Lecture 6

More potentials

6.1 Introduction

Finally, in this lecture we are going to discuss potential wells. We are going to review briefly the infinite potential well, and then the finite one.

In the examples that we have seen in the previous lecture, the energy could take any value from zero to infinity - these are examples of *continuous spectra*. In the case of potential wells, we will find, in addition, bound states with only discrete values of the energy - i.e. states that are labelled by an integer.

6.2 Infinite potential well

This is a simple problem, that we have already seen in problem sheet 2. Let us review its solution, breaking it down into logical steps.

Physical setting The system we consider here is a single particle that evolves in the potential

$$V(x) = \begin{cases} 0, & \text{for } -\frac{a}{2} < x < \frac{a}{2}\,, \\ \infty, & \text{otherwise}\,. \end{cases} \tag{6.1}$$

The potential is sketched in Fig. 6.1. Note that the infinite potential well is completely specified by its width a. Therefore we expect the physics of this system to depend on a, and on the particle mass m.

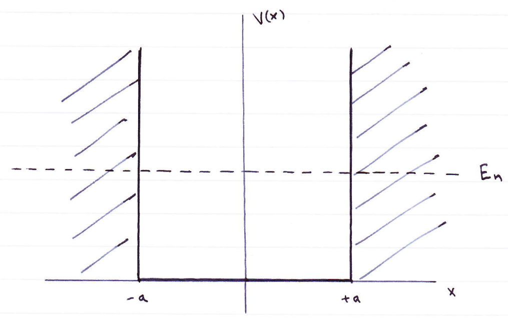

Figure 6.1: Infinite well potential.

As discussed in the previous lecture, if the walls were of finite height $V > E$, the wave function outside the wall would be of the form $e^{-\tilde{p}|x|/\hbar}$, and we would need to impose continuity at the boundary. We will consider this case in the next section. As the height of the potential barrier tends to infinity, we have that $\tilde{p} \to \infty$, and hence the wave function outside the potential $e^{-\tilde{p}|x|/\hbar} \to 0$. In other words we expect the wave function to vanish outside the potential well, thereby implying that the probability of finding the particle outside the well is exactly zero: the particle is confined inside the container.

We want to find the stationary states of this system, i.e. we want to solve the time-independent Schrödinger equation.

Eigenvalue equation In order to find the stationary states we need to solve the eigenvalue problem for the Hamiltonian, which turns the physical problem above into a well-defined mathematical problem. We need to find the solutions of the free particle equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)\,, \tag{6.2}$$

with the boundary conditions:

$$\psi(a/2) = \psi(-a/2) = 0\,. \tag{6.3}$$

All the information about the system is encoded in Eqs. (6.2), (6.3). In order to extract this information we need to solve the equation.

Solution of the eigenvalue problem Setting $k = \sqrt{\frac{2mE}{\hbar^2}}$, Eq. (6.2) becomes the familar equation:

$$\psi''(x) = -k^2\psi(x)\,. \tag{6.4}$$

The generic solution is a linear superposition of plane waves:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}\,. \tag{6.5}$$

So far, the solution of the eigenvalue problem looks very similar to the solutions we discussed for the potential barriers in the previous lecture. The peculiar features of the infinite well are encoded in the boundary conditions specified in Eq. (6.3). The latter can be written as:

$$\psi(a/2) = Ae^{ika/2} + Be^{-ika/2} = 0\,, \tag{6.6}$$

$$\psi(-a/2) = Ae^{-ika/2} + Be^{ika/2} = 0\,, \tag{6.7}$$

Eq. (6.6) yields

$$A = -Be^{-ika}\,.$$

Replacing this result in Eq. (6.7) we obtain:

$$\sin(ka) = 0\,, \tag{6.8}$$

where we see that the boundary conditions actually restrict the possible values of k, and hence of the possible energy values. In order to satisfy Eq. (6.8), we need:

$$ka = n\pi, \qquad n \text{ integer}\,. \tag{6.9}$$

Hence, finally, the solutions of the time-independent Schrödinger equation in the infinite well are:

$$u_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), & n \text{ even}\,, \\ \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right), & n \text{ odd}\,, \end{cases} \tag{6.10}$$

where n is an integer from 1 to ∞. We see from the explicit expression of the solutions that $n = 0$ is excluded because the wave function would vanish identically.

