

## THE CENTRAL POTENTIAL

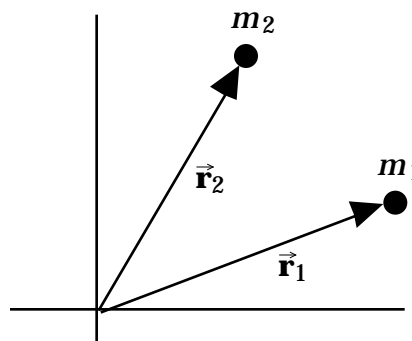
Consider two particles interacting with a force which depends only on the magnitude of the distance between them. Such a force is called a **central force** and the associated potential is called a **central potential**.

This two-body problem is easily reduced to a one-body problem, reducing the number of variables from 6 to 3 (in fact, this can be done even when the potential is not central), and the one-body problem can then be reduced to a one-dimensional problem, the kind we like best.

Let us first look at the problem according to classical (Newtonian) mechanics. The equations of motion of the particles are

$$m_1 \ddot{\mathbf{r}}_1 = \ddot{\mathbf{F}}_{1\text{int}} + \ddot{\mathbf{F}}_{1\text{ext}} = - \nabla_{\mathbf{r}_1} U(|\mathbf{r}_1 - \mathbf{r}_2|) + \ddot{\mathbf{F}}_{1\text{ext}}$$

$$m_2 \ddot{\mathbf{r}}_2 = \ddot{\mathbf{F}}_{2\text{int}} + \ddot{\mathbf{F}}_{2\text{ext}} = - \nabla_{\mathbf{r}_2} U(|\mathbf{r}_1 - \mathbf{r}_2|) + \ddot{\mathbf{F}}_{2\text{ext}}$$



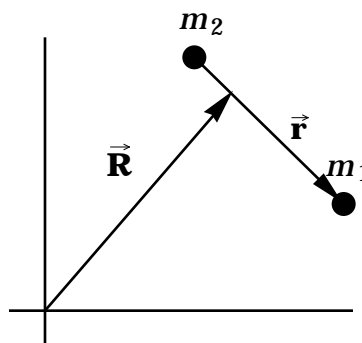
We change to the center-of-mass coordinates

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

$$\mathbf{r}_1 = \mathbf{R} + \frac{m_2}{m_1 + m_2} \mathbf{r}$$

$$\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}$$

$$\mathbf{r}_2 = \mathbf{R} - \frac{m_1}{m_1 + m_2} \mathbf{r}$$



$$M \ddot{\mathbf{R}} = \ddot{\mathbf{F}}_{1\text{ext}} + \ddot{\mathbf{F}}_{2\text{ext}}$$

and get the new equations of motion

$$\mu \ddot{\mathbf{r}} = - \nabla U(r) = - \hat{\mathbf{r}} \frac{dU}{dr}$$

(1)

where  $M = m_1 + m_2$  and  $\mu = \frac{m_1 m_2}{m_1 + m_2}$  [The second of eqs. (1) has been simplified so that it only applies for special external forces, such as gravitational. In most cases of interest, the external forces are negligible].

To find the relative motion, we have only to solve the problem of a single particle of mass  $\mu$  (the reduced mass) in the central potential  $U(\mathbf{r})$ .

It is easy to show from equations (1) that

$$\frac{d}{dt}(\vec{\mathbf{r}} \times \mu \dot{\vec{\mathbf{r}}}) = \dot{\vec{\mathbf{r}}} \times \mu \dot{\vec{\mathbf{r}}} + \vec{\mathbf{r}} \times \mu \ddot{\vec{\mathbf{r}}} = 0$$

Therefore the quantity  $\vec{\mathbf{L}} = \vec{\mathbf{r}} \times \mu \dot{\vec{\mathbf{r}}}$  is a constant of the motion. It is called the angular momentum in the center of mass frame.

A great advantage of the vector notation used above is that it is valid for all coordinate systems. Here it is convenient to use spherical coordinates  $r, \theta, \varphi$  which are related to the familiar Cartesian coordinates  $x, y, z$  by

$$x = r \sin \theta \cos \varphi$$

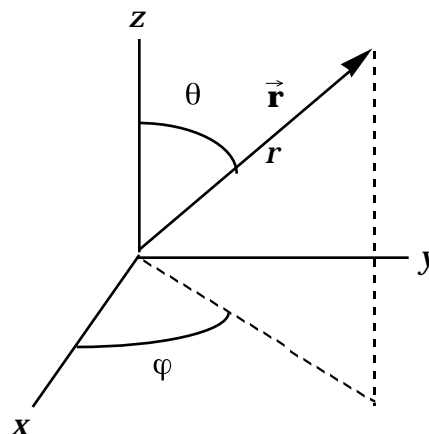
$$y = r \sin \theta \sin \varphi$$

$$z = r \cos \theta$$

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$\theta = \arccos [z/r] = \arctan [(x^2 + y^2)^{1/2}/z]$$

$$\varphi = \arctan (y/x)$$



This is the notation universally used in physics and chemistry. I am extremely sorry that math books use a different notation with  $\theta$  and  $\varphi$  interchanged.

