

1.2.2: The Schrodinger Equation

The Schrödinger Equation for the H Atom

Let us now go from an electron in a 1-dimensional box to the electron in the hydrogen atom. What is similar and what is different between these two cases. A similarity is that the electron is confined in an atom just like the electron is confined in the 1D box. Thus, like in the 1-dimensional box the electron should behave like a standing wave. While in the one-dimensional box there is only one coordinate to consider, there are three coordinates to consider for the electron in the atom. This is because an atom is spherical and thus three coordinates x, y, and z are necessary to describe a position within the atom. A second major difference is that the potential energy of the electron is zero at any position within the box, while it is not zero in the hydrogen atom. This is because in an atom there are attractive Coulomb forces between the nucleus and the electron. The further away the electron is from the nucleus the higher its potential energy. This is because it takes energy to pull the electron away from the nucleus.



Figure 1.2.12 Erwin Schrödinger (1887-1961), Nobel Prize 1933 (Attribution: Nobel foundation [Public domain] commons.wikimedia.org/wiki/F...ger_(1933).jpg)

We therefore need to modify the Schrödinger equation that we used previously for the one-dimensional box the following way. Firstly, we need to expand the operator for the kinetic energy from one to three dimensions and introduce the coordinates y and z in addition to x. Secondly, we have to add an operator for the potential energy to the equation. The potential energy is the Coulomb energy between the proton and the electron. It is similar to the term we previously used for the calculation of the potential energy of the electron in the Bohr model. Instead of the radius r we use now the square root of the sum of the square of the three coordinates x, y, and z, to indicate the Coulomb energy of the electron at any position within the atom. Our wave function will now be a function of three coordinates x, y, and z. This means our wave function will now be three-dimensional and represent three-dimensional standing waves. Three-dimensional waves are harder to imagine compared to 1-dimensional ones, but have the same properties, which are that the position of the crests, troughs, and nodes does not move.

$$\left[\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) \frac{-\hbar^2}{8\pi^2m} + \frac{e^2}{4\pi\epsilon_0 \sqrt{x^2 + y^2 + z^2}} \right] \Psi(x,y,z) = E \Psi(x,y,z)$$

Operator for kinetic energy + Operator for potential energy
(Coulomb energy)

Equation 1.2.9 Schrödinger equation for the H atom.

In order to get the wave functions for the electron we need to solve the Schrödinger equation for the hydrogen atom. To do so, we need to think about the boundary conditions for the wave function. One condition is that the square of the wave function approaches zero when we go very far from the nucleus, and r, the distance from the nucleus approaches infinite. Secondly, like in the one-dimensional box, the integral over the square of the wave function must be one. This is because the probability to find the electron somewhere in the atom must be 100%. Thirdly, it would be sensible to assume that the wave function must be continuously differentiable and single valued (Fig. 1.2.13).

Boundary conditions for Ψ :

$$\Psi^2 = 0 \text{ for } r \rightarrow \infty$$

$$\int \Psi^2 dr = 1$$

-continuously differentiable and single valued

Figure 1.2.13 Boundary conditions for the wave function of the electron in the hydrogen atom.

The Spherical Polar Coordinate System

The mathematical process to solve the Schrödinger equation is beyond the scope of this course and you are referred to Physical Chemistry classes and textbooks for the details. We shall only provide a brief outline of the process here. It is mathematically simpler to solve the Schrödinger equation in spherical polar coordinates instead of cartesian coordinates. Therefore, we obtain the solutions of the Schrödinger equation, the wavefunctions, in polar coordinates. The position of a point is specified by three numbers: the *radial distance* of that point from a fixed origin, its *polar angle* measured from a fixed zenith direction, and the *azimuthal angle* of its orthogonal projection on a reference plane that passes through the origin and is orthogonal to the zenith, measured from a fixed reference direction on that plane (Fig. 1.2.14).

