

## Lecture 10

# Central potential

## 10.1 Introduction

We are now ready to study a generic class of three-dimensional physical systems. They are the systems that have a central potential, i.e. a potential energy that depends only on the distance  $r$  from the origin:  $V(\underline{r}) = V(r)$ . If we use spherical coordinates to parametrize our three-dimensional space, a central potential does *not* depend on the angular variables  $\theta$  and  $\phi$ .

An example of central potential is the Coulomb potential between electrically charged particles:

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}. \quad (10.1)$$

## 10.2 Stationary states.

As usual, the dynamics of the system is encoded in the solutions of the time-independent Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] u(\underline{r}) = Eu(\underline{r}). \quad (10.2)$$

We have denoted the mass of the particle by  $\mu$  in order to avoid confusion with the magnetic quantum number  $m$ , which will appear in the solutions below.

It is clearly convenient to use spherical coordinates, and write the Laplacian as:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}. \quad (10.3)$$

The key observation to solve the eigensystem in Eq. (10.2) is that we can use Eq. (8.19) and rewrite the Laplacian as:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} \hat{L}^2, \quad (10.4)$$

and thus the eigenvalue equation becomes:

$$\frac{\hbar^2}{2\mu} \left[ -\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{\hbar^2 r^2} \hat{L}^2 \right] u(r, \theta, \phi) = (E - V(r)) u(r, \theta, \phi). \quad (10.5)$$

**Separation of variables.** We have already seen that the eigenfunctions of the operator  $\hat{L}^2$  are the spherical harmonics  $Y_l^m(\theta, \phi)$ . Therefore it makes sense to look for a solution of the time-independent Schrödinger equation by separating the solution into:

$$u(r, \theta, \phi) = R(r) Y_l^m(\theta, \phi). \quad (10.6)$$

We have written the general solution  $u(\underline{r})$  as the product of a radial function  $R(r)$ , which depends only on the radius  $r$ , times the spherical harmonics. The latter encode all the angular dependence of the solutions  $u(\underline{r})$ .

Using Eq. (8.21), we can rewrite Eq. (10.5) as an ordinary differential equation for the function  $R(r)$ :

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{\ell(\ell+1)}{r^2} R + \frac{2\mu}{\hbar^2} [E - V(r)] R = 0. \quad (10.7)$$

Note that the magnetic quantum number  $m$  does not enter in the equation for the radial wave function  $R$ . Hence each energy level will have a  $(2\ell+1)$ -fold degeneracy.

**Equation for the radial wave function.** Let us now discuss the solution for the radial part of the equation. The radial equation is simplified by the substitution:

$$R(r) = \frac{\chi(r)}{r}; \quad (10.8)$$

inserting Eq. (10.8) into Eq. (10.7) yields:

$$\frac{d^2 \chi}{dr^2} + \left[ \frac{2\mu}{\hbar^2} (E - V(r)) - \frac{\ell(\ell+1)}{r^2} \right] \chi(r) = 0. \quad (10.9)$$

We have obtained a one-dimensional eigenvalue problem: Eq. (10.9) is the time-independent Schrödinger equation for a one-dimensional system in the potential:

$$V_l(r) = V(r) + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2}. \quad (10.10)$$

This is simply the sum of the three-dimensional potential  $V(r)$  and a “centrifugal” term:

$$\frac{1}{2\mu} \frac{\hat{L}^2}{r^2}. \quad (10.11)$$

**Boundary condition for the radial wave function.** We know that the solution of the Schrödinger equation  $\psi$  must be finite. Therefore the radial part  $R(r)$  has to be finite everywhere including the origin. For this to happen we need

$$\chi(0) = 0. \quad (10.12)$$

Actually this condition turns out to be true also for a potential energy that diverges as  $r \rightarrow 0$ .

Hence the motion of a quantum system in a central potential can be reduced to a motion of a one-dimensional system in the region  $r > 0$  - remember that  $r$  is the radial coordinate and hence is always positive.

