = \dots = \frac{l^3}{3} \{ \frac{1}{3} - \frac{1}{2(n\pi)^2} \}$ . Classically,  $\langle x^2 \rangle_{cl} = \int_0^l x^2 (\frac{1}{l}) dx = [\frac{x^3}{3l}]_0^l = \frac{l^3}{3}$ . Now  $\langle x^2 \rangle_q \rightarrow \langle x^2 \rangle_{cl}$  for **large**  $n$ : this is Bohr's Correspondence Principle.

**Aside:** The general solution is  $\psi(x,t) = \sum_n C_n \psi_n(x,t)$ , where  $C_n \in \mathbf{C}$  (complex). How do we calculate the expectation value of the momentum of the particle? From *section 3.1*,  $\text{grad}\psi(\mathbf{r},t) = (i\mathbf{p}/\hbar)\psi(\mathbf{r},t)$ , where  $\psi(\mathbf{r},t) = A\exp[(i/\hbar)(\mathbf{p}\cdot\mathbf{r} - Et)]$ . *Multiplying* by  $(-i\hbar)$  gives  $-i\hbar \text{grad}\psi = \mathbf{p}\psi$ . Now, we *assume* that  $\langle \mathbf{p} \rangle = \int_R \psi^* \mathbf{p} \psi dv = \int_R \psi^* (-i\hbar) \text{grad}\psi dv$  (where  $(-i\hbar)\text{grad}$  is the **operator**,  $\mathbf{p}_{op}$ ); and we assume that it is *true* for all normalised  $\psi$  (not **just** for those that represent *plane waves*).

**Note:**  $\mathbf{p}$  is replaced by the operator  $(i\hbar)\text{grad}$ . In our **example**,  $\mathbf{p} = p_x \mathbf{i} \Leftrightarrow \mathbf{i}(-i\hbar) \frac{\partial}{\partial x}$ . So  $p_x = -i\hbar \frac{\partial}{\partial x}$ . Now  $\langle p_x \rangle = \int_R \psi^* (-i\hbar) \frac{\partial}{\partial x} \psi dv =$  (putting  $\psi = \psi_n$ )  $= \int_{-\infty}^{\infty} \psi_n^* (-i\hbar) \frac{\partial}{\partial x} (\psi_n) dx =$  (*1-dimensional*)  $= \int_0^l ((\sqrt{2/l})\sin(n\pi x/l)\exp(-iE_n t/\hbar))^* (-i\hbar) \frac{\partial}{\partial x} [(\sqrt{2/l})\sin(n\pi x/l)\exp(-iE_n t/\hbar)] dx = (-\hbar)^2/l \int_0^l \sin(n\pi x/l) \frac{\partial}{\partial x} (\sin(n\pi x/l)) dx = \dots = 0 = \langle p_x \rangle_{cl}$ . What **about**  $\langle p^2/2m \rangle (= \langle KE \rangle)$ ? We *have the following*:  $\int_R \psi^* [-i\hbar \nabla] \cdot (-i\hbar \nabla) / 2m \psi dv = (\frac{2}{l}) \int_0^l (\hbar^2/2m) \sin(n\pi x/l) \frac{\partial^2}{\partial x^2} (\sin(n\pi x/l)) dx = (\frac{2}{l}) (\hbar^2/2m) \times (-\frac{n^2\pi^2}{l^2}) \int_0^l \sin^2(n\pi x/l) dx = \dots = \frac{1}{2m} (\hbar\pi/l)^2 n^2 (= E_n)$ .

## Examples

**Q:** A **particle** of mass  $m$  moves in an *infinitely* deep square well potential given by  $V(x) = 0$  for  $0 \leq x \leq l$ ; and  $V(x) = \infty$  for  $x < 0$  and  $x > l$ . Solve the *Schrodinger* time independent equation for the energy *eigenvalues*  $E_n$ , and the corresponding normalised *eigenfunctions*  $u_n(x)$  given by the following:  $E_n = ((\hbar\pi)^2/2m l^2) n^2$ ;  $u_n(x) = (\sqrt{2/l})\sin(n\pi x/l)$  for  $0 \leq x \leq l$ ; and  $u_n(x) = 0$  for  $x < 0$  and  $x > l$ , where  $n = 1, 2, 3, \dots$

**A:** This was solved in the 27/10/2000 lecture. Also have a look at the *solution sheet* in the file. In general, the *TISE* is  $Hu(\mathbf{r}) = Eu(\mathbf{r})$ , where  $H = (-\hbar^2/2m)\nabla^2 + V(\mathbf{r})$ . In *one dimension*, we have  $(-\hbar^2/2m) \frac{d^2u}{dx^2} + V(x)u(x) = Eu(x)$ . For  $x < 0$  and  $x > l$ , we have  $0 = 0$ . For  $0 \leq x \leq l$ , we have  $(-\hbar^2/2m) \frac{d^2u}{dx^2} = E_n u_n(x)$ ;  $\dots$ ;  $\frac{d^2u}{dx^2} = (2mE/\hbar^2)u_n = 0$ . Then set  $k^2$ , and *continue* to solve as in the lecture.

**Q:** If  $u_m$  and  $u_n$  are the wave functions corresponding to *two energy states* of a particle confined to a **one-dimensional** box with infinite sides, show that  $\int_{-\infty}^{\infty} u_m^* u_n dx = 0$ , with  $m \neq n$  (use the *expression* for  $u_n$  given in a **previous** question). **A:** It is obvious that  $\int_0^l u_m^* u_n dx = \int_l^\infty u_m^* u_n dx = 0$  from the *definition* of  $u_n(x)$ .

So we want  $\int_0^l u^*_m u_n dx = \int_0^l (\sqrt{2/l} \sin(m\pi x/l)) (\sqrt{2/l} \sin(n\pi x/l)) dx = 2/l \int_0^l \sin(m\pi x/l) \sin(n\pi x/l) dx$ . Now  $\sin A \sin B = 1/2 (\cos(A+B) - \cos(A-B))$ , so that  $= 2/l \int_0^l 1/2 [\cos((m+n)\pi x/l) - \cos((m-n)\pi x/l)] dx = 1/l \int_0^l \cos((m-n)\pi x/l) - \cos((m+n)\pi x/l) dx = 1/l [\sin((m-n)\pi x/l) / (m-n)\pi - \sin((m+n)\pi x/l) / (m+n)\pi]_0^l = 1/(m-n)\pi \sin((m-n)\pi) - 1/(m+n)\pi \sin((m+n)\pi) - (0/(m-n)\pi \sin(0) - 0/(m+n)\pi \sin(0)) = 1/(m-n)\pi \sin((m-n)\pi) - 1/(m+n)\pi \sin((m+n)\pi)$ . As  $\sin k\pi = 0$  for any integer  $k$ , then  $1/(m-n)\pi \sin((m-n)\pi) - 1/(m+n)\pi \sin((m+n)\pi) = 0$  for all  $m$  and  $n$ , *excluding*  $m = n$ , as in this case,  $1/(m-n)\pi \sin((m-n)\pi) = 1/0 \sin(0)$  — which is *not allowed*. **Conclusion:**  $\int_{-\infty}^{\infty} u^*_m u_n dx = 0$ , with  $m \neq n$ . **QED.**

Q: Write down the *general solution*,  $\psi(x,t)$ , of the *time-dependent Schrodinger equation* for the particle in question 3 above, in terms of the **eigenvalues**  $E_n$ , and the corresponding **eigenfunctions**  $u_n(x)$  of the *time-independent Schrodinger equation*. If, at  $t = 0$ ,  $\psi(x,0) = \sin^3(\pi x/l)$  for  $0 \leq x \leq l$ , and  $\psi(x,0) = 0$  for  $x < 0$  and  $x > l$ , show that for  $t > 0$ , we have  $\psi(x,t) = 3a u_1(x) \exp(-iE_1 t/\hbar) - a u_3(x) \exp(-iE_3 t/\hbar)$ , where  $a = (\sqrt{l/32})$ . **Hint:**  $4\sin^3(\theta) = 3\sin(\theta) - \sin(3\theta)$ .

A: The *general solution* is given by  $\psi(\underline{r},t) = \sum_E a_E \psi_E(\underline{r},t)$ , where  $a_E \in \mathbf{C}$ , *depending* on  $E$ ; and  $\psi_E(\underline{r},t) = u_E(\underline{r}) \exp(-iEt/\hbar)$ . So  $\psi(x,t) = \sum_n a_n \psi_n(x,t)$ ;  $\psi(x,t) = \sum_n a_n u_n(x) \exp(-iE_n t/\hbar)$ . **When**  $t = 0$ ,  $\psi(x,0) = \sum_n a_n \sqrt{2/l} \sin(n\pi x/l) \exp(0)$  for  $0 \leq x \leq l$ , and  $\psi(x,0) = 0$  for  $x < 0$  and  $x > l$ .

So **for**  $0 \leq x \leq l$ ,  $\sin^3(\pi x/l) = \sum_n a_n \sqrt{2/l} \sin(n\pi x/l)$ ;  $(1/4)(3\sin(\pi x/l) - \sin(3\pi x/l)) = \sum_n a_n \sqrt{2/l} \sin(n\pi x/l)$ ;  $3\sin(\pi x/l) - \sin(3\pi x/l) = \sum_n a_n \sqrt{2/l} \sin(n\pi x/l)$ . Now *choose*  $a_0 = 0$ ,  $a_1 = \sqrt{l/32}(3)$ ,  $a_2 = 0$ ,  $a_3 = -\sqrt{l/32}$ , and  $a_4 = a_5 = \dots = 0$ . Let  $a = \sqrt{l/32}$ , so that all  $a_i = 0$ , except  $a_1 = 3a$ , and  $a_3 = -a$ . Now, let us get back to the *general solution*:  $\psi(x,t) = \sum_n a_n u_n(x) \exp(-iE_n t/\hbar)$ . But now we *know the values of all* the  $a_n$ , so that  $\psi(x,t) = 3a u_1(x) \exp(-iE_1 t/\hbar) - a u_3(x) \exp(-iE_3 t/\hbar)$ , where  $a = \sqrt{l/32}$ . **QED.**

Q: For the *particle* in question 3 above, calculate the **expectation value**  $\langle x \rangle$  of the  $x$ -co-ordinate of the particle in the  $n^{\text{th}}$  stationary state  $u_n(x)$ , and *compare* with the corresponding classical value. A: Recall that  $u_n(x) = \sqrt{2/l} \sin(n\pi x/l)$  for  $0 \leq x \leq l$ , and  $u_n(x) = 0$  for  $x < 0$  and  $x > l$ . Therefore,  $\langle x \rangle = \int_{-\infty}^{\infty} x (u_n(x))^2 dx = \int_0^l x [\sqrt{2/l} \sin(n\pi x/l)]^2 dx = 2/l \int_0^l x \sin^2(n\pi x/l) dx$ .

Let  $I = \int_0^l x \sin^2(n\pi x/l) dx$ . Evaluate by *parts*: Let  $u = x$ ,  $du/dx = 1$ ;  $dv/dx = \sin^2(n\pi x/l)$ ,  $v$ : as  $\cos 2A = 1 - 2\sin^2 A$ , then  $\sin^2 A = 1/2(1 - \cos 2A)$ , so that  $\sin^2(n\pi x/l) = 1/2(1 - \cos(2n\pi x/l))$ . Therefore,  $v = \int (1/2)(1 - \cos(2n\pi x/l)) dx = 1/2 \int [1 - \cos(2n\pi x/l)] dx = 1/2 [x - \sin(2n\pi x/l) / (2n\pi)]$ , so that  $I = uv - \int v du/dx dx = [x/2 (x - \sin(2n\pi x/l) / (2n\pi))]_0^l - \int_0^l 1/2 (x - \sin(2n\pi x/l) / (2n\pi)) dx = [\dots]_0^l - 1/2 [x^2/2 + (l/(2n\pi))^2 \cos(2n\pi x/l)]_0^l = [1/2 (l^2 - l^2 \sin(2n\pi))] - 0 - 1/2 [l^2/2 + (l/(2n\pi))^2 \cos(2n\pi)] + 1/2 [(l/(2n\pi))^2 \cos(0)]$ . Notes: the **blue** bit is zero, and the **red** bits are 1.

Therefore,  $I = [1/2(l)] - 1/2 [l^2/2 + (l/(2n\pi))^2] + 1/2 [(l/(2n\pi))^2] = l^2/2 - l^2/4 - 1/2 (l/(2n\pi))^2 + 1/2 (l/(2n\pi))^2 = l^2/4$ . So  $\langle x \rangle = 2/l I = (2/l)(l^2/4) = l/2$ . **Classically**, the probability of the particle being anywhere between 0 and  $l$  is constant. The p.d.f. is  $1/l$  for  $0 \leq x \leq l$ , and 0 *everywhere* else. Therefore,  $\langle x \rangle_{cl} = \int_{-\infty}^{\infty} x p(x) dx = \int_0^l x/l dx = [x^2/2l]_0^l = l/2 = \langle x \rangle_q$ . Conclusion: we get the **same** values using *quantum* or *classical* methods.

**Q: Repeat** the above question for the *expectation value*  $\langle x^2 \rangle$ . Comment on your results.

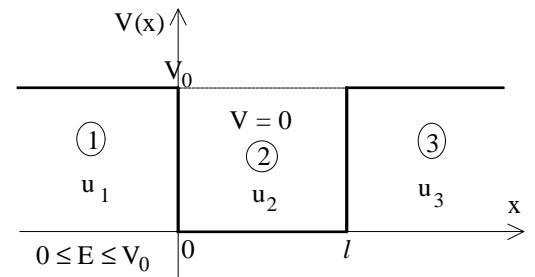
**A:**  $\langle x^2 \rangle = \int_0^l x^2 \sin^2(n\pi x/l) dx = \int_0^l x^2 \sin^2(n\pi x/l) dx$ . Evaluate the integral  $I$  by **parts** again: let  $u = x^2$ ,  $du/dx = 2x$ ;  $dv/dx = \sin^2(n\pi x/l)$ , and  $v = \frac{1}{2}(x - \frac{l}{2n\pi})\sin(2n\pi x/l)$ , as before. Substituting into the *integral*, we get  $I = \dots = \frac{l^3}{6} + \int_0^l x(\frac{l}{2n\pi})\sin(2n\pi x/l) dx$ .