Physical interpretation We can now look at our solutions and discuss the physical properties that are embodied in the mathematical expressions.

The values of the energy are:

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2ma^2}, \qquad n = 1, 2, \ldots\,. \tag{6.11}$$

Solutions are labelled by an integer: this is an example of a discrete spectrum.

Note that the eigenfunctions u_n are also eigenstates of the momentum operator, the values of the momentum are:

$$p_n = n\frac{\pi\hbar}{a}\,. \tag{6.12}$$

Note that the lowest value of the energy is greater than zero. This is a consequence of the uncertainty principle. The particle is confined inside a box of size a. Hence the maximum uncertainty in the determination of its position is a, which implies that the minimum uncertainty in the value of the momentum is $\Delta p \geq 2\pi\hbar/a$. As a consequence the particle has a kinetic energy

$$E \sim (\Delta p)^2/(2m)\,. \tag{6.13}$$

The kinetic energy that stems from the uncertainty principle is called *zero point energy*. A striking manifestation is the existence of liquid Helium all the way down to $T = 0$. In order to have solid Helium, we need to localize the particles in a lattice. This localization entails a zero point energy, which becomes large for light particles, as shown by Eq. (6.13). In the case of Helium the zero point energy is so large that the interatomic forces can no longer constrain the particles in a lattice, and the system remains in a liquid state.

6.3 Parity

By inspecting the energy eigenstates in Eq. (6.10) we see that

$$u_n(-x) = u_n(x), \quad n \text{ odd}, \tag{6.14}$$
$$u_n(-x) = -u_n(x), \quad n \text{ even}. \tag{6.15}$$
$$\tag{6.16}$$

Under the parity operations defined in Eq. (3.30) the eigenfunctions $u_n(x)$ are multiplied by a constant $(-1)^{n+1}$, i.e. they are eigenstate of the parity operator $\mathcal{P}$, with eigenvalue $(-1)^{n+1}$. The eigenvalue is called the parity of the state. States with parity $(+1)$ are called *even*, states with parity (-1) are called *odd*.

For a potential that is symmetric under parity, you can readily prove that:

$$\hat{\mathcal{P}}\hat{H}\psi(x) = \hat{H}\hat{\mathcal{P}}\psi\,, \tag{6.17}$$

for any wave function ψ, which is the same as saying that $\left[\hat{\mathcal{P}}, \hat{H}\right] = 0$.

As a consequence of the commutation relation, for each eigenstate of the Hamiltonian u_n, we can construct another eigenstate of $\hat{H}$ with the *same* eigenvalue by acting with $\hat{\mathcal{P}}$ on it:

$$\begin{aligned}\hat{H}\hat{\mathcal{P}}u_n(x) &= \hat{\mathcal{P}}\hat{H}u_n(x) \\ &= \hat{\mathcal{P}}\left(E_n u_n(x)\right) \\ &= E_n \hat{\mathcal{P}}u_n(x)\,.\end{aligned} \tag{6.18}$$

We can then construct the states

$$\left(1 \pm \hat{\mathcal{P}}\right) u_n(x)\,, \tag{6.19}$$

which are simultaneous eigenstates of $\hat{H}$ and $\hat{\mathcal{P}}$. Notice that the result above does not necessarily imply that the energy levels are doubly-degenerate, since one of the linear combinations defined in Eq. (6.19) could vanish. The main result to remember here is the following.