In this coordinate system we find that

$$p_r = \mu \dot{r} \quad p_\theta = \mu r \dot{\theta} \quad p_\varphi = \mu r \sin \theta \dot{\varphi}$$

$$L_r = 0 \quad L_\theta = -r p_\varphi = -\mu r^2 \sin \theta \dot{\varphi} \quad L_\varphi = r p_\theta = \mu r^2 \dot{\theta}$$

Combining these yields  $p^2 = p_r^2 + \frac{L^2}{r^2}$

Thus the kinetic energy can be written

$$K = \frac{p^2}{2\mu} = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} \quad (2)$$

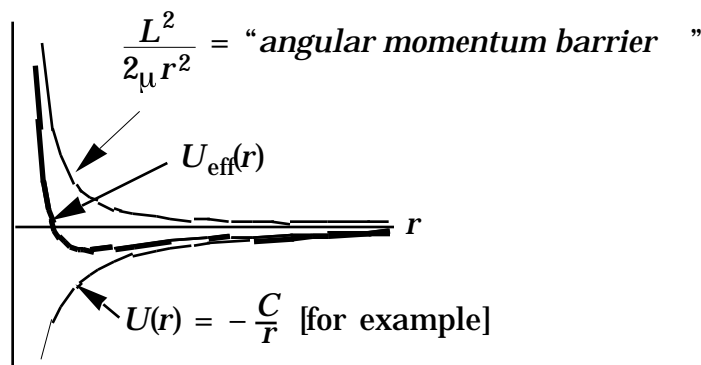
where the last form is particularly useful because  $L^2$  is a constant of the motion. In fact, the total energy  $E$  and the angular momentum  $\vec{\mathbf{L}}$  are the two most useful constants of the motion for the particle in a central potential.

The classical conservation of energy equation can now be written

$$\frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} + U(r) = E = \text{constant.}$$

Often the angular momentum term, really a part of the kinetic energy, is included with the potential energy to form a new “effective potential”.

$$U_{\text{eff}}(r) = U(r) + \frac{L^2}{2\mu r^2} \quad \frac{p_r^2}{2\mu} + U_{\text{eff}}(r) = E \quad (3)$$



Thus we have reduced the problem of two particles interacting with a central potential to a one-dimensional problem with a single fictitious particle moving in an effective potential. We could stay with classical mechanics and solve the problem with the potential  $U(r) = -C/r$  and obtain the Kepler laws, but we must leave some things for Physics 320. The reason we have gone this far is that nearly all of this carries over into quantum mechanics.

The generalization of the Schrödinger equation to 3 dimensions is easy. In one dimension we replaced the  $x$ -component of momentum by the operator

$$p_{x, \text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

and similarly for other variables, substituted into the conservation of energy equation and “operated” on the wave function  $\Psi(x, t)$ . Now we do the obvious things for  $p_y$

and  $p_z$  to get  $\vec{p}_{\text{op}} = \frac{\hbar}{i} \vec{\nabla}$ .

where the **gradient**, or **del** operator  $\vec{\nabla}$  has components  $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$  in rectangular coordinates. In vector notation, valid for any coordinate system, the Schrödinger equation becomes

$$\boxed{-\frac{\hbar^2}{2\mu} \nabla^2 \Psi(\vec{r}, t) + U(\vec{r}, t) \Psi(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t)}$$

**Time-dependent Schrödinger equation**

Whenever the potential energy is independent of time, the usual separation of variables leads at once to  $\Psi(\vec{r}, t) = \psi(\vec{r}) e^{-iEt/\hbar}$  where  $\psi(\vec{r})$  is the solution to

$$\boxed{-\frac{\hbar^2}{2\mu} \nabla^2 \psi(\vec{r}) + U(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})}$$

**Time-independent Schrödinger equation**

We see that the kinetic energy term contains the Laplacian operator  $\nabla^2$ . In

rectangular coordinates this is simply  $\nabla^2\psi = \frac{\partial^2}{\partial x^2}\psi + \frac{\partial^2}{\partial y^2}\psi + \frac{\partial^2}{\partial z^2}\psi$

and problems involving rectangular symmetry can be solved in the usual way.

To deal with central potentials it is more convenient to use spherical coordinates.