Now let  $J = \int_0^l x(\frac{l}{2n\pi})\sin(2n\pi x/l) dx$ . By **parts** again, let  $u = x/l$ ,  $du/dx = 1/l$ ;  $dv/dx = \sin(2n\pi x/l)$ , and  $v = -\frac{1}{2n\pi}\cos(2n\pi x/l)$ . So  $J = \dots = -\frac{l^3}{(2n\pi)^2}$ ; and therefore,  $I = \frac{l^3}{6} + J = \frac{l^3}{6} - \frac{l^3}{(2n\pi)^2}$ . **Conclusion:**  $\langle x^2 \rangle = \frac{2}{l} I = \frac{2}{l} (\frac{l^3}{6} - \frac{l^3}{(2n\pi)^2}) = \frac{l^2}{3} (1 - \frac{1}{(2n\pi)^2})$ . *Classically*, with the same pdf as before,  $\langle x^2 \rangle_{cl} = \int_0^l x^2/l dx = \frac{l^2}{3}$ . The *quantum* expectation value will be **smaller** in magnitude than the *classical* expectation value. However, as  $n \rightarrow \infty$ ,  $\langle x^2 \rangle_q \rightarrow \frac{l^2}{3} = \langle x^2 \rangle_{cl}$ . This is "Bohr's Correspondence Principle".

3rd November 2000

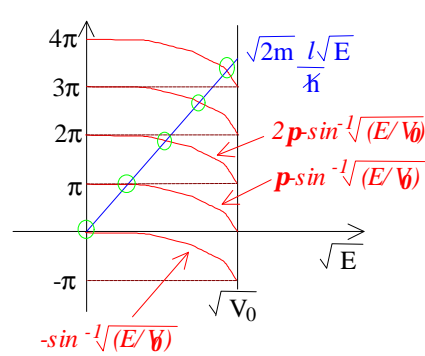
### 3.6: Square Well with Finite Potential Walls

The TISE is  $(-\hbar^2/2m)(d^2u/dx^2) + Vu = Eu$  (---(1)). In **region 1**,  $d^2u_1/dx^2 - k_1^2 u_1 = 0$  (---(2)), where  $k_1^2 = (2m\hbar^{-2})(V_0 - E)$  (---(3)).  $[e^{\pm k_1 x}, k_1 > 0]$ . In **region 2**,  $d^2u_2/dx^2 + k_2^2 u_2 = 0$  (---(4)), where  $k_2^2 = 2mE/\hbar^2$  (---(5)). In **region 3**,  $d^2u_3/dx^2 - k_3^2 u_3 = 0$  (---(6)), where  $k_3^2 = (2m\hbar^{-2})(V_0 - E)$  (---(7))  $[e^{\pm k_3 x}]$ .



In region 1, the *solutions* which remain finite as  $x \rightarrow -\infty$  are:  $u_1(x) = Ae^{+k_1 x}$  (---(8)) ( $k_1 > 0$ ). In region 3, ... as  $x \rightarrow +\infty$  are  $u_3(x) = Ce^{-k_3 x}$  (---(9)) ( $k_3 > 0$ ). In region 2,  $u_2 = B\sin(k_2 x + \epsilon)$  (---(10)). (Note: A, B, C and  $\epsilon$  are *arbitrary* constants). We require the **continuity** of  $u(x)$  and  $du/dx$  across the *boundaries* of the regions, i.e.  $d/dx[\ln(u(x))] = u'(x)/u(x)$  must be *continuous* across the boundaries.

Now  $u_1'(x)/u_1(x)|_{x=0} = u_2'(x)/u_2(x)|_{x=0}$ ;  $Ak_1 e^{k_1 x}/Ae^{k_1 x}|_{x=0} = Bk_2 \cos(k_2 x + \epsilon)/B\sin(k_2 x + \epsilon)|_{x=0}$ ;  $k_1 = k_2 \cot(\epsilon)$  (---(11)). *Similarly*,  $u_2'(x)/u_2(x)|_{x=l} = u_3'(x)/u_3(x)|_{x=l} \Rightarrow k_2 \cot(k_2 l + \epsilon) = -k_3$  (---(12)). Now (3), (5) and (11)  $\Rightarrow \cot(\epsilon) = k_1/k_2 = (\sqrt{(V_0 - E)/E})$ , so that  $\sin(\epsilon) = (\sqrt{E})/(\sqrt{V_0})$  (---(13))  $\Rightarrow \epsilon = \sin^{-1}(\sqrt{E/V_0}) + n_1\pi$  (---(14)), where  $n_1 = 0, \pm 1, \pm 2, \dots$

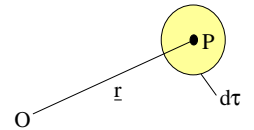


Also, **equation** (12)  $\Rightarrow \cot(k_2 l + \epsilon) = -k_3/k_2 = (5)$ , (7)  $\sqrt{V_0} \sqrt{V_0 - E} = -\sqrt{(V_0 - E)/\sqrt{E}}$ . Therefore,  $\sin(k_2 l + \epsilon) = -\sqrt{E}/\sqrt{V_0}$ ;  $k_2 l + \epsilon = -\sin^{-1}(\sqrt{E/V_0}) + n_2\pi$  (---(15)), where  $n_2 = 0, \pm 1, \pm 2, \dots$ . Now (14) and (15)  $\Rightarrow k_2 l = (5) = (\sqrt{(2mE/\hbar^2)})l = -2\sin^{-1}(\sqrt{E/V_0}) + n\pi$  ( $n = n_2 - n_1$ ). Alternatively,  $(l\hbar)\sqrt{(2mE)} = n\pi - 2\sin^{-1}(\sqrt{E/V_0})$  (---(16)), where  $n = 0, \pm 1, \pm 2, \dots$ . **No** negative  $n$  solutions. With  $n = 0$ , the only solution is  $E = 0 \Rightarrow u_1(x) = u_2(x) = u_3(x) = 0$  for *all*  $x$ . (Not physically acceptable).

### 3.7: The General Principles of Quantum Mechanics for a Single Particle

**Reference:** Rae, Chapter 4. Consider a particle of mass  $m$  moving in space under the action of a *conservative force*, with potential function  $V(\underline{r}, t)$ . **(P1)**. The quantum mechanical behaviour of the particle is *completely specified* by a complex-valued, square integrable wave (or state) function  $\psi(\underline{r}, t)$ .

**Remarks:** A square integrable function  $\psi$  satisfies  $0 < \int_{\text{all space}} |\psi|^2 d\tau = \int_{\text{all space}} \psi^* \psi d\tau < \infty$  (---(1)). The norm,  $\|\psi\|$ , of  $\psi$ , is defined by  $\|\psi\| = [\langle \psi | \psi \rangle]^{1/2}$  (---(2)), where  $\langle \psi | \psi \rangle = \int_{\text{all space}} \psi^* \psi d\tau$  (---(3)). If the norm of  $\psi$  is **unity**, then  $\psi$  is said to be *normalised*, and every wave function may be **normalised**, since  $\|d\psi\| = 1$  if  $d = (\langle \psi | \psi \rangle)^{-1/2}$ . If  $\psi$  is normalised, then  $|\psi(\underline{r}, t)|^2 d\tau$  denotes the *probability* that the particle lies in the volume element  $d\tau$  around the point with position vector  $\underline{r}$  at time  $t$ .



**(P2)**. Provided the particle is not *disturbed* (by, for example, a measurement), then the wave function  $\psi$  satisfies the time-dependent Schrödinger Equation,  $H_{\text{op}} \psi = \hbar \frac{\partial \psi}{\partial t}$  (---(4)), a *linear Equation*; where  $H_{\text{op}} = (-\hbar^2/2m)\nabla^2 + V$  (---(5));  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  (---(6)); and  $\hbar = h/2\pi$ , where  $h$  is *Planck's constant*,  $(1.054589 \pm 0.000006) \times 10^{-34}$  Js.

**Remarks:**  $H_{\text{op}}$  is called the *Hamiltonian* operator for the particle in the potential  $V$ . The fact that equation (4) is **linear** implies that  $\psi = \sum_{n=1}^{\infty} C_n \psi_n$  (---(7)) is a solution of  $\psi_n$ , for  $n = 1, 2, \dots$ , where the  $C_n$  are *arbitrary* complex constants. The set of **all** solutions of (4) form a function space called a *Hilbert* space,  $H$ .

**(P3)**. To a dynamical variable, or observable,  $A(x, y, z, p_x, p_y, p_z, t)$ , there *corresponds* an operator  $A_{\text{op}}$ , given by  $A_{\text{op}} = A(x, y, z, -i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z}, t)$  (---(8)), where  $p_x, p_y$  and  $p_z$  are the *Cartesian* components of the momentum  $\underline{p}$  of the particle.

**Remark:**  $A_{\text{op}}$  is a linear operator *acting* on  $H$ :  $A_{\text{op}}(c_1 \psi_1 + c_2 \psi_2) = c_1 (A_{\text{op}} \psi_1) + c_2 (A_{\text{op}} \psi_2)$  (---(9)), where  $c_1$  and  $c_2$  are arbitrary complex constants;  $\psi_1, \psi_2 \in H$ ; and  $A_{\text{op}}$  possesses a *complete set of orthonormal eigenfunctions*, which correspond to real eigenvalues, i.e.  $A_{\text{op}}$  is a **Hermitian** operator:  $\langle A_{\text{op}} \psi | \phi \rangle = \int_{\text{all space}} (A_{\text{op}} \psi)^* \phi d\tau = \int_{\text{all space}} \psi^* (A_{\text{op}} \phi) d\tau = \langle \psi | A_{\text{op}} \phi \rangle$ , for any  $\psi, \phi$  in  $H$  (---(10)). Further, we have  $A_{\text{op}} \phi_n = a_n \phi_n$  (---(11)), where  $n = 1, 2, \dots$ ; the **red**  $\phi_n$  are *orthonormal* eigenfunctions which imply the basis of  $H$ ; the  $a_n$  are real; and  $\langle \phi_n | \phi_m \rangle = \delta_{nm}$  (---(12)), where  $\delta_{nm} = 1$  when  $n = m$ , and  $\delta_{nm} = 0$  when  $n \neq m$ .

(Aside: for a **square** well,  $u_n = \sqrt{(2/l)} \sin(n\pi x/l)$ , for  $n = 1, 2, \dots, \infty$ ). Further, the set  $\{\phi_n\}$  is complete, i.e. for any  $\psi$  in  $H$ ,  $\psi = \sum_{n=1}^{\infty} c_n \phi_n$  (---(13)), where  $c_n = \langle \phi_n | \psi \rangle$  (---(14)). Now  $\langle \phi_m | \psi \rangle = \langle \phi_m | \sum_n c_n \phi_n \rangle = \sum_n c_n \langle \phi_m | \phi_n \rangle$  (red = (12) =  $\delta_{nm}$ ) =  $c_m$ . Therefore,  $c_m = \langle \phi_m | \psi \rangle$ .

**(P4).** The only *possible results* of the measurement of a dynamical variable, A, on the particle in the state  $\psi$ , are the eigenvalues  $a_n$  of  $A_{op}$ . If  $\psi$  is normalised, then (13)  $\Rightarrow \sum_{n=1}^{\infty} |c_n|^2 = 1$  (---(15)), and the *probability* of the result of the measurement of A being  $a_k$  is  $|c_k|^2$ . Immediately **after** the measurement, if  $a_k$  is obtained, then the *state function* of the particle is  $\phi_k$ .

Important Remarks. (R1): If  $V$  is independent of  $t$ , then the time  $t$  may be separated from the spatial co-ordinates  $x, y$  and  $z$  in equation (4), to give  $H_{op}u(\underline{r}) = Eu(\underline{r})$  (---(16)), and  $\psi(\underline{r},t) = u(\underline{r})\exp(-iEt/\hbar)$  (---(17)), where  $E$  (the *energy*) is the separation constant. Equation (16) is called the *time independent Schrödinger equation*.

(R2): The *total energy* of the particle is given by  $E = T+V = \frac{1}{2}m\mathbf{v}^2 + V(\underline{r}) = \frac{\mathbf{p}^2}{2m} + V(\underline{r}) = \frac{1}{2m}(p_x^2+p_y^2+p_z^2) + V(x,y,z)$  (---(18)). Making *correspondence*,  $p_\alpha \rightarrow -i\hbar \frac{\partial}{\partial \alpha}$ , for  $\alpha = x, y, z$ . Then  $E \rightarrow E_{op} = (18) = (-\hbar^2/2m)(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(x,y,z)$  (---(19)). But, from (5), (6) and (19),  $E_{op} = H_{op}$  (---(20)), so that  $H_{op}$  is the operator *corresponding* to the **total** energy of the particle.

(R3): If the state  $\psi$  of the particle is *simultaneously* an eigenfunction of  $A_{op}$  and of  $B_{op}$ , corresponding to *observables* A and B:  $A_{op}\psi = a\psi$  (---(21a)), and  $B_{op}\psi = b\psi$  (---(21b)), then *measuring A and B* (in any order) will yield  $a$  for A, **and**  $b$  for B — with certainty. The state  $\psi$  remains *undisturbed* by the measurements.

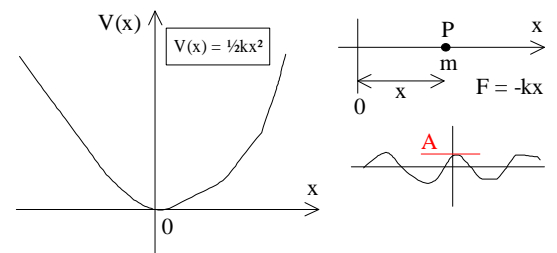
A and B are said to be simultaneously measurable, or compatible, if  $A_{op}$  and  $B_{op}$  possess a **complete set of common eigenfunctions**. Further, this occurs iff  $A_{op}$  and  $B_{op}$  commute:  $[A_{op}, B_{op}] = A_{op}B_{op} - B_{op}A_{op} = 0$  (---(22)). So A and B cannot be *simultaneously measured*, i.e. are **incompatible**, if  $A_{op}$  and  $B_{op}$  do not commute, i.e. if  $[A_{op}, B_{op}] \neq 0$ .

### Examples of Non-Commuting Operators

Consider  $x, \frac{\partial}{\partial x}$ :  $[x, \frac{\partial}{\partial x}]\psi(x) = (\text{by definition}) = x(\frac{\partial}{\partial x}(\psi)) - \frac{\partial}{\partial x}(x\psi) = x\frac{\partial\psi}{\partial x} - ((\frac{\partial x}{\partial x})\psi + x\frac{\partial\psi}{\partial x}) = (\text{because } \frac{\partial x}{\partial x} = 1) = x\frac{\partial\psi}{\partial x} - 1\psi - x\frac{\partial\psi}{\partial x} = -1\psi$ , where  $\psi$  is arbitrary. So  $[x, \frac{\partial}{\partial x}] = -1$ ; and  $[x, p_x] = [x, (-i\hbar)\frac{\partial}{\partial x}] = (-i\hbar)[x, \frac{\partial}{\partial x}] = -i\hbar(-1) = i\hbar$ . ( $p_x = -i\hbar \frac{\partial}{\partial x}$ ). Therefore,  $[x, p_x] = i\hbar \neq 0$ , so  $x$  and  $p_x$  are **not** compatible — thus they cannot be *consistently simultaneously measured*.

