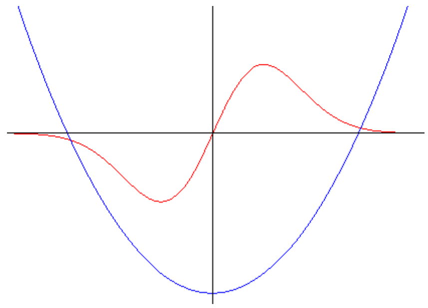
Modern Physics

Schrödinger's equation

Problem 1.- Consider the wavefunction for a simple harmonic oscillator:
$\psi = Axe^{-m\omega x^2/2\hbar}$



Substitute it in the Schrödinger equation (given below) and calculate the energy.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

Solution: The derivatives are:

$$\frac{d\psi}{dx} = Ae^{-m\omega x^2/2\hbar} - Am\omega x^2/\hbar e^{-m\omega x^2/2\hbar}$$

$$\frac{d^2\psi}{dx^2} = -Am\omega x/\hbar e^{-m\omega x^2/2\hbar} - 2Am\omega x/\hbar e^{-m\omega x^2/2\hbar} + Am^2\omega^2 x^3/\hbar^2 e^{-m\omega x^2/2\hbar}$$

$$\frac{d^2\psi}{dx^2} = \frac{Am\omega x}{\hbar}\left(-3 + mx^2\omega/\hbar\right)e^{-m\omega x^2/2\hbar}$$

Substituting in the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{Am\omega x}{\hbar}\left(-3 + mx^2\omega/\hbar\right)e^{-m\omega x^2/2\hbar} + \frac{1}{2}m\omega^2 x^2 Axe^{-m\omega x^2/2\hbar} = EAxe^{-m\omega x^2/2\hbar}$$

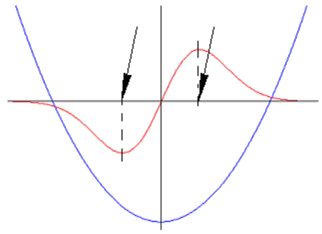
Simplifying:

$$\frac{3\hbar^2}{2m}\frac{m\omega}{\hbar} - \frac{\hbar^2}{2m}\frac{m\omega^2}{\hbar}\left(mx^2/\hbar\right) + \frac{1}{2}m\omega^2 x^2 = E$$

$$\frac{3\hbar}{2}\frac{\omega}{1} - \frac{\hbar}{2}\frac{\omega^2}{1}\left(mx^2/\hbar\right) + \frac{1}{2}m\omega^2 x^2 = E \rightarrow E = \frac{3}{2}\hbar\omega$$

Problem 1a.- The wavefunction $\psi_1 = Axe^{-\alpha x^2/2}$ satisfies the Schrödinger equation (independent of time) for a particle in the potential of a simple harmonic oscillator. The wavefunction and the potential are shown schematically in the figure. Indicate the position(s) where you have the maximum probability of finding the particle.

Solution:



Problem 2.- The wavefunction of the only electron of hydrogen in the first excited state and with quantum numbers $l = 0$ and $m_l = 0$ is given (in spherical coordinates) by the formula:

$\psi = \frac{1}{4\sqrt{2\pi}a^{3/2}}\left[2 - \frac{r}{a}\right]e^{-r/2a}$, where "a" is the Bohr radius

Find the places where the probability of finding the electron is zero.

Solution: The probability of finding a particle is proportional to the wavefunction squared:

$$P \;\alpha\; |\psi|^2 = \frac{1}{32\pi a^3}\left[2 - \frac{r}{a}\right]^2 e^{-r/a}$$

We notice that this probability is zero when $r=2a$ and when $r \to \infty$

Problem 3.- The wavefunction of a free electron (free means V=0) is given by:

$$\Psi(x) = Ce^{-i2\pi x/1.5nm}$$

Calculate its kinetic energy.

Solution: Replacing this wavefunction in Schrödinger's equation we get:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \to -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(Ce^{-i2\pi x/1.5nm}\right) + V(x)\left(Ce^{-i2\pi x/1.5nm}\right) = E\left(Ce^{-i2\pi x/1.5nm}\right)$$

But the particle is free, so the potential is zero: $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(Ce^{-i2\pi x/1.5nm}\right) = E\left(Ce^{-i2\pi x/1.5nm}\right)$, which means that:

$$E = \frac{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(Ce^{-i2\pi x/1.5nm}\right)}{\left(Ce^{-i2\pi x/1.5nm}\right)} = -\frac{\hbar^2}{2m}\left(\frac{-i2\pi}{1.5nm}\right)^2 = \frac{4\pi^2\hbar^2}{2m(1.5nm)^2}$$

With the values of mass and Planck's constant, we get:

$$E = \frac{(6.62\times10^{-34}\,Js)^2}{2(9.1\times10^{-31}\,kg)(1.5\times10^{-9}\,m)^2} = \mathbf{1.07 \times 10^{-19}\ J}$$

Problem 3a.- The wavefunction of a free electron is given by:

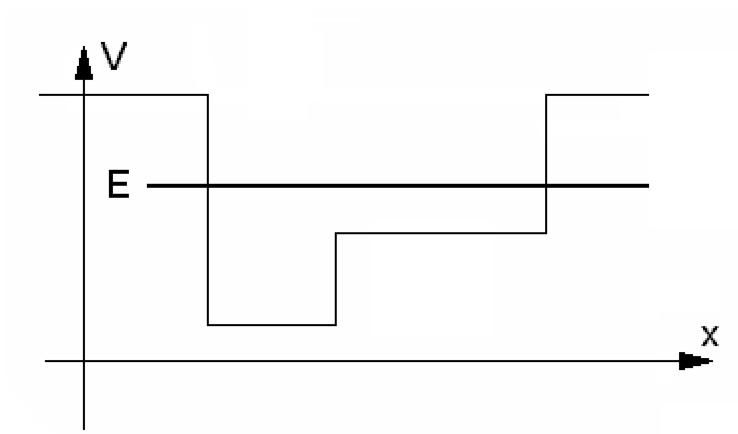
$$\Psi(x,t) = C\sin\left(\frac{2\pi\ x}{1.54\ \text{nm}}\right)$$

Calculate its kinetic energy.

Solution: The wavelength of the electron is 1.54 nm, we can use that to calculate the momentum and energy:

$$p = \frac{h}{\lambda} \rightarrow K.E. = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{(6.62\times10^{-34}\,Js)^2}{2(9.1\times10^{-31}\,kg)(1.54\times10^{-9}\,m)^2} = \mathbf{1.015\times10^{-19}\ J}$$

Problem 4.- How would the wavefunction look like for a particle with energy E in a potential V as follows:



Problem 5.- Given an electron whose wavefunction at t=0 is:

$$\Psi(x,0) = A\sin(x) + \frac{A}{2}\sin(2x)$$

Find the places in the range [0, 2π] where the electron will not be found and the places where we will have the maximum probability of finding it at t=0.