Then the Laplacian operator becomes

$$\nabla^2\psi = \left[ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right) \right] \psi$$

Note that 
$$\hat{p}_{\text{op}}^2 = \left( \frac{\hbar \vec{\nabla}}{i} \right) \left( \frac{\hbar \vec{\nabla}}{i} \right) = -\hbar^2 \nabla^2 = \hat{p}_{r\text{op}}^2 + \frac{L_{\text{op}}^2}{r^2} \quad K_{\text{op}} = \frac{p_{\text{op}}^2}{2\mu} = \frac{p_{r\text{op}}^2}{2\mu} + \frac{L_{\text{op}}^2}{2\mu r^2}$$

where  $\vec{L}_{\text{op}} = \vec{r} \times \vec{p}_{\text{op}} = \vec{r} \times \frac{\hbar \vec{\nabla}}{i}$  is the angular momentum operator.

There is a very strong resemblance to the classical equations (2). It is not surprising that angular momentum is conserved in both classical and quantum mechanics. The conservation laws for energy, linear momentum, and angular momentum represent deep symmetries in nature.

Our final form for the Schrödinger equation for a particle in a central potential is

$$-\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \psi(r, \theta, \varphi) + \frac{L_{\text{op}}^2}{2\mu r^2} \psi(r, \theta, \varphi) + U(r) \psi(r, \theta, \varphi) = E \psi(r, \theta, \varphi)$$

To solve this formidable-looking partial differential equation, it is possible to separate the variables. The solutions are well known. There is a set of functions called the spherical harmonics  $Y_{lm}(\theta, \varphi)$  which have the properties

$$L_{\text{op}}^2 Y_{lm}(\theta, \varphi) = l(l+1) \hbar^2 Y_{lm}(\theta, \varphi) \quad \text{and} \quad L_{z\text{op}} Y_{lm}(\theta, \varphi) = m \hbar Y_{lm}(\theta, \varphi)$$

where  $l$  can take on the values  $0, 1, 2, 3, \dots$  and for a given  $l$ ,  $m$  can take on the values  $-l, -l+1, \dots, l$ .

Thus if we let  $\psi(r, \theta, \varphi) = R_l(r) Y_{lm}(\theta, \varphi)$

$$-\frac{\hbar^2}{2\mu} \left[ \frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{dR_l}{dr} - \frac{l(l+1)}{r^2} R_l \right] + U(r) R_l = E R_l(r)$$

or 
$$-\frac{\hbar^2}{2\mu} \left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right] R_l(r) + \left[ U(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R_l(r) = E R_l(r) \quad (4)$$

There is one more simplification possible:

Let  $R_l(r) = \frac{u_l(r)}{r}$  [which requires  $u_l(0) = 0$ ] and

$$-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} u_l(r) + U_{\text{eff}}(r)u_l(r) = Eu_l(r) \quad \text{where } U_{\text{eff}}(r) = U(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad (5)$$

Note how similar this is to equation (3).

It is conventional to choose the arbitrary additive constant in  $U(r)$  so that  $U(r) \rightarrow 0$  as  $r \rightarrow \infty$ . Then free states are states of positive energy and bound states are states of negative energy. This convention is not possible if  $U(r)$  as  $r \rightarrow \infty$ , as is the case for the harmonic oscillator potential.

In any case, the requirements on the behavior of the wave function at the boundaries as  $r$  approaches zero and infinity will impose quantization on bound states. The bound state solutions of eq. (4) or (5) may be labeled by a **radial quantum no.**  $n_r$ .

We may choose to let  $n_r$  be the number of nodes in  $R_l(r)$ . Then, for each  $l$  we have  $n_r = 0, 1, 2, 3, \dots$ . The energy levels depend on the two quantum nos.,  $n_r$  and  $l$ . Since the quantum no.  $m$  may take any value from  $-l$  to  $l$  in steps of unity, there are  $2l + 1$  states at each energy level  $E_{n_r, l}$ . Thus we say that each energy level is  $(2l + 1)$ -fold **degenerate**.

All of the above assumes only that the potential is a central one. For a few special (but common) potentials there is additional degeneracy. In the case of the Coulomb potential  $U(r) = -\frac{\text{Const}}{r}$ , it is found that the energy levels depend only on the combination  $(n_r + l + 1)$ :

$$E_{n_r, l} = -\frac{\text{constant}}{(n_r + l + 1)^2}$$

Then it is possible to define a **principal quantum number**

$$n = n_r + l + 1 \quad (6)$$

and to write  $E_n = -\frac{\text{constant}}{n^2}$ . From the definition, eq. (6), we see that  $n = l + 1$  or

$l = n - 1$ . The degeneracy of each energy level  $n$  is

$$g_n = \sum_{l=0}^{n-1} \sum_{m=-l}^l 1 = \sum_{l=0}^{n-1} (2l + 1) = n^2$$

[This must be multiplied by two for particles of spin 1/2, such as electrons or neutrons.]