### 3.8: The Harmonic Oscillator in 1-Dimension

Classical Solution.  $m \frac{d^2x}{dt^2} = -kx$  (---(1))  $\Rightarrow \ddot{x} + \omega^2x = 0 \Rightarrow x = A\sin(\omega t + \epsilon)$  (---(2)), where  $\omega^2 = (k/m)$  (---(3)). In the *diagram*,  $T = \frac{2\pi}{\omega} = 2\pi\sqrt{(m/k)}$ . Quantum Mechanical solution. STIE:  $((-\hbar^2/2m)\frac{d^2}{dx^2} + V(x))u(x) = Eu(x) = (\text{using } V(x) = \frac{1}{2}kx^2) = (-\hbar^2/2m)\frac{d^2u}{dx^2} + \frac{1}{2}kx^2u(x) = Eu(x)$  (---(4))  
**Aside:**  $\psi(\underline{r},t) = u(x)T(t) = u(x)\exp(-iEt/\hbar)$ , so that  $T(t) = \exp(-iEt/\hbar)$ .



Simplify by setting  $\alpha^4 = mk/\hbar^2$  (A);  $\lambda = (2E/\hbar)/\omega$  (B) ( $= (2E/\hbar)\sqrt{(m/k)}$ );  $\xi = \alpha x$  ( $\alpha > 0$ ) (C); and  $\omega^2 = k/m$  (D) (---(set 5)). So (4) becomes  $d^2u/d\xi^2 + (\lambda - \xi)^2 u = 0$  (---(6)). Check:  $(-\hbar^2/2m)d^2u/dx^2 + (1/2kx^2 - E)u(x) = 0$ ;  $d^2u/dx^2 + (-kmx^2/\hbar^2 + 2mE/\hbar^2)u(x) = 0$ ;  $d^2u/dx^2 + (-\alpha^4 x^2 + 2m/\hbar \omega/\hbar^2)u(x) = 0$ ;  $d^2u/dx^2 + (-\xi^2 \alpha^2 + \lambda m \omega/\hbar)u(x) = 0$ .

Now  $d^2u/dx^2 + (-\xi^2 \alpha^2 + \lambda m/\hbar \sqrt{(k/m)})u(x) = 0$ ;  $d^2u/dx^2 + (-\xi^2 \alpha^2 + (\lambda/\hbar)\sqrt{(mk)})u(x) = 0$ ;  $d^2u/dx^2 + (-\xi^2 \alpha^2 + \alpha^2 \lambda)u(x) = 0$ ;  $d^2u/dx^2 + \alpha^2(\lambda - \xi^2)u(x) = 0$ ;  $1/\alpha^2 d^2u/dx^2 + (\lambda - \xi^2)u(x) = 0$ . **Now**  $d^2/dx^2(u) = d^2/d\xi^2(u) d\xi^2/dx^2$ . And  $\xi = x\alpha$ , so that  $\xi^2 = x^2 \alpha^2$ ;  $d\xi^2/dx^2 = \alpha^2$ . Therefore,  $d^2/dx^2(u) = d^2/d\xi^2(u)(\alpha^2)$ ;  $d^2u/d\xi^2(\alpha^2)/(\alpha^2) + (\lambda - \xi^2)u(x) = 0$ ;  $d^2u/d\xi^2 + (\lambda - \xi^2)u = 0$ . **QED.**

**Boundary Conditions:**  $u \rightarrow 0$  as  $\xi \rightarrow \pm\infty$  (---(7)). (6) does not possess a general solution in terms of a **finite** number of simple functions. A solution in series does exist, but if an attempt were to be made on (6) as it stands, then a **3 term** recurrence relation would result, which is *difficult* to handle. Instead, we will proceed as follows:

**When**  $\xi \rightarrow \pm\infty$ , i.e.  $|\xi| \gg \lambda$ , then (6)  $\rightarrow d^2u/d\xi^2 - \xi^2 u = 0$  (---(8)), which, as  $\xi \rightarrow \pm\infty$ , has **solutions**  $u(x) = \xi^n \exp(\pm 1/2 \xi^2)$  (---(9)) for arbitrary n. From (7), we **must** have  $u(\xi) \rightarrow \xi^n \exp(-1/2 \xi^2)$  (---(10)) as  $\xi \rightarrow \pm\infty$ . Therefore, we try a solution for equation (6) given by  $u(\xi) = f(\xi) \exp(-1/2 \xi^2)$  (---(11)). Now (11) in (6)  $\Rightarrow d^2f/d\xi^2 - 2\xi df/d\xi + (\lambda - 1)f = 0$  (---(12)).

Try a *series* solution:  $f(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$  (---(13)). Now (13) in (12)  $\Rightarrow \sum_{n=0}^{\infty} \xi^n \{(n+1)(n+2)a_{n+2} - 2na_{n+1} + (\lambda - 1)a_n\} = 0$  (for all  $x \in \mathbf{R}$ )  $\Rightarrow a_{n+2} = \frac{(2n+1-\lambda)}{(n+1)(n+2)} a_n$  (---(14)), which is a *2-term recurrence* relation **connecting** alternate terms. Set  $a_0$  and  $a_1$  *independently*. As  $\xi \rightarrow \pm\infty$ , the behaviour is as follows:  $\lim_{n \rightarrow \infty} (a_{n+2}/a_n) = (14) = 2/n$  (---(15)). Now  $\exp(+\xi^2) = \sum_{n \text{ even}} b_n \xi^n \Rightarrow (b_{n+2}/b_n) \rightarrow 2/n$  as  $n \rightarrow \infty$ . So, for *large* n, the behaviour of the series (13) **approaches** that of  $\exp(+\xi^2)$ . So as  $\xi \rightarrow \pm\infty$ , (13) will **tend** to infinity (like  $\exp(+\xi^2)$ ). Hence  $u(\xi) = f(\xi) \exp(-1/2 \xi^2) \sim \exp(+\xi^2) \exp(-1/2 \xi^2) = \exp(+1/2 \xi^2) \rightarrow \infty$  as  $\xi \rightarrow \pm\infty$ .

This can *only be avoided* by **truncating** the series, i.e. by setting  $\lambda = 2N+1$  (---(16)), where N is *some non-negative integer*. The other series will *still* be infinite, so we specifically set it to be **zero**: From (16), (5) and (3),  $E (= E_N) = (\hbar\omega/2)\lambda = (16) = (N+1/2)\hbar\omega$ , where  $N = 0, 1, 2, 3, \dots$

14th November 2000

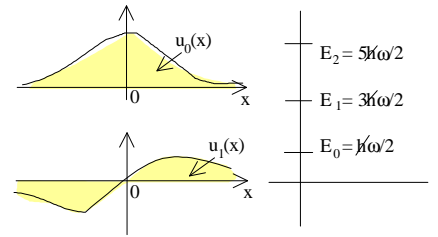
$f(\xi)$  is a *polynomial* of degree N, containing either only **even** powers of  $\xi$ , or only **odd** powers of  $\xi$  — Hermite polynomials of degree N:  $H_N(\xi)$ . The *eigenfunctions* are as follows:  $u(\xi) = (\xi = \alpha x) = u(\alpha x) = A_n \exp(-(\alpha x)^2) H_n(\alpha x)$  (---(18)), where  $A_n$  are *constants*.

## Hermite Polynomials

Hermite polynomials **satisfy** the differential equation (equation (12), with x replacing  $\xi$ , and  $(\lambda - 1) = 2n$ )  $d^2/dx^2 H_n(x) - 2x d/dx H_n(x) + 2n H_n(x) = 0$  (---(19)). *Properties* of these polynomials may be deduced from the **generating** function,  $F(x,s)$ , defined by  $F(x,s) = \exp(-s^2 + 2xs) = \sum_{n=0}^{\infty} (H_n(x)/n!) s^n$  (---(20)). It then *follows* that  $dH_n(x)/dx = 2n H_{n-1}(x)$  (---(21)), and that  $H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x)$  (---(22)), for  $n = 1, 2, 3, \dots$ . Further,  $\int_{-\infty}^{\infty} H_m(x) H_n(x) \exp(-x^2) dx = \sqrt{(\pi)} 2^n n! \delta_{mn}$  (---(23)).

This can be used to show that the **normalisation** constant  $A_n$  in (18) is  $A_n = \sqrt{\frac{a}{\sqrt{\pi} 2^n n!}}$  (---(24)), i.e.  $1 = \int_{x=-\infty}^{x=\infty} u_n^*(\alpha x) u_n(\alpha x) dx = (\xi = \alpha x) = \int_{\xi=-\infty}^{\xi=\infty} \frac{1}{\alpha} u_n^*(\xi) u_n(\xi) d\xi = (A_n \text{ real}) = \frac{1}{\alpha} \int_{-\infty}^{\infty} A_n^2 H_n^2(\xi) (\exp(-1/2 \xi^2))^2 d\xi = (A_n^2/\alpha) \int_{-\infty}^{\infty} H_n^2(\xi) \exp(-\xi^2) d\xi = (23, \text{ with } m = n) = (A_n^2/\alpha) (\sqrt{\pi} 2^n n!) \Rightarrow A_n = \sqrt{\frac{a}{\sqrt{\pi} 2^n n!}}$ .

Consider the first 4 eigenvalues and eigenfunctions.  $E_0 = E_N =$  (with  $N = 0$ )  $= \frac{1}{2} \hbar \omega$ . Now  $u_0(\xi) = u_0(\alpha x) = A_0 H_0(\alpha x) \exp(-1/2(\alpha x)^2) = (H_0(\alpha x) = a_0 = 1) = (\sqrt{(\alpha)/\pi^{1/4}}) 1 \cdot \exp(-1/2(\alpha x)^2) = (\sqrt{(\alpha)/\pi^{1/4}}) \exp(-1/2 \alpha^2 x^2) = u_0(x)$ . Aside remember the **relations** implied by (5):  $\alpha^4 = m k / \hbar^2$  and  $\omega^2 = k / m \Rightarrow \alpha^4 = m^2 \omega^2 / \hbar^2$ ;  $\alpha = (m \omega / \hbar)^{1/2}$ . Now for  $N = 1$ , we have  $E_1 = (1 + 1/2) \hbar \omega = 3 \hbar \omega / 2$ ;  $u_1(\xi) = u_1(\alpha x) = (\sqrt{(\alpha/2)/\pi^{1/4}}) (\alpha x) \cdot \exp(-1/2 \alpha^2 x^2)$  (---(25)).



17th November 2000

**Recap:**  $F(x,s) = \exp(-s^2+2xs) = \sum_{n=0}^{\infty} (H_n(x)/n!) s^n$  (---(20), RHS uniformly convergent);  $(dH_n(x)/dx) = 2nH_{n-1}(x)$  (---(21, with  $n = 1, 2, 3, \dots$ ; and  $H_0(x) = 0$ );  $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$  (---(22)); and  $(d^2H_n(x)/dx^2) - (2x dH_n(x)/dx) + 2nH_n(x) = 0$  (---(19)). We want to **verify** the above expressions. Now  $(20) \Rightarrow \frac{\partial}{\partial x} (\exp(-s^2+2xs)) = \sum_{n=0}^{\infty} \frac{1}{n!} (dH_n(x)/dx) s^n$

$$\Rightarrow 2s \cdot \exp(-s^2+2xs) = \Rightarrow (\text{by } 20) 2s (\sum_{n=0}^{\infty} \frac{1}{n!} H_n(x) s^n) = \sum_{n=0}^{\infty} \frac{1}{n!} (dH_n(x)/dx) s^n \Rightarrow \sum_{n=0}^{\infty} (2H_n(x)/n!) s^{n+1} = \sum_{n=0}^{\infty} \frac{1}{n!} H'_n(x) s^n = H'_0(x) + \sum_{n=1}^{\infty} \frac{1}{n!} H'_n(x) s^n = H'_0(x) + \sum_{m=0}^{\infty} \frac{1}{(m+1)!} H'_{m+1}(x) s^{m+1} \Rightarrow H'_0(x) + (\sum_{n=0}^{\infty} \frac{1}{(n+1)!} H'_{n+1}(x) s^{n+1} - (2H_n(x)/n!) s^{n+1}) = 0 \Rightarrow H'_0(x) + (\sum_{n=0}^{\infty} \frac{1}{(n+1)!} H'_{n+1}(x) - (2H_n(x)/n!)) s^{n+1} = 0 \text{ for all } s$$

$$\Rightarrow H'_0(x) = 0; \frac{1}{(n+1)!} H'_{n+1} - (2H_n(x)/n!) = 0 \quad (n = 0, 1, 2, \dots), \text{ so that } H'_{n+1}(x) = \frac{2(n+1)!}{n!} H_n(x) \Rightarrow H'_{n+1}(x) = 2(n+1)H_n(x) \quad (n = 0, 1, 2, \dots) \Rightarrow (\text{using } m = n+1) H'_m(x) = 2mH_{m-1}(x) \quad (m = 1, 2, \dots, \infty) \Rightarrow (\text{as } m \rightarrow n) H'_n(x) = 2nH_{n-1}(x) \quad (n = 1, 2, \dots, \infty) \Rightarrow (\text{because } H'_0(x) = 0) H'_n(x) = 2nH_{n-1}(x), \quad n = 0, 1, 2, \dots$$

$$\text{Now } (20) \Rightarrow (\text{differentiating w.r.t. } s) (-2s+2x) \exp(-s^2+2xs) = \sum_{n=1}^{\infty} (H_n(x)/n!) n s^{n-1} \Rightarrow 2(x-s) \sum_{n=0}^{\infty} ((H_n(x)/n!) s^n) = \sum_{n=1}^{\infty} (H_n(x)/n!) n s^{n-1} \Rightarrow \sum_{n=0}^{\infty} (2xH_n(x)/n!) s^n - \sum_{n=0}^{\infty} (2H_n(x)/n!) s^{n+1} - \sum_{n=1}^{\infty} (\frac{n}{n!}) H_n(x) s^{n-1} = 0 \Rightarrow \sum_{n=1}^{\infty} [2x/n! H_n(x) - 2/(n-1)! H_{n-1}(x) - (n+1)/n! H_{n+1}(x)] s^n + 2xH_0(x)/0! - 1/1! H_1(x) = 0 \text{ for all } s \text{ (change of indices: } m = n+1, \text{ then } n = m; m = n-1, \text{ then } n = m)$$

$$\Rightarrow 2xH_0(x) - H_1(x) = 0; \frac{2x}{n!} H_n(x) - \frac{2}{(n-1)!} H_{n-1}(x) - \frac{1}{n!} H_{n+1}(x) = 0 \Rightarrow H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (n = 1, 2, 3, \dots). \text{ Now } (19) \Rightarrow H''_n(x) - 2xH'_n(x) + 2nH_n(x) = (21) = (2nH_{n-1}(x))' - 2x(2nH_{n-1}(x)) + 2nH_n(x) = (21) = 2n2(n-1)H_{n-2}(x) - 4xnH_{n-1}(x) + 2nH_n(x) = (22, \text{ with } n \rightarrow n-1) = H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x) = (22) = 2n[2xH_{n-1}(x) - H_n(x)] - 4xnH_{n-1}(x) + 2nH_n(x) = 0. \text{ QED.}$$

Now for the proof of  $\int_{-\infty}^{\infty} H_m(x) H_n(x) \exp(-x^2) dx = \sqrt{\pi} 2^n n! \delta_{nm}$ . Consider  $\int_{-\infty}^{\infty} F(x,s) F(x,t) \exp(-x^2) dx$ . Now  $\int_{-\infty}^{\infty} \exp(-s^2+2xs) \exp(-t^2+2xt) \exp(-x^2) dx * = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} [H_m(x)/m!] [H_n(x)/n!] s^m t^n \exp(-x^2) dx = \sum_{n,m=0}^{\infty} (s^m t^n / m! n!) \int_{-\infty}^{\infty} H_m(x) H_n(x) \exp(-x^2) dx$ . Now  $* = \exp[-x^2 - s^2 - t^2 + 2xs + 2xt] = \exp[-(x-s-t)^2 + 2st] = \exp(2st) \exp(-(x-s-t)^2)$ . So  $\int_{-\infty}^{\infty} \exp(-x^2) \exp(-s^2+2xs) \exp(-t^2+2xt) dx = \exp(2st) \int_{-\infty}^{\infty} \exp(-(x-s-t)^2) dx$ .

