

0.1 Examples of the Stationary Schrödinger Equation

We now want to solve the Schrödinger equation

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + E_{\text{pot}}\psi = E\psi$$

for a few simple, one-dimensional problems. These examples will illustrate the description of classical particles as waves and the following physical consequences.

0.1.1 The Free Particle

A particle is said to be free, if it is moving in a constant potential ϕ_0 , because then $\mathbf{F} = -\nabla E_{\text{pot}}$ means that no forces are acting on the particle. Through a suitable choice of the zero point energy we can set $\phi_0 = 0$, i.e. $E_{\text{pot}} = 0$, and thus get the Schrödinger equation for a free particle

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad (1)$$

The total energy $E = E_{\text{kin}} + E_{\text{pot}}$ is because of E_{pot} now

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Thus (1) gets reduced to

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

which has the general solution

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (2)$$

The time-dependent wave function

$$\psi(x, t) = \psi(x) \cdot e^{-i\omega t} = Ae^{i(kx - \omega t)} + Be^{-i(kx + \omega t)} \quad (3)$$

represents the superposition of a planar wave travelling in the $+x$ and $-x$ direction.

The coefficients A and B are the amplitudes of those waves, which are determined by the boundary conditions. For example, the wave function of electrons which are emitted from a cathode in $+x$ direction towards a detector, will have $B = 0$, since there are no particles moving in $-x$. From this experimental setup we know that the electrons are found along the length L of the path between cathode and detector. This means their wave function can only be different from zero in this region of space. Using the normalization condition we get

$$\int_0^L |\psi(x)|^2 dx = 1 \\ \implies A^2 \cdot L = 1 \implies A = \frac{1}{\sqrt{L}}$$

To determine the location of a particle at time t more accurately, we will have to construct *wave packets* in place of planar waves (2)

$$\psi(x, t) = \int_{k_0 - \Delta k/2}^{k_0 + \Delta k/2} A(k) e^{i(kx - \omega t)} dk \quad (4)$$

The location uncertainty of this packet at $t = 0$ is

$$\Delta x \geq \frac{\hbar}{2\Delta p_x} = \frac{1}{2\Delta k}$$

and depends on the pulse width $\Delta p_x = \hbar\Delta k$. The larger k is, the more certainly $\Delta x(t = 0)$ can be determined, but the faster the wave packet spreads.

Experimentally, this can be illustrated as follows: If we apply a short voltage pulse to the cathode at time $t = 0$, then electrons can start travelling towards the detector at this instance. The emitted electrons have a velocity distribution Δv , such that electrons with differing velocities v will not necessarily be in the same location x at a later point in time t . Instead they are spread over the interval $\Delta x(t) = t \cdot \Delta v$. The velocity distribution is described by $\Delta v \propto \Delta k$ of the wave packet, such that the location uncertainty Δx

$$\frac{d(\Delta x(t))}{dt} = \Delta v(t = 0) = \frac{\hbar}{m} \Delta k(t = 0)$$

changes proportionally to the initial impulse uncertainty.

0.1.2 Potential Step

We are still considering particles like in the previous example, however we introduce a potential step at $x = 0$. This means we are considering the potential

$$\phi(x) = \begin{cases} 0, & x < 0 \\ \phi_0 & x \geq 0 \end{cases}$$