The normalization condition for the radial wave function is:

$$\int_0^\infty |R(r)|^2 r^2 dr = \int_0^\infty |\chi(r)|^2 dr = 1. \quad (10.13)$$

### 10.3 Physical interpretation.

The solution of the one-dimensional problem in Eq. (10.9) is entirely determined by the value of the energy  $E$ . Given that the angular part is given by the spherical harmonics  $Y_\ell^m$ , we obtain that the three-dimensional wave function is entirely determined by the values of  $E, \ell, m$ .

The eigenstates can be written as:

$$u_{n\ell m}(r) = R_{n\ell}(r)Y_\ell^m(\theta, \phi), \quad (10.14)$$

where  $n$  indicates the allowed values of the energy  $E$  as usual. As already noted above, the magnetic quantum number does not enter in the radial equation, and therefore the solution  $R_{n\ell}(r)$  only depends on the two indices  $n$  and  $\ell$ .

Let us discuss the behaviour of the solution  $R$  near the origin for a potential such that:

$$\lim_{r \rightarrow 0} (V(r)r^2) = 0, \quad (10.15)$$

i.e. for a potential that diverges in the origin *at most* as  $1/r^2$ . We shall look for a solution of the form:

$$R(r) = \text{const} \cdot r^s. \quad (10.16)$$

Substituting Eq. (10.16) into Eq. (10.7), and neglecting terms that vanish in the limit  $r \rightarrow 0$ , we find:

$$s(s+1) = \ell(\ell+1). \quad (10.17)$$

The latter has two solutions for  $s$ :

$$s = \ell, \quad \text{or} \quad s = -(\ell+1). \quad (10.18)$$

Clearly the solution with  $s = -(\ell+1)$  is divergent at the origin  $r = 0$  and therefore does not satisfy the boundary condition for the radial wave function. Hence, close to the origin, the solutions with angular momentum  $\ell$  are proportional to  $r^\ell$ .

The probability density for a particle to be at a distance  $r$  from the origin is given by:

$$|R|^2 r^2 \simeq r^{2(\ell+1)}. \quad (10.19)$$

The larger the angular momentum, the more rapidly the probability goes to zero at  $r = 0$ .

### 10.4 Quantum rotator

Let us conclude this lecture with a simple example of physical relevance: the quantum rotator. The quantum rotator is a quantum system made of two particles of mass  $m_1$  and  $m_2$  separated

by a fixed distance  $r_e$ . It is a simple but effective description of the rotational degrees of freedom of a diatomic molecule. By solving the time-independent Schrödinger equation we are going to find the rotational energy levels, i.e. the energy levels of the molecule in the limit where we neglect the vibrational energy.

Let us choose the centre-of-mass of the molecule as the origin of the reference frame. The state of the system is completely specified by two angles  $\theta$  and  $\phi$  that specify the orientation of the axis of the molecule with respect to the axis of the reference frame, as illustrated in Fig. 10.1.