**[Aside:**  $\int_{-\infty}^{\infty} e^{-x^2} = \sqrt{\pi}$ ): Let  $x = y-a$ , so that  $dx = dy$ , and  $\int_{y=-\infty}^{y=\infty} e^{-(y-a)^2} dy = \sqrt{\pi}$  again]. Now  $\sum_{m,n=0}^{\infty} (s^m t^n / m! n!) \int_{-\infty}^{\infty} H_m(x) H_n(x) \exp(-x^2) dx = \sqrt{\pi} \exp(2st) = \sqrt{\pi} \sum_{n=0}^{\infty} (2st)^n / n! \Rightarrow$  (comparing the coefficients of  $s^m t^n$ )  $\int_{-\infty}^{\infty} H_m(x) H_n(x) e^{-x^2} dx = 0$  ( $m \neq n$ ). **When**  $m = n$ ,  $\int_{-\infty}^{\infty} H_n(x) H_n(x) e^{-x^2} dx = \sqrt{\pi} (2^n / n!)$ ;  $\int_{-\infty}^{\infty} (H_n(x))^2 e^{-x^2} dx = \sqrt{\pi} 2^n n!$ .

### Assignment 3

**Q: Find**  $\langle x \rangle$ ,  $\langle x^2 \rangle$ ,  $\langle p_x \rangle$  and  $\langle p_x^2 \rangle$  for the 1-dimensional harmonic oscillator in the normalised ground state eigenfunction of the energy. **Hence** show that  $\Delta x \Delta p_x = \hbar / 2$ , where  $(\Delta x)^2 = \langle x^2 \rangle - (\langle x \rangle)^2$ , and  $(\Delta p_x)^2 = \langle p_x^2 \rangle - (\langle p_x \rangle)^2$ . **A:** For the ground state,  $u_0(x) = [\sqrt{(\alpha)/\pi}^{1/4}] \exp(-1/2 \alpha x^2)$ , a normalised ground state wave function, with  $\alpha = \sqrt{(m\omega\hbar)}$ .

Now  $\langle x \rangle_{u_0(x)} = \int_{-\infty}^{\infty} u_0^*(x) x u_0(x) dx = \int_{-\infty}^{\infty} x [\sqrt{(\alpha)/\pi}^{1/4}] \exp(-1/2 \alpha x^2) [\sqrt{(\alpha)/\pi}^{1/4}] \exp(-1/2 \alpha x^2) dx = \int_{-\infty}^{\infty} x \alpha / \sqrt{\pi} \exp(-\alpha x^2) dx = \alpha / \sqrt{\pi} \int_{-\infty}^{\infty} x \exp(-\alpha x^2) dx = \alpha / \sqrt{\pi} [-1/2 \alpha \exp(-\alpha x^2)]_{-\infty}^{\infty} = \alpha / \sqrt{\pi} [0 - 0] = 0$ . Alternatively, use *symmetry* because of the **odd** integrand. Now  $\langle x^2 \rangle_{u_0(x)} = \int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2) dx$ . Now let  $u = x$ ,  $du/dx = 1$ ;  $dv/dx = x \exp(-\alpha x^2)$ ,  $v = 1/2 \alpha \exp(-\alpha x^2)$ .

So  $\langle x^2 \rangle_{u_0(x)} = \alpha / \sqrt{\pi} \{ [x(-1/2 \alpha \exp(-\alpha x^2))]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} -1/2 \alpha \exp(-\alpha x^2) dx \} = -\alpha / \sqrt{(\pi) 2 \alpha^2} [x \exp(-\alpha x^2)]_{-\infty}^{\infty} + \alpha / \sqrt{(\pi) 2 \alpha^2} \int_{-\infty}^{\infty} \exp(-\alpha x^2) dx$ . Now for the RHS, let  $y = \alpha x$ , so that  $dy = \alpha dx$ . It follows that  $\int_{-\infty}^{\infty} \exp(-\alpha x^2) dx = \int_{-\infty}^{\infty} \exp(-y^2) dy / \alpha = 1/\alpha \int_{-\infty}^{\infty} \exp(-y^2) dy = \sqrt{\pi} / \alpha$ . **Therefore**,  $\langle x^2 \rangle_{u_0(x)} = -\alpha / \sqrt{(\pi) 2 \alpha^2} [x \exp(-\alpha x^2)]_{-\infty}^{\infty} + \alpha \sqrt{(\pi)} / \sqrt{(\pi) 2 \alpha^2} = -\alpha / \sqrt{(\pi) 2 \alpha^2} [0] + 1/2 \alpha^2 = 1/2 \alpha^2$ .

Now  $\langle p_x \rangle_{u_0(x)} = \int_{-\infty}^{\infty} u_0^*(x) (-i \hbar d/dx) u_0(x) dx = \int_{-\infty}^{\infty} (\sqrt{(\alpha)/\pi}^{1/4}) \exp(-1/2 \alpha x^2) [-i \hbar d/dx ((\sqrt{(\alpha)/\pi}^{1/4}) \times \exp(-1/2 \alpha x^2))] dx = \int_{-\infty}^{\infty} (\sqrt{(\alpha)/\pi}^{1/4}) \exp(-1/2 \alpha x^2) (-i \hbar) ((\sqrt{(\alpha)/\pi}^{1/4}) (-1/2 \alpha \cdot 2x) \exp(-1/2 \alpha x^2)) dx = \int_{-\infty}^{\infty} (\sqrt{(\alpha)/\pi}^{1/4}) \exp(-1/2 \alpha x^2) [-i \hbar (\sqrt{(\alpha)/\pi}^{1/4}) - \alpha x \exp(-1/2 \alpha x^2)] dx = \int_{-\infty}^{\infty} (\alpha / \sqrt{(\pi)}) \exp(-1/2 \alpha x^2) (\hbar \alpha^2) \times x \exp(-1/2 \alpha x^2) dx = i \hbar \alpha^3 / \sqrt{(\pi)} \int_{-\infty}^{\infty} x \exp(-\alpha x^2) dx = 0$ . So  $\langle p_x \rangle_{u_0(x)} = 0$ .

And  $\langle p_x^2 \rangle_{u_0(x)} = \int_{-\infty}^{\infty} u_0^*(x) (-i \hbar d/dx)^2 u_0(x) dx = \int_{-\infty}^{\infty} u_0^*(x) (\hbar^2 d^2/dx^2) u_0(x) dx = \int_{-\infty}^{\infty} (\sqrt{(\alpha)/\pi}^{1/4}) \times \exp(-1/2 \alpha x^2) (-\hbar^2 \times d^2/dx^2 [(\sqrt{(\alpha)/\pi}^{1/4}) \exp(-1/2 \alpha x^2)]) dx = \dots = \alpha \hbar^2 / \sqrt{\pi} \int_{-\infty}^{\infty} \exp(-1/2 \alpha x^2) \times [\exp(-1/2 \alpha x^2) - \alpha x^2 \exp(-1/2 \alpha x^2)] dx = \alpha \hbar^2 / \sqrt{(\pi)} \int_{-\infty}^{\infty} \exp(-\alpha x^2) dx + \alpha \hbar^2 / \sqrt{(\pi)} \int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2) dx = (\alpha^3 \hbar^2 / \sqrt{(\pi)}) (\sqrt{\pi} / \alpha) + (\alpha^5 \hbar^2 / \sqrt{(\pi)}) (1/2 \alpha^2 (\sqrt{\pi} / \alpha)) = \alpha^2 \hbar^2 - \alpha^2 \hbar^2 / 2 = \alpha^2 \hbar^2 / 2$ . Therefore,  $(\Delta x)^2 = 1/2 \alpha^2$ , and  $(\Delta p_x)^2 = \alpha^2 \hbar^2 / 2$ , so that  $\Delta x \Delta p_x = \sqrt{[(\Delta x)^2 (\Delta p_x^2)]} = \sqrt{\hbar^2 / 4} = \hbar / 2$ . **QED.**

**Q: Find**  $\langle x \rangle$ ,  $\langle x^2 \rangle$ ,  $\langle p_x \rangle$  and  $\langle p_x^2 \rangle$  for the 1-dimensional infinitely deep square well potential in the normalised  $n^{\text{th}}$  eigenfunction of the energy. **Hence** show that  $\Delta x \Delta p_x = d \hbar$ , where  $(\Delta x)^2 = \langle x^2 \rangle - (\langle x \rangle)^2$ ;  $(\Delta p_x)^2 = \langle p_x^2 \rangle - (\langle p_x \rangle)^2$ ; and  $d_n^2 = n^2 \pi^2 / 12 - 1/2$ . **Comment** on the **least** value of  $d_n$  in the light of Heisenberg's Uncertainty Principle.

**A:** For the 1-dimensional infinitely deep square well, the **normalised**  $n^{\text{th}}$  eigenfunction of the energy is given by  $u_n(x) = \sqrt{(2/l)} \sin(n\pi x/l)$  for  $0 \leq x \leq l$ ; and  $u_n(x) = 0$  for  $x < 0$  and  $x > l$ . Now  $\langle x \rangle =$  (calculated in previous examples)  $= l/2$ . And  $\langle x^2 \rangle =$  (calculated in previous examples)  $= l^2 (1/3 - 1/2(n\pi)^2)$ . So  $(\Delta x)^2 = l^2 (1/3 - 1/2(n\pi)^2) - (l/2)^2 = l^2 / 12 - l^2 / 2(n\pi)^2$ .

Now  $\langle p_x \rangle$  is given by  $\int \sqrt{\langle l \rangle} \sin(n\pi x/l) (-i\hbar \frac{d}{dx}) \sqrt{\langle l \rangle} \sin(n\pi x/l) dx = -2\hbar/l \int_0^l \sin(n\pi x/l) \frac{d}{dx} (\sin(n\pi x/l)) dx = -i\hbar n\pi/l \int_0^l 2\sin(n\pi x/l) \cos(n\pi x/l) dx = -i\hbar n\pi/l^2 \int_0^l \sin(2n\pi x/l) dx = (-i\hbar n\pi/l^2) \times [-1/2n\pi \cos(2n\pi x/l)]_0^l = (-i\hbar n\pi/l) (-1/2n\pi) [\cos(2n\pi) - \cos(0)] = 0$ . And  $\langle p_x^2 \rangle = \int_0^l \sqrt{\langle l \rangle} \sin(n\pi x/l) (-i\hbar \frac{d}{dx})^2 \sqrt{\langle l \rangle} \sin(n\pi x/l) dx = \dots = (\hbar n\pi/l)^2$ .

Therefore, we have  $(\Delta p_x)^2 = (\hbar n\pi/l)^2 - (0)^2 = (\hbar n\pi/l)^2$ . Now  $(\Delta x)^2 (\Delta p_x)^2 = (l^2/12 - l^2/2(n\pi)^2) (\hbar n\pi/l)^2 = \dots = \hbar^2 (n^2\pi^2/12 - 1/2)$ ;  $(\Delta x)^2 (\Delta p_x)^2 = \hbar^2 d_n^2$ . It follows that  $\Delta x \Delta p_x = \sqrt{\hbar^2 d_n^2} = \hbar d_n$ . **QED**. Now **Heisenberg's Uncertainty Principle** says that  $\Delta x \Delta p_x \geq 1/2 \hbar \Rightarrow d_n \geq 1/2$ ;  $d_n^2 \geq 1/4$ ;  $n^2\pi^2/12 - 1/2 \geq 1/4$ ;  $n^2\pi^2/12 \geq 3/4$ ;  $n^2\pi^2 \geq 9$  (---(1)). For  $n = 1, 2, 3, \dots$ , we see that (1) holds *true*. However, for  $n = 0$ ,  $0 \geq 9$ . This agrees with the **lectures**, where we saw that the case  $n = 0$  was physically unacceptable.

**Q:** Show that in **any** eigenstate of the energy for the *1-dimensional harmonic oscillator*,  $\langle \text{Potential Energy} \rangle = \langle \text{Kinetic Energy} \rangle$ . (Hint: use the *properties* of the **Hermite** polynomials).  
**A:** Now  $Hu_n = E_n u_n$  (---(1)), where  $H = (\hbar^2/2m) \frac{d^2}{dx^2} + 1/2 kx^2$  (---(2)); and  $u_n(x) = A_n H_n(\alpha x) \exp(-1/2(\alpha x)^2)$  (---(3),  $n = 0, 1, 2, \dots$ ), where  $A_n = \sqrt{(\alpha/\sqrt{\pi}) 2^{-n} n!}$ ; (---(4)),  $\alpha = (mk\hbar^2)^{1/4}$  (---(5)); and  $\omega = (k/m)^{1/2}$  (---(6)).

The  $u_n$  given by (3), with  $A_n$  given by (4) and (5), are *normalised*, i.e.  $\int_{-\infty}^{\infty} u_n^* u_n dx = 1$ . From (2),  $PE = V = 1/2 kx^2$  (---(7)), and  $KE = p^2/2m = (\hbar^2/2m) \frac{d^2}{dx^2}$  (---(8)). **Consider**  $\langle PE \rangle$ .  $\langle PE \rangle = \int_{-\infty}^{\infty} u_n^* (PE) u_n dx = \int_{-\infty}^{\infty} u_n^* 1/2 kx^2 u_n dx$  (---(8)). (3) and (4) in (8)  $\Rightarrow \langle PE \rangle = (\alpha/\sqrt{\pi}) 2^{-n} n! \int_{-\infty}^{\infty} x^2 H_n^2(\alpha x) e^{-\alpha^2 x^2} dx = (\text{using } \zeta = \alpha x) = C \int_{-\infty}^{\infty} [\zeta H_n(\zeta)]^2 e^{-\zeta^2} d\zeta$  (---(10)), where  $C = k/\sqrt{\pi} 2^{-n-1} n! \alpha^2 = (5)$ , (6)  $= \hbar\omega/\sqrt{\pi} 2^{n+1} n!$  (---(11)).

