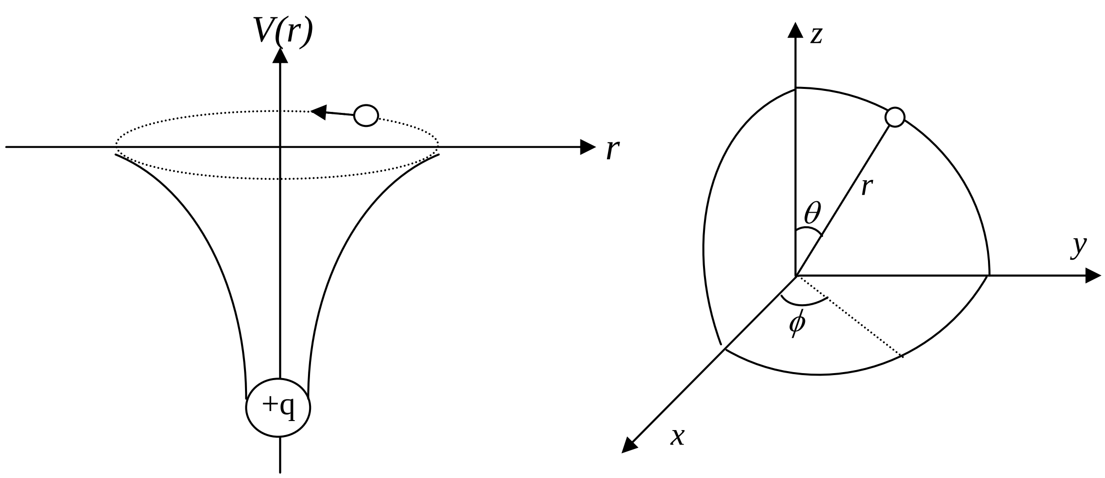
Example 2:

Apply Schrodinger equation on a hydrogen atom:

A hydrogen atom is represented by a nucleus with charge +q and an electron with charge –q. The electron orbits around the nucleus. Suppose the distance between the nucleus and the electron is *r*, then the electron has a potential energy of

$$V(r) = \frac{-q^2}{4\pi\varepsilon_0 r}$$

Since the electron and the nucleus may not stay on the same plane, this becomes a three-dimensional problem.



Using spherical coordinate system, the Schrodinger equation is,

$$\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) + \left[E - V(r,\theta,\phi)\right]\psi(r,\theta,\phi) = 0$$

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

Separate variables using,

$$\psi(r,\theta,\phi) = R(r)\cdot\Theta(\theta)\cdot\Phi(\phi)$$

Where $R(r)$, $\Theta(\theta)$ and $\Phi(\phi)$ are *r*-dependent, θ-dependent and ϕ-dependent functions. This process is very similar to that used to solve Maxwell's equations with boundary conditions: the Schrodinger equation can be separated into 3 equations, each having a single variable.

As an example, the ϕ-dependent equation is,

$$\Phi(\phi) + m^2\phi = 0$$

and its solutions are,

$$\Phi(\phi) = e^{jm\phi}$$

Since the solution must be single-valued and the spherical coordinate, ϕ is repeated after every 2π, or say, the single-valued region is $\phi \in (0,2\pi)$. So that m must be integer $m = 0, \pm1, \pm2, \pm3 \ldots$

Similarly, the equation for $\Theta(\theta)$ and R(r) can also be solved, each having its own integer selection rule. Then the overall solution is,

$$\psi_{nlm}(r,\theta,\phi) = R_n(r)\cdot\Theta_l(\theta)\cdot\Phi_m(\phi)$$

Here *n*, l, and *m* are commonly referred to as "quantum numbers" and the relationship between is,

n = 1, 2, 3, … (principle quantum number)

l = 0, 1, 2, 3… (n-1) (azimuthal quantum number)

m = 0, ±1, … $\pm(l-1)$, $\pm l$ (magnetic quantum number)

The simplest case of the solution is for n = 1, l = 0 and m = 0:

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right)$$

Where a_0 is the Bohr radius.

Recall that $|\psi_{100}|^2$ is the probability density function in [m^{-3}].

Now, we are interested in the probability of finding the electron within a ball shall with a radius r. This probability is,

$$P_r = \int_0^{2\pi} d\theta \int_0^{\pi} |\psi_{100}(r)|^2 r^2 \sin\phi d\phi = 4\pi r^2 |\psi_{100}(r)|^2 = \frac{4r^2}{a_0^3} \exp\left(-\frac{2r}{a_0}\right)$$

This is a Maxwellian distribution.

Physical meaning:

The location of the electron has the highest probability on the obit at r = a_0 (for n = 1, l = 0 and m = 0), while it is possible to be away from this orbit but with a smaller probability. This agrees with the Heisenberg uncertainty Principle (position uncertainty).

In general, the 3 quantum numbers n, l and m combine to form a quantum state [n, l, m]. For example, [1, 0, 0] is a quantum state and [2, 1, -1] is also a quantum state.

In addition, because of the spin of the electron (self-spin), which has two possible spin directions, so the more general quantum state has 4 dimensions [n, l, m_e , m_s], where the quantum number of spin, m_s can be $m_s = \pm 1/2$.