> If the Hamiltonian is symmetric under parity, i.e. if $[\hat{\mathcal{P}}, \hat{H}] = 0$, then there exists a set of eigenfunctions of $\hat{H}$ that are also eigenstates of $\hat{\mathcal{P}}$. Or, equivalently, we can find a complete basis of eigenstates of $\hat{H}$ made of either even or odd functions of the position x.

6.4 Finite potential well

The final example that we are going to discuss is the finite potential well, which corresponds to the potential:

$$V(x) = \begin{cases} -V_0, & \text{for } |x| < a/2\,, \\ 0, & \text{otherwise}\,. \end{cases} \tag{6.20}$$

Once again we have a potential that is symmetric under parity, $V(-x) = V(x)$. Therefore we can choose to look for solutions of the energy eigenvalue equation that are also parity eigenstates.

As discussed previously, energy eigenvalues must be larger than $-V_0$. This means that we can have states with $-V_0 < E < 0$; they are called *bound states*: the wave function for these states decays exponentially at large $|x|$, so that the probability of finding the particle outside the well becomes rapidly very small. On the other hand, states with $E > 0$ correspond to incident plane waves that are distorted by the potential. We will concentrate on the bound states here.

The Schrödinger equation reads:

$$\psi'' = \begin{cases} -\frac{2m}{\hbar^2} E\psi \\ -\frac{2m}{\hbar^2}(E + V_0)\psi \, . \end{cases} \tag{6.21}$$

The main difference between the infinite and the finite well comes from the fact that the wave function does not have to vanish outside the classically allowed region $|x| < a/2$. As we discussed before, the wave function for $|x| > a/2$ will decay exponentially.

For $-V_0 < E < 0$, the even parity solutions are of the form:

$$\psi(x) = \begin{cases} A\cos(px/\hbar), & |x| < a/2 \\ Ce^{-\bar{p}x/\hbar}, & x > a/2 \\ Ce^{\bar{p}x/\hbar}, & x < -a/2 \, , \end{cases} \tag{6.22}$$

while the odd parity solutions are:

$$\psi(x) = \begin{cases} A\sin(px/\hbar), & |x| < a/2 \\ Ce^{-\bar{p}x/\hbar}, & x > a/2 \\ -Ce^{\bar{p}x/\hbar}, & x < -a/2 \, . \end{cases} \tag{6.23}$$

As usual we have introduced the momenta:

$$p = \sqrt{2m(E + V_0)} \, , \qquad \bar{p} = \sqrt{-2mE} \, . \tag{6.24}$$

(Remember that we are looking for bound states, and hence $E < 0$.)

Once again the values of E cannot be arbitrary, they are determined when we impose the continuity condition. Imposing continuity of the wave function and its derivative in the even parity sector, we obtain:

$$\begin{aligned} A\cos\left(\frac{pa}{2\hbar}\right) &= Ce^{-\bar{p}a/(2\hbar)} \, , \\ -\frac{p}{\hbar} A\sin\left(\frac{pa}{2\hbar}\right) &= -\frac{\bar{p}}{\hbar} Ce^{-\bar{p}a/(2\hbar)} \, . \end{aligned}$$

Dividing the bottom equation by the top one, we obtain the quantization condition for the energy levels:

$$p \tan\left(\frac{pa}{2\hbar}\right) = \bar{p}\,. \tag{6.25}$$

Similarly in the odd parity sector we obtain:

$$p \cot\left(\frac{pa}{2\hbar}\right) = -\bar{p}\,. \tag{6.26}$$

The graphical solution of these equations is discussed in problem sheet 3.

The main physical features of this system is that there is always at least one even bound state. For very small V_0, i.e. for a shallow well, you can show that

$$E = -\frac{mV_0^2 a^2}{2\hbar^2}\,. \tag{6.27}$$

6.5 Summary

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

- Detailed solution of the infinite potential well.
- Logical steps, mathematical tools, interpretation.
- Zero point energy.
- Potentials symmetric under parity.
- Using parity to solve the finite potential well.