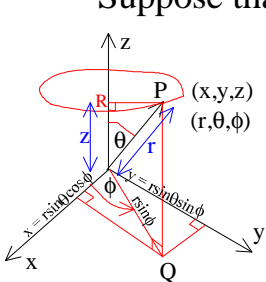
Now use the *properties of the Hermite polynomials*:  $\frac{d}{d\zeta} H_n(\zeta) = 2n H_{n-1}(\zeta)$  (---(12)); and  $H_{n+1}(\zeta) = 2\zeta H_n(\zeta) - 2n H_{n-1}(\zeta)$  (---(13), with  $n = 1, 2, 3, \dots$ ). So  $\int_{-\infty}^{\infty} H_n(\zeta) H_n(\zeta) \exp(-\zeta^2) d\zeta = \sqrt{\pi} 2^n n! \delta_{nn}$  (---(14)). (13) in (10)  $\Rightarrow \langle PE \rangle = C/4 \int_{-\infty}^{\infty} (H_{n+1}(\zeta) + 2n H_{n-1}(\zeta))^2 e^{-\zeta^2} d\zeta = (C/4) [\int_{-\infty}^{\infty} H_{n+1}^2(\zeta) e^{-\zeta^2} d\zeta + 2 \int_{-\infty}^{\infty} H_{n+1}(\zeta) (2n) H_{n-1}(\zeta) e^{-\zeta^2} d\zeta + 4n^2 \int_{-\infty}^{\infty} H_{n-1}^2(\zeta) e^{-\zeta^2} d\zeta]$  (---(15)).

(14) in (15)  $\Rightarrow \langle PE \rangle = (C/4) [\sqrt{\pi} 2^{n+1} (n+1)! + 4n^2 \sqrt{\pi} 2^{n-1} (n-1)!] = C \sqrt{\pi} 2^{n-1} n! [n+1+n] = C \sqrt{\pi} 2^{n-1} n! (2n+1)$ . (11) and (16)  $\Rightarrow \langle PE \rangle = (\hbar\omega/\sqrt{\pi} 2^{n+1} n!) \sqrt{\pi} 2^{n-1} n! (2n+1) = 1/2 (n+1/2) \hbar\omega = 1/2 E_n$ . Now (1)  $\Rightarrow \langle H \rangle = E_n$ . **But**  $H = KE + PE$  — therefore,  $\langle H \rangle = \langle KE \rangle + \langle PE \rangle$ , where  $\langle KE \rangle + \langle PE \rangle = (n+1/2) \hbar\omega$ . But we *know*  $\langle PE \rangle$ , so  $\langle KE \rangle = E_n - 1/2 E_n = 1/2 E_n$ . Therefore,  $\langle KE \rangle = \langle PE \rangle$ . **QED**. (We can also calculate  $\langle KE \rangle$  directly, but calculating the  $\langle PE \rangle$  is easier).

21st November 2000

### 3.9: Spherically Symmetrical Potentials

Suppose that the **potential** function  $V(\underline{r})$  is *spherically symmetrical*, i.e.  $V(\underline{r}) = V(r)$  (---(1)). To **exploit** equation (1), we use *spherical polar*  $\underline{r} = \overrightarrow{OP}$  co-ordinates,  $(r, \theta, \phi)$ . In the **diagram**,  $z = r \cos\theta$ ,  $y = r \sin\theta \sin\phi$ , and  $x = r \sin\theta \cos\phi$ , for  $0 \leq r < \infty$ ,  $0 \leq \theta \leq 2\pi$ , and  $0 \leq \phi < 2\pi$ . Now we need the *Laplacian* operator:  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = 1/r^2 \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + 1/r^2 \sin\theta \frac{\partial}{\partial \theta} (\sin\theta \frac{\partial}{\partial \theta}) + 1/r^2 \sin^2\theta \frac{\partial^2}{\partial \phi^2}$  (---(2)). [Use e.g.  $\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi}$ , and  $\frac{\partial}{\partial r} = \frac{\partial x}{\partial r} \frac{\partial}{\partial x} + \frac{\partial y}{\partial r} \frac{\partial}{\partial y} + \frac{\partial z}{\partial r} \frac{\partial}{\partial z}$ ].



The **TISE** is  $(-\hbar^2/2m)[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial u}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial u}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}]u + V(r)u = Eu$  (---(3)), where  $u = u(r,\theta,\phi)$ . By *separation of variables*,  $u(r,\theta,\phi) = R(r)Y(\theta,\phi)$  (---(4)). (4) in (3)  $\Rightarrow \frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) + \{(2m/\hbar^2)(E-V(r))-\lambda/r^2\}R = 0$  (---(5)), and  $\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial Y}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} + \lambda Y = 0$  (---(6)), where  $\lambda$  is the *separation constant*.

Again, by **separating** variables,  $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$  (---(7)). (6) and (7)  $\Rightarrow \frac{1}{\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta}) + (\lambda-\mu/\sin^2\theta)\Theta = 0$  (---(8)), and  $\frac{d^2\Phi}{d\phi^2} + \mu\Phi = 0$  (---(9)), where  $\mu$  is **another** separation constant. (9) may be *integrated* immediately to give  $\Phi = (\text{const})\exp(\pm i\sqrt{\mu}\phi)$  (---(10)), and for  $\Phi$  to be *single valued*, then  $\Phi(\phi+2n\pi) = \Phi(\phi)$ , for  $n = 1, 2, 3, \dots$ , i.e.  $\exp(\pm i2n\pi\sqrt{\mu}) = 1$ ; or  $\sqrt{\mu}$  must be *integral*,  $m$ , say, i.e.  $\Phi = (\text{const})\exp(\pm im\phi)$  (---(11)).

**Putting**  $\mu = m^2$  in (8), and *setting*  $w = \cos\theta$ , we get  $\frac{d}{dw}[(1-w^2)\frac{dP}{dw}] + (\lambda-m^2/(1-w^2))P = 0$  (---(12)), where  $P(w) = \Theta(\theta)$ . Now it can be **shown** that for *finite* solutions to (12), and for  $0 \leq \theta \leq \pi$ , i.e.  $-1 \leq w \leq 1$ , then  $\lambda$  must take on **certain** integral values given by  $\lambda = l(l+1)$  (---(13)), where  $l = 0, 1, 2, 3, \dots, \infty$  s.t.  $l \geq |m|$ .

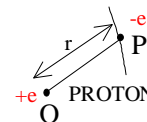
The solutions are then **labelled** by  $P_l^m(w)$ , and are known as Associated Legendre Functions (see the *book* for details). **Therefore**,  $Y(\theta,\phi) = Y_l^m(\theta,\phi) = P_l^m(\cos\theta)\exp(im\phi)$  (---(14)), where  $|m| \leq l$ ;  $l = 0, 1, 2, \dots, \infty$ ; and the **red** expression is known as the Spherical Harmonics. So  $\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) + \{(2m/\hbar^2)(E-V(r)) - l(l+1)/r^2\}R = 0$  (---(15)), for  $l = 0, 1, 2, 3, \dots$

The **energy**  $E$  only appears in (15). The *spherical harmonic solutions*,  $Y_l^m(\theta,\phi)$ , are the same for all *potentials*  $V(r)$ . For each value of  $l$ , there are  $2l+1$  *linearly independent spherical harmonics* ( $Y_l^m$ ) as  $|m| \leq l$ , i.e.  $m = -l, -l+1, \dots, -1, 0, 1, \dots, l-1, l$ . ( $2l+1$  values). So the energy levels  $E$  are then at *least*  $(2l+1)$ -fold **degenerate**.

24th November 2000

### 3.10: The Hydrogen Atom

The hydrogen *atom* consists of a single electron orbiting a single proton. As a first approximation, consider the mass of the **proton** to be infinitely large compared to the mass of the electron — then the *centre* of mass of the atom will coincide with the centre of the proton. The potential of the **electron** in the field of attraction of the proton is  $V(r) = (-e^2/(4\pi\epsilon_0))/r$  (---(1)), in SI Units ( $\epsilon_0 =$  *permittivity* of free space), where  $e$  is the magnitude of the **electronic** charge, and  $r$  is the distance between the *proton* and the *electron*.



Using (1) in equation 3.9.15  $\Rightarrow \frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) + \{2m/\hbar^2(E+((e^2/4\pi\epsilon_0)/r))-\lambda/r^2\}R = 0$  (---(2)). **Simplify** (2) by setting  $\alpha_n^2 = -8mE/\hbar^2$  (---(3)), with  $\alpha_n > 0$ , where  $\alpha_n$  is real since we are looking for **bound state solutions** of (2), which implies that  $E < 0$ , and that  $n = -\alpha_n(e^2/4\pi\epsilon_0)/4E$  (---(4)). Now change the **independent** variable from  $r$  to  $\rho$ , where  $\rho = \alpha_n r$  (---(5)).

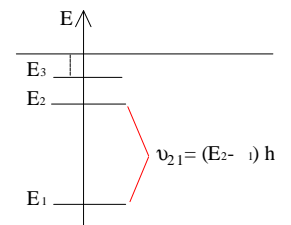
(3) to (5) in (2)  $\Rightarrow \frac{1}{\rho^2} \frac{d}{d\rho} (\rho^2 \frac{dR}{d\rho}) + \{ \frac{n}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \} R = 0$  (---(6)), for  $0 \leq r < \infty$ . As in the *Harmonic oscillator*, we consider the **behaviour** of (6) for large  $\rho$ . (6)  $\rightarrow \frac{d^2 R}{d\rho^2} - \frac{R}{4} = 0$  (---(7)), which has *solutions*  $R = \exp(\pm \frac{1}{2}\rho)$  (---(8)). (Try  $R = Ae^{\lambda\rho}$ , so that  $A(\lambda^2 - \frac{1}{4})e^{\lambda\rho} = 0$ ). Now  $R(\rho)$  must *remain finite everywhere*, so we must take the -ve sign in (8), and then try a **solution** of (6) of the form  $R(\rho) = F(\rho)\exp(-\frac{1}{2}\rho)$  (---(9)), where  $F(\rho)$  is to be **found**. (9) in (6)  $\Rightarrow \frac{d^2 F}{d\rho^2} + (\frac{2}{\rho} - 1) \frac{dF}{d\rho} + (\frac{n-1}{\rho} - \frac{l(l+1)}{\rho^2}) F = 0$  (---(10)).

**Frobenius Series Solutions.** Equation (10) has a *regular singularity* at  $\rho = 0$ , so that a Frobenius series solution can be **attempted** by setting  $F(\rho) = \sum_{m=0}^{\infty} a_m \rho^{m+\sigma}$  (---(11)), where  $a_0 \neq 0$ . (11) in (10)  $\Rightarrow (\rho^{\sigma-2}) a_0 [\sigma(\sigma+1) - l(l+1)] = 0$  (---(12)), where the **red** part is the indicial equation. ( $\rho^{m+\sigma-1}$ ,  $m = 0, 1, 2, \dots$ ) gives  $\{ a_{m+1} [(m+\sigma+1)(m+\sigma+2) - l(l+1)] - a_m (m+\sigma-n+1) \} = 0$  (---(13)). And  $a_0 \neq 0$ , so that (12)  $\Rightarrow \sigma = l$ , or  $\sigma = -(l+1)$  (the 2nd is **not** allowed).

**Reject** the negative values of  $\sigma$ , since  $\rho^{-(l+1)} \rightarrow \infty$  as  $\rho \rightarrow 0$ . So setting  $\sigma = l$  in (13)  $\Rightarrow a_{m+1}/a_m = \frac{(m+l-n+1)}{[(m+l+1)(m+l+2) - l(l+1)]}$  (---(14)). (14)  $\Rightarrow \lim_{m \rightarrow \infty} (a_{m+1}/a_m) = 1/m$  (---(15)). Now **observe** that  $\exp(+\rho) = \sum_{r=0}^{\infty} b_r \rho^r$ , where  $b_r = 1/r!$ , and  $b_{r+1}/b_r = \frac{1}{(r+1)!} / \frac{1}{r!} = \frac{r!}{(r+1)!} = \frac{1}{r+1}$ . *Therefore*,  $\lim_{r \rightarrow \infty} b_{r+1}/b_r = 1/r$  (---(16)). So as  $\rho \rightarrow \infty$ ,  $F(\rho) = \sum_{m=0}^{\infty} a_m \rho^{m+l} \sim \exp(\pm \rho)$ . So  $R(\rho) = F(\rho)\exp(-\frac{1}{2}\rho) \sim \exp(+\rho)\exp(-\frac{1}{2}\rho) = \exp(+\frac{1}{2}\rho)$  as  $\rho \rightarrow \infty$ . So  $R(\rho) \rightarrow \infty$  as  $\rho \rightarrow \infty$ , not physically acceptable — we must have **finite** solutions.

The only way to *avoid* this is to cut off the series for  $F(\rho)$ , i.e. let  $n = m+l+1$ , then  $a_{m+1} = 0 = a_{m+2} = a_{m+3} = \dots$  ( $m = 0, 1, 2, \dots$ ). Therefore, a solution for  $R$  will **exist** if  $n > l$ , and will be of the form  $R_{n,l}(\rho) = \exp(-\rho/2) \rho^l L_{n,l}(\rho)$  (---(17)), where the **red** bit is  $F(\rho)$ . Now  $L_{n,l}(\rho) = \sum_{m=0}^{n-l-1} a_m \rho^m$  (---(18), Associated Laguerre Polynomials), and the  $a_m$  are given by (14).

**Replacing**  $\rho$  by  $\alpha_n r$ , we get  $R_{n,l}(\alpha_n r) = (\alpha_n r)^l \exp(-\alpha_n r/2) L_{n,l}(\alpha_n r)$  (---(19)). ( $n = 1, 2, 3, \dots, \infty$ ;  $l = 0, 1, 2, \dots, n-1$ ). From (4) and (3) [ $\alpha_n^2 = -8mE/\hbar^2$  (---(3));  $n = (-\alpha_n(e^2/4\pi\epsilon_0))/4E$  (---(4))],  $E = -\alpha_n^2 \hbar^2 / 8m = (4) = (\hbar^2 / 8m) \times (16E^2 n^2 / (e^2/4\pi\epsilon_0)^2)$ . So  $E = [-m(e^4/(4\pi\epsilon_0)^2)/2\hbar^2]^{1/2} = E_n$  (---(20)), independent of the  $l$ -value. ( $n = 1, 2, 3, \dots$ ).