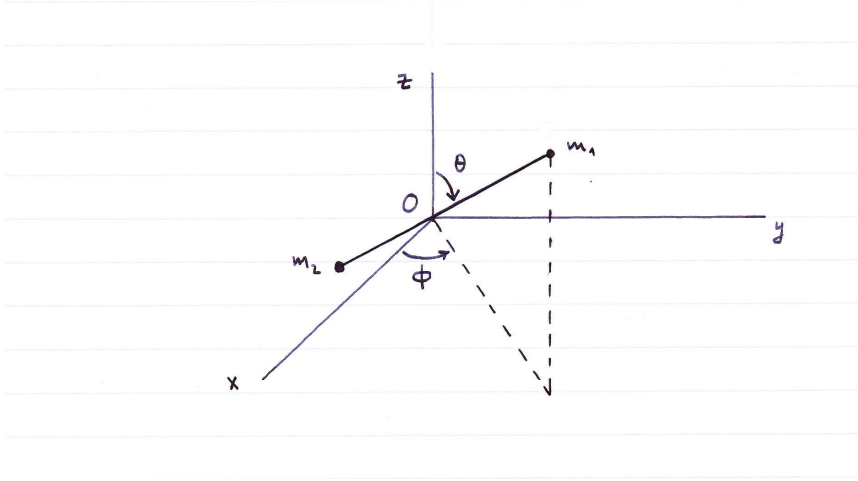


Figure 10.1: Rotator in three-dimensional space. The length of the axis between the two atoms is fixed to be  $r_e$ . The origin of the reference frame is chosen to coincide with the centre-of-mass of the system, denoted by  $O$  in the figure. The direction of the axis of the rotator is completely specified by the two angles  $\theta$  and  $\phi$ .

The distance from the origin to the first mass is denoted by  $r_1$ , and similarly the distance from the origin to the second mass is  $r_2$ . Since we are neglecting the vibrational degrees of freedom both  $r_1$  and  $r_2$  are constant, and clearly  $r_1 + r_2 = r_e$ . Since we have chosen the origin of the reference frame to be the centre-of mass of the system we also have:

$$m_1 r_1 = m_2 r_2, \quad (10.20)$$

and therefore:

$$r_1/m_2 = r_2/m_1 = r_e/(m_1 + m_2). \quad (10.21)$$

The moment of inertia of this system is simply:

$$I = m_1 r_1^2 + m_2 r_2^2 \equiv \mu r_e^2, \quad (10.22)$$

where we have introduced the reduced mass:

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}. \quad (10.23)$$

In classical mechanics the angular momentum of the system is given by:

$$|\underline{L}| = I\omega_R, \quad (10.24)$$

where  $\omega_R$  is the angular velocity of the system. The energy can be expressed as:

$$H = \frac{1}{2}I\omega_R^2 = \frac{L^2}{2I} = \frac{L^2}{2\mu r_e^2}. \quad (10.25)$$

Eq. (10.25) is the starting point to define the Hamiltonian for the quantum rotator. According to the general principles defined at the beginning of the course, we define the Hamiltonian operator as:

$$\hat{H} = \frac{\hat{L}^2}{2\mu r_e^2}, \quad (10.26)$$

where  $\hat{L}^2$  is the operator associated to the square of the angular momentum - see Eq. (8.19). The reduced mass  $\mu$  and the radius of the molecule  $r_e$  are constants that define the physical system under study: different diatomic molecules have different reduced masses, or sizes.

Note that the wave function of the system does not depend on  $r$  since we are neglecting the vibrations of the molecule. So the state of the quantum system is described by a wave function  $\psi(\theta, \phi)$  that depends only on the angular variables.

The Hamiltonian for the diatomic molecule is proportional to  $\hat{L}^2$ ; we have already computed the eigenvalues and the eigenfunctions of  $\hat{L}^2$  when we discussed the angular momentum. The stationary states are:

$$\hat{H}Y_\ell^m(\theta, \phi) = \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}Y_\ell^m(\theta, \phi). \quad (10.27)$$

The constant  $B = \hbar/(4\pi\mu r_e^2)$  is usually called the “rotational constant”. It has the dimensions of a frequency (**check this!**). The energy levels are therefore:

$$E_\ell = Bh\ell(\ell+1). \quad (10.28)$$

More details about the quantum rotator can be found in problem sheet 5. We shall see that this rather simple model allows us to make physical predictions about the behaviour of diatomic molecules.

## 10.5 Summary

As usual, we summarize the main concepts introduced in this lecture.

- Time-independent equation for a system in a central potential.
- Separation of variables.
- Reduction to a one-dimensional problem, effective potential, boundary condition.
- Solutions for the stationary states and their generic properties.
- Quantum rotator.