28th November 2000

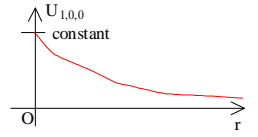
*Section 3.9, Equation 4*  $\Rightarrow u(r, \theta, \phi) = R_{n,l}(\alpha_n r) Y_l^m(\theta, \phi)$ , where  $n = 1, 2, \dots, \infty$ ;  $l = 0, 1, 2, \dots, n-1$ ; and  $m = -l, -l+1, \dots, -1, 0, 1, \dots, l-1, l$ . The *ground state energy* of the H-atom is given by  $E_1 = -me^4(4\pi\epsilon_0)^2/2\hbar^2$ , where  $n$  is the **principal quantum number**. For  $n = 1$ , there is only **one** ( $u_{1,0,0}$ ) eigenfunction *corresponding* to  $E_1$ . For  $n = 2$ , we have  $U_{2,0,0}$ ,  $U_{2,1,-1}$ ,  $U_{2,1,0}$ , and  $U_{2,1,1}$ , i.e. there are four *linearly independent eigenfunctions* corresponding to eigenvalue  $E_2$ .

### Degeneracy of $E_n$

$E_n$  does **not** depend on the  $l$ -value (*nor* the  $m$ -value), where  $0 \leq l \leq n-1$ . Let  $d$  be the *degeneracy* of  $E_n$ , the **total** number of linearly independent eigenfunctions ( $U_{n,l,m}$ ) corresponding to  $E_n$ . Therefore,  $d = \sum_{l=0}^{n-1} (2l+1) = 2 \sum_{l=0}^{n-1} l + \sum_{l=0}^{n-1} 1 = 2(1+n-1)(n-1)/2 + n = n(n-1) + n = n^2$ .

## Radial Wave Functions (Not Normalised)

**Recall:**  $L_{n,l}(\alpha_n r) = \sum_{m=0}^{n-l-1} a_m(\alpha_n r)^m$  (---(18),  $m$  here is just an index); and  $a_{m+1}/a_m = \frac{(m-n+l+1)}{[(m+l+1)(m+l+2)-l(l+1)]}$  (---(14), with  $m = 0, 1, 2, \dots$ ). Now  $E_1, U_{1,0,0} \Leftrightarrow n = 1, l = 0, m = 0$ . (14)  $\Rightarrow a_1/a_0 = \frac{(0-1+0+1)}{[(0+0+1)(0+0+2)-0(0+1)]} = 0/2 \Rightarrow a_1 = 0$  ( $a_0 \neq 0$ ). So  $L_{1,0}(\alpha_1 r) = a_0$ , and so  $R_{1,0}(\alpha_1 r) = (\alpha_1 r)^0 \exp(-\alpha_1 r/2) a_0 = (a_0) \exp(-\alpha_1 r/2)$ . Further,  $Y_0^0(\theta, \phi) = (\text{constant}) \times 1$ . Therefore,  $U_{1,0,0}(r, \theta, \phi) = (\text{const}) \exp(-\alpha_1 r/2) = \text{spherically symmetrical}$ , for  $0 \leq r < \infty$ .



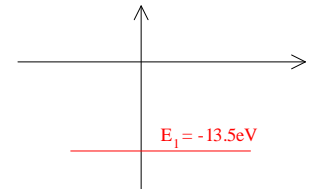
Consider  $R_{n,l}(\alpha_n r)$ . Here,  $n = 1, 2, \dots, \infty$ ; and  $l = 0, 1, \dots, n-1$ . **Case E<sub>1</sub>:**  $R_{1,0} = (\text{constant}) \exp(-\alpha_1 r/2)$ . **Case E<sub>2</sub>:**  $R_{2,0}(\alpha_2 r) = (\text{constant})(1 - (\alpha_2 r/2)) \exp(-\alpha_2 r/2)$ , where the red bit is  $L_{2,0}(\alpha_2 r)$ . And  $R_{2,1}(\alpha_2 r) = (\text{constant})(\alpha_2 r) \exp(-\alpha_2 r/2)$  (where the blue bit is  $L_{2,1}(\alpha_2 r)$ ), etc. **Spherical Harmonics**,  $Y_l^m(\theta, \phi)$  (*un-normalised*):  $Y_0^0(\theta, \phi) = (\text{constant}) \times 1$ ;  $Y_1^0(\theta, \phi) = (\text{constant}) \times \cos\theta$ ; and  $Y_1^{\pm 1}(\theta, \phi) = (\text{constant}) \sin\theta \exp(\pm i\phi)$ .

1st December 2000

## Bohr Radius

The *Bohr Radius* is given by  $a_0 = \hbar^2 / (me^2 / 4\pi\epsilon_0)$ , where  $e$  is the *magnitude of the electronic charge*;  $m$  is the *rest mass of the electron*; and  $a_0$  is approximately  $0.528 \times 10^{-8} \text{cm}$ . **Recall** that  $\rho = \alpha r$  (---(5, with  $\alpha > 0$ ), where  $\alpha^2 = -8mE/\hbar^2$  (---(3)). Now  $E = E_n = [-me^4 / (4\pi\epsilon_0)^2] / 2\hbar^2 n^2$  (---(20), with  $n = 1, 2, 3, \dots, \infty$ ). (20) in (3)  $\Rightarrow \alpha^2 = -8m/\hbar^2 \times \{ [-me^4 / (4\pi\epsilon_0)^2] / 2\hbar^2 \}^{1/n^2} = [2me^2 / (4\pi\epsilon_0)] \hbar^{-2} n^2$ , where  $\alpha = (2/a_0)^{1/n}$ . Therefore,  $\rho = \alpha r$ , so that  $\rho = (2/a_0)(r/n)$  for  $n = 1, 2, 3, \dots, \infty$ .

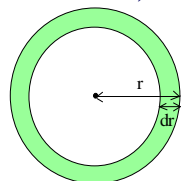
Consider the ground state,  $n = 1$ . (20)  $\Rightarrow E_1 = [-me^4 / (4\pi\epsilon_0)^2] / 2\hbar^2 (= \text{the ionisation energy of the Hydrogen atom}) = -13.5 \text{eV}$ , where  $1 \text{eV} = 1.6 \times 10^{-12} \text{ergs} = 1.6 \times 10^{-19} \text{J}$ .



## Wave Function

For  $n = 1$ ,  $u_{1,0,0} = (\text{constant}) R_{1,0}(\alpha r) Y_0^0(\theta, \phi)$ . ( $c, e^{-\alpha r/2}, 1$ ). So  $u_{1,0,0} = C e^{-\alpha r/2}$ , where  $\alpha = (n = 1) = (2/a_0)^{1/n} = 2/a_0$ . Therefore,  $u_{1,0,0} = C e^{-r/a_0}$ . ( $a_0$ , the **Bohr Radius**, is approximately  $0.53 \times 10^{-8} \text{cm}$ ). Q: Find the  $C$  so that  $u_{1,0,0}$  is *normalised*. A: Now  $1 = \int_{\text{all space}} |u_{1,0,0}|^2 dv (= I) = \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} |C|^2 e^{-2r/a_0} r^2 \sin\theta dr d\theta d\phi$ , where  $r^2 \sin\theta$  comes from the **Jacobian** (*from the transformation*).

It follows that  $1 = |C|^2 \int_{r=0}^{\infty} e^{-2r/a_0} r^2 dr \int_{\theta=0}^{\pi} \sin\theta d\theta \int_{\phi=0}^{2\pi} d\phi$ . We evaluate the **first** integral *by parts*, and we get  $a_0^3/4$ . The **second** integral is  $[-\cos\theta]_0^{\pi} = 1 - (-1) = 2$ ; while the **third** integral is  $[\phi]_0^{2\pi} = 2\pi$ . Therefore,  $1 = |C|^2 (a_0^3/4)(2)(2\pi) \Rightarrow |C| = (\pi^{1/2} a_0^{3/2})^{-1}$ . So  $u_{1,0,0}$  (*normalised*) =  $[e^{i\delta} / \pi^{1/2} a_0^{3/2}] e^{-r/a_0}$ , where  $c = |C| e^{i\delta}$  for  $0 \leq \delta < 2\pi$ . **Take**  $\delta = 0$  without loss of generality w.r.t. *expectation* values, etc., then **from** the diagram,  $I = \int_{r=0}^{\infty} |C|^2 e^{-2r/a_0} 4\pi r^2 dr$  (where the red bit is the *volume element for the case of spherical symmetry in the integrand*) =  $|C|^2 4\pi \int_{r=0}^{\infty} r^2 e^{-2r/a_0} dr$ .



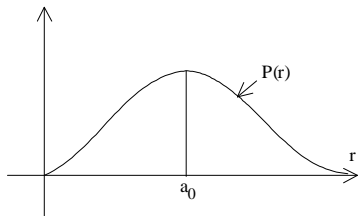
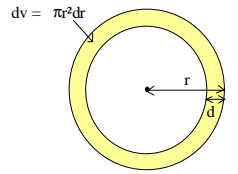
# Tutorial

Q: Find the *average value* (or expectation value)  $\langle r \rangle_{u_{1,0,0}} = \int_{\text{allspace}} (u_{1,0,0}^*(r)(u_{1,0,0}(r))dv$ , where  $u_{1,0,0} = (1/\pi^{1/2}a_0^{3/2})e^{-r/a_0}$ . A:  $\langle r \rangle_{u_{1,0,0}} = \int_{\text{allspace}} ((1/\pi^{1/2}a_0^{3/2})e^{-r/a_0})^2 r dv = \int_{\text{allspace}} (1/\pi a_0^3) e^{-2r/a_0} r dv = 1/\pi a_0^3 \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} e^{-2r/a_0} r (r^2 \sin\theta) dr d\theta d\phi = 1/\pi a_0^3 \int_{r=0}^{\infty} r^3 e^{-2r/a_0} dr \times \int_{\theta=0}^{\pi} \sin\theta d\theta \int_{\phi=0}^{2\pi} d\phi = (\text{red} = 2, \text{blue} = 2\pi) = 4\pi/\pi a_0^3 \int_{r=0}^{\infty} r^3 e^{-2r/a_0} dr$ . Now let  $J = \int_{r=0}^{\infty} r^3 e^{-2r/a_0} dr$ .

Let us evaluate J *by parts*. First, let  $u = r^3$ , so that  $du/dr = 3r^2$ . Then, let  $dv/dr = e^{-2r/a_0}$ , so that  $v = (a_0/2)e^{-2r/a_0}$ . It follows that  $J = [(r^3 a_0 / 2) e^{-2r/a_0}]_0^{\infty} - \int_0^{\infty} (3r^2 a_0 / 2) e^{-2r/a_0} dr = [0 - 0] - \int_0^{\infty} (3r^2 a_0 / 2) e^{-2r/a_0} dr$ . Let K be the purple integral, and *evaluate it by parts*. Let  $u = 3r^2 a_0 / 2$ , so that  $du/dr = 3ra_0$ . And let  $dv/dr = e^{-2r/a_0}$ , so that  $v = (a_0/2)e^{-2r/a_0}$ . Therefore,  $K = [(3r^2 a_0^2 / 4) e^{-2r/a_0}]_0^{\infty} - \int_0^{\infty} (3ra_0^2 / 2) e^{-2r/a_0} dr = [0 - 0] - \int_0^{\infty} (3ra_0^2 / 2) e^{-2r/a_0} dr$ .

Let L be the green integral, and evaluate it by **parts**. Let  $u = (3ra_0^2/2)$ , so that  $du/dr = 3a_0^2/2$ . And let  $dv/dr = e^{-2r/a_0}$ , so that  $v = (a_0/2)e^{-2r/a_0}$ . It follows that  $L = [(3ra_0^3/4) e^{-2r/a_0}]_0^{\infty} - \int_0^{\infty} (3a_0^3/4) e^{-2r/a_0} dr = [0 - 0] - \int_0^{\infty} (3a_0^3/4) e^{-2r/a_0} dr$ . Therefore,  $J = \int_0^{\infty} (3a_0^3/4) e^{-2r/a_0} dr = [(3a_0^4/8) e^{-2r/a_0}]_0^{\infty} = (3a_0^4/8)(0) - (3a_0^4/8)(1)$ . It follows that  $J = 3a_0^4/8$ , and so  $\langle r \rangle_{u_{1,0,0}} = 4/a_0^3 (3a_0^4/8) = 3a_0/2$ .

Q: Find the *most probable value* of r in the ground state. A: Let  $P(r)dr$  denote the **probability** that the electron, in the ground state, lies between r and r+dr from the nucleus. This implies that  $P(r)dr = |u_{1,0,0}|^2 dv$ , where  $dv = 4\pi r^2 dr$ . Find P(r), and hence its *maximal* value for  $0 \leq r < \infty$ . So  $P(r)dr = |u_{1,0,0}|^2 4\pi r^2 dr = ((1/\pi^{1/2}a_0^{3/2})e^{-r/a_0})^2 4\pi r^2 dr = (1/\pi a_0^3) e^{-2r/a_0} 4\pi r^2 dr$ ;  $P(r) = (4/a_0^3) r^2 e^{-2r/a_0}$ .



Now  $dP(r)/dr = 2r(4/a_0^3)e^{-2r/a_0} + (4r^2/a_0^3)(-2/a_0)e^{-2r/a_0} = re^{-2r/a_0}((8/a_0^3) - (8r/a_0^4))$ . So either  $r = 0$  (gives a **minimum**);  $r = \infty$  (gives a **minimum**); or  $8r/a_0^4 = 8/a_0^3$ ;  $r = a_0$ . This is a **maximum** (we can check the 2nd derivative), and, further, is a **global** maximum because of the *differentiability* of the function across its domain.

## Assignment 4

Q: Given the *radial equation* for the **H-atom** in the form  $(1/r^2)d/dr(r^2 dR/dr) + \{(2m/\hbar^2)(E + (e^2/4\pi\epsilon_0/r)) - l(l+1)/r^2\}R = 0$  (---(1)), make the *substitutions*  $\alpha^2 = -8mE/\hbar^2$  (---(2));  $n = (-\alpha e^2/4\pi\epsilon_0)/4E$  (---(3)); and  $\rho = \alpha r$  (---(4)), to give  $(1/\rho^2)d/d\rho(\rho^2 dR/d\rho) + (n/\rho - 1/4 - l(l+1)/\rho^2)R = 0$ . Let  $R(\rho) = \exp(-1/2\rho)F(\rho)$ , and show that  $d^2F/d\rho^2 + (2/\rho - 1)dF/d\rho + ((n-1)/\rho - l(l+1)/\rho^2)F = 0$ .

Let  $F(\rho) = \rho^\sigma \sum_{m=0}^{\infty} a_m \rho^m$  ( $a_0 \neq 0$ ), and show that  $\sigma(\sigma+1) - l(l+1) = 0$ ; and that  $a_{m+1}[(m+\sigma+1)(m+\sigma+2) - l(l+1)] = a_m(m+\sigma-n+1)$ . Deduce that when  $\sigma = l$ , and when n is a *positive integral*, then the series for F(ρ) is finite. Show that  $R(\rho) = R_{n,l}(\rho)$ , where  $0 \leq l \leq n-1$ ;  $n = 1, 2, \dots$ ; and hence show that  $R_{1,0}(\rho) = (\text{constant})e^{-\rho/2}$ ,  $R_{2,0}(\rho) = (\text{constant})(1-\rho/2)e^{-\rho/2}$ ,  $R_{2,1}(\rho) = (\text{constant})\rho e^{-\rho/2}$ ,  $R_{3,0}(\rho) = (\text{constant})(1-\rho+\rho^2/6)e^{-\rho/2}$ ,  $R_{3,1}(\rho) = (\text{constant})(1-\rho/4)\rho e^{-\rho/2}$ , and  $R_{3,2}(\rho) = (\text{constant})\rho^2 e^{-\rho/2}$ .

A: (4)  $\Rightarrow \rho^2 = \alpha^2 r^2$ , so that  $r^2 = \rho^2/\alpha^2$ . **Substituting** for  $r^2$  in (1), we get  $(\alpha^2/\rho^2)^{d/d\rho}(\rho^2/\alpha^2)^{dR/d\rho} + \{2m\hbar^2(E + (e^2/4\pi\epsilon_0)/r) - \alpha^2 l(l+1)/\rho^2\}R = 0$ . **Now**  $d/d\rho = d/d\rho \cdot d\rho/dr = d/d\rho(\alpha) = \alpha^{d/d\rho}$  (---(6)). **Substituting** for  $d/d\rho$ , gives  $\alpha^2/\rho^2 \cdot d/d\rho(\rho^2)^{dR/d\rho} + \{2m\hbar^2/\rho^2 + (2me^2/(4\pi\epsilon_0))/r^2 - \alpha^2 l(l+1)/\rho^2\}R = 0$ . **Now use** (2) to (4) to replace stuff in the  $\{..\}$ , giving  $(\alpha^2/\rho^2)^{d/d\rho}(\rho^2)^{dR/d\rho} + \{-\alpha^2/4 + \alpha^2 n/\rho - \alpha^2 l(l+1)/\rho^2\}R$ . **Divide** through by  $\alpha^2$  to get the result

Now let  $R = \exp(-1/2\rho)F$ , so that  $dR/d\rho = -1/2\exp(-1/2\rho)F + \exp(-1/2\rho)dF/d\rho$ . **Substitute** for  $R$  and  $dR/d\rho$  above to give  $(1/\rho^2)^{d/d\rho}(\rho^2(-1/2\exp(-1/2\rho)F + \exp(-1/2\rho)dF/d\rho)) + (n/\rho - 1/4 - l(l+1)/\rho^2)\exp(-1/2\rho)F = 0$ . **Differentiate** again; collect **like terms**; and **factorise**, to give  $\exp(-1/2\rho)\{d^2F/d\rho^2 + (2/\rho - 1)dF/d\rho + ((n-1)l(l+1)/\rho^2)F\} = 0$ . Now **either A or B** is zero, so we have our **second** result from the solution  $B = 0$ .

Now let  $F(\rho) = \rho^\sigma \sum_{m=0}^{\infty} a_m \rho^m$ , with  $a_0 \neq 0$ , i.e.  $F(\rho) = \sum_{m \geq 0} a_m \rho^{m+\sigma}$ . Now use the *Frobenius method* to solve the D.E. Let  $F(\rho) = \sum_{m \geq 0} a_m \rho^{m+\sigma}$  (---(A)), so that  $dF/d\rho = \sum_{m \geq 0} a_m(m+\sigma)\rho^{m+\sigma-1}$  (---(B)), and  $d^2F/d\rho^2 = \sum_{m \geq 0} a_m(m+\sigma)(m+\sigma-1)\rho^{m+\sigma-2}$  (---(C)). **Substituting** from (A), (B) and (C) into the D.E. **gives**  $\sum_{m \geq 0} a_m(m+\sigma)(m+\sigma-1)\rho^{m+\sigma-2} + \sum_{m \geq 0} 2a_m(m+\sigma)\rho^{m+\sigma-2} - \sum_{m \geq 0} a_m(m+\sigma)\rho^{m+\sigma-1} + \sum_{m \geq 0} (n-1)a_m\rho^{m+\sigma-1} - \sum_{m \geq 0} l(l+1)a_m\rho^{m+\sigma-2} = 0$ , i.e.  $\sum_{m \geq 0} \rho^{m+\sigma-2}[a_m(m+\sigma)(m+\sigma-1) + 2a_m(m+\sigma) - l(l+1)a_m] + \sum_{m \geq 0} \rho^{m+\sigma-1}[(n-1)a_m - a_m(m+\sigma)] = 0$ .

To get the *indicial equation*, we look for the lowest power of  $\rho$ . Here, it is  $\sigma-1$  (when  $m = 0$ ), and its **coefficient** (which must be zero) is given by  $a_0\sigma(\sigma-1) + 2a_0(\sigma) - a_0l(l+1) = 0$ . Now  $a_0 \neq 0$ , so we can *divide through by it*, giving  $\sigma(\sigma-1) + 2\sigma - l(l+1) = 0$ ;  $\sigma(\sigma+1) - l(l+1) = 0$ . Note that **one** solution for this equation is  $\sigma = l$ .

Now let us look at the *coefficient* for the **general** term,  $\rho^{m+\sigma-1}$ . It has *coefficient*  $[(n-1)-(m+\sigma)]a_m + a_{m+1}[((m+1+\sigma)((m+1)+\sigma-1) + 2((m+1)+\sigma) - l(l+1))] = 0$ ;  $[(n-1)-(m+\sigma)]a_m + a_{m+1}[\{(m+\sigma+1)[m+1+\sigma-1+2]\} - l(l+1)] = 0$ ;  $[(n-1)-(m+\sigma)]a_m + a_{m+1}[(m+\sigma+1)(m+\sigma+2) - l(l+1)] = 0$ ;  $a_{m+1}[(m+\sigma+1)(m+\sigma+2) - l(l+1)] = a_m[m+\sigma-n+1]$ .

Following the route of the **lectures** in substituting  $\sigma = l$  into the *above*; finding the **limit**  $\lim_{m \rightarrow \infty} (a_{m+1}/a_m)$ ; *comparing* to  $\exp(+\rho)$ ; and then letting  $n = m+l+1$  to **terminate** the series, we get that a solution for  $R$  will *exist* if  $n > l$ , and will be of the **form**  $R_{n,l}(\rho) = \exp(-\rho/2)\rho^l L_{n,l}(\rho)$  (for  $n = 1, 2, 3, \dots$ ;  $l = 0, 1, 2, \dots, n-1$ ), where  $L_{n,l}(\rho) = \sum_{m=0}^{n-l-1} a_m \rho^m$ , and  $a_{m+1} = \frac{(m+l-n+1)}{[(m+l+1)(m+l+2)-l(l+1)]} a_m$ .

**Now**  $R_{1,0}(\rho) = \exp(-\rho/2)\rho^0 L_{1,0}(\rho) = \exp(-\rho/2)L_{1,0}(\rho)$ , and  $L_{1,0}(\rho) = \sum_{m=0}^0 a_m \rho^m = a_0(1)$ , so that  $R_{1,0}(\rho) = a_0 \exp(-\rho/2) = (\text{constant})\exp(-\rho/2)$ . **Now**  $R_{2,0}(\rho) = \exp(-\rho/2)(1)L_{2,0}(\rho)$ , and  $L_{2,0}(\rho) = \sum_{m=0}^1 a_m \rho^m = a_0 + \rho a_1$ , where  $a_1 = (0+0-2+1)a_0/[(0+0+1)(0+0+2)-0(0+1)] = -a_0/2$ , so that  $L_{2,0}(\rho) = a_0 - (a_0/2)\rho$ , and therefore  $R_{2,0}(\rho) = \exp(-\rho/2)[a_0 - 1/2 a_0 \rho] = (\text{constant})\exp(-\rho/2)[1 - \rho/2]$ .

**Now**  $R_{2,1}(\rho) = \exp(-\rho/2)\rho L_{2,1}(\rho)$ , and  $L_{2,1}(\rho) = \sum_{m=0}^0 a_m \rho^m = a_0$ , so that  $R_{2,1}(\rho) = (\text{constant})\exp(-\rho/2)\rho$ . **Now**  $R_{3,0}(\rho) = \exp(-\rho/2)(1)L_{3,0}(\rho)$ ;  $L_{3,0}(\rho) = \sum_{m=0}^2 a_m \rho^m = a_0 + \rho a_1 + \rho^2 a_2$ ;  $a_1 = (0+0-3+1)a_0/[(0+0+1)(0+0+2)-0(0+1)] = -2/2 a_0 = -a_0$ ; and  $a_2 = (1+0-3+1)a_1/[(1+0+1)(1+0+2)-0(0+1)] = -1(-a_0)/6 = a_0/6$ , so that  $L_{3,0}(\rho) = a_0 + \rho(-a_0) + \rho^2(a_0/6) = a_0(1 - \rho + \rho^2/6)$ , and therefore  $R_{3,0}(\rho) = (\text{constant})\exp(-\rho/2)(1 - \rho + \rho^2/6)$ .

**Now**  $R_{3,1}(\rho) = \exp(-\rho/2)(\rho)L_{3,1}(\rho)$ ;  $L_{3,1}(\rho) = \sum_{m=0}^1 a_m \rho^m = a_0 + \rho a_1$ ; and  $a_1 = (0+1-3+1)a_0 / [(0+1+1)(0+1+2)-1(1+1)] = -a_0/6-2 = -a_0/4$ , so that  $L_{3,1}(\rho) = a_0 - (a_0/4)\rho$ , and therefore  $R_{3,1}(\rho) = (\text{constant})\exp(-\rho/2)\rho(1-\rho/4)$ . **Now**  $R_{3,2}(\rho) = \exp(-\rho/2)(\rho^2)L_{3,2}(\rho)$ , and  $L_{3,2}(\rho) = \sum_{m=0}^0 a_m \rho^m = a_0$ , so that  $R_{3,2}(\rho) = (\text{constant})\exp(-\rho/2)\rho^2$ . **QED.**

5th December 2000

## Past Paper

**Q:** Starting from the *definition of the Hamiltonian function* in terms of the **Lagrangian** function, derive **Hamiltonian's** canonical equations of motion for a conservative holonomic system with  $n$  degrees of freedom. **A:** Book work — see the notes earlier, and BLD's solution.

**Q:** Show that if the Hamiltonian function is *not* an *explicit function of time*, then it is constant during the motion. **A:** Now  $H = H(q_1, \dots, q_n, p_1, \dots, p_n)$ , so that  $\partial H / \partial t = 0$ . **Now**  $dH/dt = \sum_{\sigma=1}^n ((\partial H / \partial p_{\sigma}) \dot{q}_{\sigma} + (\partial H / \partial q_{\sigma}) \dot{p}_{\sigma}) = \sum_{\sigma=1}^n ((\partial H / \partial q_{\sigma}) (\partial H / \partial p_{\sigma}) + (\partial H / \partial p_{\sigma}) (-\partial H / \partial q_{\sigma})) = 0$ . **QED.**

**Q:** The Lagrangian function of a **particle** of mass  $m$  and charge  $q$  moving in the  $xy$ -plane subject to a *constant uniform magnetic field* of intensity  $B$  (directed along the positive  $z$ -axis) is given by  $L = \frac{1}{2}m(\dot{r}^2 + (r\dot{\theta})^2) + (qB/2)(r^2\dot{\theta})$ , where  $r$  and  $\theta$  denote the **polar** co-ordinates of the particle in the  $xy$ -plane. Find expressions for the *generalised momenta*  $p_r$  and  $p_{\theta}$ ; show that the Hamiltonian function  $H$  is **given** by  $H = \frac{1}{2m}[p_r^2 + (p_{\theta}/r)^2 + (qBr/2)^2 - qBp_{\theta}]$ ; and write down the **canonical** equations of motion.

**A:** This is similar to *previous* examples. Remember that you must express  $H$  in terms of the  $p_r$  and the  $p_{\theta}$ . At the end, we get the *canonical equations*  $\dot{r} = p_r/m$ ;  $\dot{\theta} = (p_{\theta}/mr^2) - \omega/m$  (we have *previously* defined  $\omega = qB/2$ );  $\dot{p}_r = (p_{\theta}^2/mr^3) - (\omega^2 r/m)$ ; and  $\dot{p}_{\theta} = -\partial H / \partial \theta = 0$ . Now the **last** equation implies that  $p_{\theta} = \text{constant}$  (after integrating).

**Q:** If at  $t = 0$ ,  $r = a$ ;  $\dot{r} = u$ ; and  $\dot{\theta} = 0$ , show that  $H = mu^2/2$ . Deduce that if  $u = \sqrt{3qBa/(4m)}$ , then the motion is *bounded* by the circles  $r = a/2$  and  $r = 2a$ . **A:** We have already **found** that  $dH/dt = 0 \Rightarrow H = \text{constant}$ . Now substituting into an equation during the **derivation** for  $H$ , we find our result,  $H = mu^2/2$ .

From *previous calculations*,  $p_{\theta} = mr^2\dot{\theta} + \omega r^2 = C = 0 + \omega a^2$  (substituting in *initial conditions*). **Now**  $mu^2/2 = H = (m/2)(\dot{r}^2 + r^2[\omega a^2 - \omega r^2/mr^2]^2) \Rightarrow \dot{r}^2 = u^2 - (\omega a/m)^2(a/r - r/a)^2 \geq 0$ . Now given  $\sqrt{3qBa}/4m = \sqrt{3\omega a}/2m$ . (...)  $\Rightarrow$  (using  $x = r/a$ )  $(1/x - x)^2 \leq (3/2)^2 \Rightarrow -3/2 \leq (1/x - x) \leq 3/2$ . Taking the **LHS extremity**,  $-3/2 = 1/x - x \Rightarrow x^2 - 3x/2 - 1 = 0$ ;  $(x-2)(x+1/2) = 0$ ;  $x = 2$  or  $x = -1/2$ . Take the *first* solution,  $r = 2a$ . **Reject** the second — we cannot have  $r < 0$ . Taking the **RHS extremity**,  $1/x - x = 3/2$ ;  $x^2 + 3x/2 - 1 = 0$ ;  $(x+2)(x-1/2) = 0$ ;  $x = -2$  (*reject*) or  $x = 1/2$  (*accept*,  $r = a/2$ ). **QED.**

**Q:** Describe an **experiment** that demonstrates the *particle-like nature* of radiation. Give a non-relativistic mathematical explanation, explaining clearly the conservation principles involved. **A:** Book Work.

Q: A particle of mass  $m$  moves in an **infinitely deep square well potential** given by  $V(x) = 0$  if  $0 \leq x \leq l$ , and  $V(x) = \infty$  if  $x < 0$  or  $l < x$ . Solve the *time-independent Schrödinger equation* to find the energy eigenvalues  $E_n$ , where  $E^n = (\hbar^2\pi^2/2ml^2)n^2$ , ( $n = 1, 2, 3, \dots$ ), and find the corresponding *normalised eigenfunctions*,  $u_n(x)$ . A: See the lecture notes.

Q: Calculate the **expectation** value  $\langle x^2 \rangle$  in the state represented by  $u_n(x)$ , and compare it to the corresponding **classical** value. A: See Assignment 3.

8th December 2000

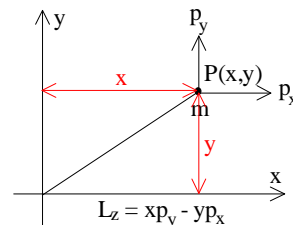
## Past Paper

Q: Write down Hamilton's *canonical equations* of motion for a conservative holonomic system of  $n$  degrees of freedom. Show that if the Hamiltonian is **not** an explicit function of time, then it is *constant* during the motion. A: Book Work.

Q: The Hamiltonian,  $H$ , for a particle of **mass**  $m$  and **charge**  $q$  moving in a **magnetic field** derived from a **vector potential**,  $\underline{A}$ , is given by  $H = \frac{1}{2m}(\underline{p} - q\underline{A})^2$ , where  $\underline{p} = (p_x, p_y, p_z)$  denotes the *generalised momentum vector*, and  $\underline{A} = (A_x, A_y, A_z)$ .

If  $\underline{A} = (-ky, kx, 0)$ , where  $k$  is a constant, show that the *corresponding quantum mechanical Hamiltonian operator* is given by  $(-\hbar^2/2m)\nabla^2 - (kq/m)\hat{L}_z + k^2q^2/2m(x^2+y^2)$ , where the **operator** corresponding to the angular momentum of the particle about the  $z$ -axis is denoted by  $\hat{L}_z$ , which is to be found.

A: **Now**  $(\underline{p} - q\underline{A})^2 = \underline{p}^2 - 2q\underline{p} \cdot \underline{A} + q^2\underline{A}^2$ . Substituting for  $\underline{p}$  and  $\underline{A}$  gives  $H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + \frac{1}{2m}(-2q)(p_x(-ky) + p_y(kx)) + \frac{q^2}{2m}((-ky)^2 + (kx)^2) = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) - \frac{(kq/m)}{2m}(xp_y - yp_x) + \frac{k^2q^2}{2m}(x^2 + y^2)$ . In the *diagram*,  $L_z$  is the classical *angular momentum* about the  $z$ -axis. The corresponding **quantum** mechanical operator,  $H_q$ , is  $p_\alpha \rightarrow -i\hbar \frac{\partial}{\partial x}$ , where  $\alpha = x, y, \text{ or } z$ .



*Substituting*,  $H_q = \frac{1}{2m}((-i\hbar)^2 \frac{\partial^2}{\partial x^2} + (-i\hbar)^2 \frac{\partial^2}{\partial y^2} + (-i\hbar)^2 \frac{\partial^2}{\partial z^2}) - \frac{(kq/m)}{2m}(x(-i\hbar) \frac{\partial}{\partial y} - y(-i\hbar) \frac{\partial}{\partial x}) + \frac{k^2q^2}{2m}(x^2 + y^2) = (-\hbar^2/2m)\nabla^2 - \frac{(kq/m)}{2m}(\hat{L}_z) + \frac{(k^2q^2)}{2m}(x^2 + y^2)$ . **QED.**

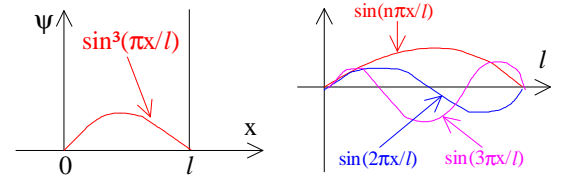
Q: Give an account of the **four basic postulates of quantum mechanics**, explaining carefully the roles of the *wave function* and the Hamiltonian, and include a brief description of the theory of measurement. Illustrate your answer by considering a **single** particle of mass  $m$  moving in a potential  $V(x, y, z)$ . A: Book Work.

Q: A particle of mass  $m$  moves in an *infinitely deep square well potential* given by  $V(x) = 0$  if  $0 \leq x \leq l$ , and  $V(x) = \infty$  if  $x < 0$  or  $x > l$ . Solve the *time-independent Schrödinger equation* to find the energy eigenvalues  $E_n$ , for  $n = 1, 2, 3, \dots, \infty$ , and show that the *corresponding eigenfunctions*,  $u_n(x)$ , are given by  $u_n(x) = \sqrt{(2/l)}\sin(n\pi x/l)$  if  $0 \leq x \leq l$ , and  $u_n(x) = 0$  if  $x < 0$  or  $x > l$ . A: Book Work.

Q: Write down the *general solution*,  $\psi(x,t)$ , of the **time-dependent** Schrödinger equation in terms of  $E_n$  and  $u_n(x)$ , for  $n = 1, 2, 3, \dots, \infty$ . If, at  $t = 0$ ,  $\psi(x,0) = \sin^3(\pi x/l)$  for  $0 \leq x \leq l$ , and  $\psi(x,0) = 0$  for  $x < 0$  and  $x > l$ , find  $\psi(x,t)$  when  $t > 0$ . A:  $\psi(x,t) = \sum_{n=1}^{\infty} c_n u_n(x) \exp(-iE_n t/\hbar)$ , where  $E_n = (\hbar^2/2m)(\pi/l)^2 n^2$ ;  $n = 1, 2, 3, \dots, \infty$ ; and  $u_n(x)$  is as **shown** in the question.

$\psi(x,0) = \sum_{n=1}^{\infty} c_n u_n(x) = \sin^3(\pi x/l)$ . Now  $4\sin^3\theta = 3\sin\theta - \sin 3\theta$ , so that  $\psi(x,0) = \frac{3}{4}\sin(\pi x/l) - \frac{1}{4}\sin(3\pi x/l) \Rightarrow c_1 \sqrt{(2/l)} = \frac{3}{4}$ ;  $c_3 \sqrt{(2/l)} = -\frac{1}{4}$ ; and  $c_n = 0$  for  $n \neq 1, 3$ . Therefore,  $\psi(x,t) = \frac{3}{4}\sqrt{(l/2)}u_1(x)\exp(-iE_1 t/\hbar) - \frac{1}{4}\sqrt{(l/2)}u_3(x)\exp(-iE_3 t/\hbar)$ . ( $c_1, c_3$ ). (Useful in an exam:  $e^{i\theta} = \cos\theta + i\sin\theta$ ;  $e^{i3\theta} = (\cos\theta + i\sin\theta)^3 = \cos(3\theta) + i\sin(3\theta)$ ; and also useful:  $\Pr(A=a_k) = |c_k|^2 / \sum_{n=1}^{\infty} |c_n|^2$ ).

Q: Deduce that a **measurement** of the energy of the particle in the *state*  $\psi(x,t)$  will yield either  $E_1$  or  $E_3$ , and find the corresponding probabilities of their occurrence. A:  $\Pr(E = E_1) = |c_1|^2 / \sum_{n=1}^{\infty} |c_n|^2 = |c_1|^2 / (|c_1|^2 + |c_3|^2) = \frac{3^2}{3^2 + (-1)^2} = \frac{9}{10}$ . **And**  $\Pr(E = E_3) = \frac{(-1)^2}{3^2 + (-1)^2} = \frac{1}{10}$  ( $= 1 - 9/10 = 1 - \Pr(E = E_1)$ ).



12th December 2000

## Past Paper

Q: Write down the *time-independent Schrödinger equation* for the hydrogen atom in SI units. Show that a **physically acceptable** spherically symmetrical solution of the form  $R(r) = A \exp(-\alpha r)$  ( $A$  and  $\alpha$  are +ve constants) exists, provided  $\alpha$  takes a *particular value to be found*. Show that the **corresponding** value of the energy is (in the usual notation)  $-me^4/\hbar^2(4\pi\epsilon_0)^2$ .

Find the *expectation value* of  $r$  in the state represented by  $R(r)$ , and compare this with the most **probable** value of  $r$  in the same state. You may assume that in spherical polar co-ordinates,  $(r, \theta, \phi)$ ,  $\nabla^2 = \{ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2} [ \frac{\partial^2}{\partial \theta^2} (\sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin\theta} \frac{\partial^2}{\partial \phi^2}) ] \}$ . (The red bit is  $L(\theta, \phi)$ , (---(4))).

A: The *TISE* for the H-atom is  $(-\hbar^2/2m)\nabla^2 u + V u = E u$  (---(1)), where  $V = (-e^2/(4\pi\epsilon_0))/r$  (---(2), SI Units). **Given**  $\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2} L(\theta, \phi)$  (---(3)), let  $u(r, \theta, \phi) = R(r) = A \exp(-\alpha r)$  (---(5)).

Now (1) to (5)  $\Rightarrow (\frac{1}{r^2}) \frac{d}{dr} (r^2 \frac{dR}{dr}) + (2m/\hbar^2)[E + (e^2/(4\pi\epsilon_0)r)]R = 0 \Rightarrow (\frac{1}{r^2}) \frac{d}{dr} (r^2(-\alpha)Ae^{-\alpha r}) + (2m/\hbar^2)(E + (e^2/(4\pi\epsilon_0)r))Ae^{-\alpha r} = 0 \Rightarrow (\frac{1}{r^2})\{2r(-\alpha) + r^2(-\alpha)^2\}Ae^{-\alpha r} + \dots = 0 \Rightarrow (\times r^2) \Rightarrow (2r(-\alpha) + \alpha^2 r^2) + (2m/\hbar^2)r^2\{E + ((e^2/(4\pi\epsilon_0))/r)\} = 0 \Rightarrow (\alpha^2 + (2mE/\hbar^2)r^2 + ([2me^2/(4\pi\epsilon_0)]/\hbar^2 - 2\alpha)r = 0$ . Note that this is for all  $r$ , where  $0 \leq r < \infty$ .

Now  **$r$  and  $r^2$  are independent**, thus both coefficients must be zero, and this implies that  $\alpha = (m/\hbar^2)e^2/(4\pi\epsilon_0)$  (---(6)), and that  $E = (-\hbar^2/2m)\alpha^2$  (---(7)). (6) in (7) implies that we have  $E = (-\hbar^2/2m)[(m/\hbar^2)e^2/4\pi\epsilon_0]^2 = -\frac{1}{2}(me^4/\hbar^2(4\pi\epsilon_0)^2) (= E_1, \text{Ground State Energy})$ . **QED**.

## Exam Paper: January 2001

### Answer 3 questions out of 5 (Questions Done: 1, 3, 4)

- (1) (a) Show that for a conservative holonomic system with  $n$  degrees of freedom, Lagrange's equations and Hamilton's equations are equivalent. **[8 marks]**
- (b) The Lagrangian function for a particle of mass  $m$  moving in the  $xy$ -plane is given by  $L = (\frac{m}{2})(\dot{r}^2 + (r\dot{\theta})^2) + (\frac{A}{2})(r^2\dot{\theta})$  where  $r, \theta$  are the polar coordinates of the particle and  $A$  is a constant.

Find expressions for the generalised momenta  $p_r, p_\theta$  and show that the Hamiltonian function  $H$  is given by  $H = (\frac{1}{2m})(p_r^2 + (p_\theta/r)^2) + (Ar/2)^2 - Ap_\theta$  and write down the canonical equations of motion. **[8 marks]**

If at  $t=0, r=a, \dot{\theta}=0$ , deduce that  $\dot{\theta} = (\frac{A}{2m})(\frac{a}{r})^2 - 1, t > 0$ . **[4 marks]**

- (2) Write a short mathematical essay describing the evidence that a theory radically different from classical theory is necessary for the description of microphysical phenomena. **[20 marks]**

- (3) A particle of mass  $m$  moves in one dimension in a time-independent potential  $V(x)$ . Apply the method of separation of variables to show that solutions  $\psi_E(x,t)$  to the time-dependent Schrödinger equation may be found in the form  $\psi_E(x,t) = U_E(x)T_E(t)$  where  $E$  denotes the separation constant,  $U_E(x)$  denotes a solution to the time-independent Schrödinger equation and  $T_E(t)$  is to be found. Give a physical interpretation of  $E$ . Hence write down the general solution to the time-dependent Schrödinger equation. **[10 marks]**

If  $V(x)$  is given by:  $V(x) = 0$  for  $0 < x < l$  and  $\infty$  for  $x \leq 0, x \geq l$  show that  $E = E_n = (\frac{1}{2m})(\frac{h\pi}{l})^2 n^2$  for  $n = 1, 2, 3, \dots$  **[10 marks]**

- (4) A particle of mass  $m$  moves in one dimension in the potential given by  $V(x) = V_0$  for  $x < 0$  and  $x > l$ ;  $0$  for  $0 \leq x \leq l$ . Show that there are only a finite number  $N$  of bound states of energy  $E < V_0$ , where  $E$  satisfies the equation  $(\frac{l}{h})\sqrt{2mE} = n\pi - 2\sin^{-1}\sqrt{E/V_0}, n = 1, 2, 3, \dots, N$ . **[18 marks]**

Contrast with the energy spectrum of a classical particle moving in the same potential. **[2 marks]**

- (5) The radial part of a bound state wave function of energy  $E < 0$  of a hydrogen atom is given by:  $R(\rho) = \exp(-\rho/2)F(\rho)$  where  $\rho = \alpha r$ ,  $\alpha^2 = (-8\mu E)/\hbar^2$  and  $F(\rho)$  satisfies  $\frac{d^2F}{d\rho^2} + \left[\frac{2}{\rho} - 1\right]\frac{dF}{d\rho} + \left[\frac{n-1}{\rho} - \frac{l(l+1)}{\rho^2}\right]F = 0$ , with  $n = -\alpha(e^2/4\pi\epsilon_0)/4E$ ,  $\mu$  and  $e$  denoting respectively the reduced electronic mass and charge, and  $l$  taking on non-negative integral values. By considering a Frobenius series solution for  $F$  show that a physically acceptable solution for  $R$  is obtained only when  $n$  taken on positive integral values and find the corresponding energy levels.

**[17 marks]**

Show that the degeneracy of the  $n^{\text{th}}$  energy level is  $n^2$ .

**[3 marks]**