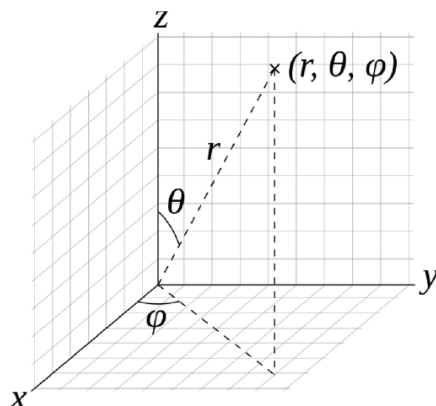


Figure 1.2.14 Illustration of the spherical polar coordinate system.

Solutions of the Schrödinger Equation

The wavefunction is then a function of r , θ and ϕ , in particular it is a product of a radial wave function which is function of r , a colatitude wave function, which is a function of θ , and an azimuthal wave function which is a function of ϕ (Eq. 1.2.10). You can see the explicit forms of the radial, colatitude, and azimuthal functions in Fig. 1.2.15.

$$\Psi(r, \theta, \phi) = R(r) \times \Theta(\theta) \times \Phi(\phi)$$

Equation 1.2.10 The wave function for the electron in the H atom as a function of r , θ and ϕ

| | | |
|--------------------------|---|--|
| Radial wave function | → | $R_{n,l} = r^l L_{n,l} e^{-r/na_0}$ |
| Colatitude wave function | → | $\Theta(\theta) = (-1)^m \sqrt{\frac{2l+1}{2\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta).$ |
| Azimuthal equation | → | $\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}.$ |

Figure 1.2.15 Explicit forms of the radial, colatitude and azimuthal functions

We do not need to understand all details here, but need to realize that these wavefunctions are functions of quantum numbers. In contrast to the electron in the one-dimensional box not only one, but three quantum numbers need to be considered. Beyond the quantum number n , which is called the principal quantum number, there is also a so-called orbital quantum number l , and a magnetic quantum number m . The quantum number n only occurs in the radial wave function, the quantum number l only occurs in the radial and colatitude function, and the quantum number m only occurs in the colatitude and the azimuthal part of the wave function. The values the orbital quantum number l can adopt depends on n , it can be between 0 and $n-1$ for a given quantum number n . The magnetic quantum number m depends on the quantum number l , and can run from $-l$ to $+l$. So, for example when n is equal to 2, l can vary between 0 and 1, and for l equal to 1, m can adopt any value between -1 and $+1$, namely $-1, 0, +1$, and $+2$ (Fig. 1.2.16).

Principal quantum number: n
 Orbital quantum number: l ($l = 0, \dots, n-1$)
 Magnetic quantum number m ($m = -l, \dots, +l$)

Figure 1.2.16 The quantum numbers of the wave function of the H atom.

These wave functions have a particular name in chemistry. They are called orbitals. One can understand an orbital as the three-dimensional wave function that describes the electron in an atom as a standing wave. Thus, an orbital is a state the electron can adopt, and when we say that an electron is in a particular orbital we mean that the electron is in a particular state.

The spin quantum number s

Within an orbital an electron can adopt two different spins described by the spin quantum number s . This quantum number is not a result of the Schrödinger equation, but was found experimentally. The spin quantum number s can adopt two values: $+1/2$ and $-1/2$. We say an electron is spin up when $s = +1/2$, and spin down when $s = -1/2$.

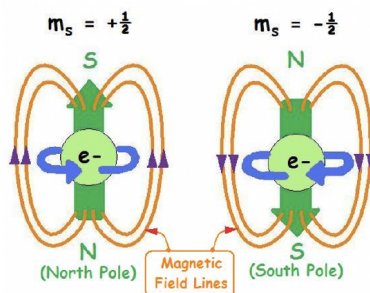


Figure 1.2.17 Electron spin (Attribution: Chemlibretexts.org
 chem.libretexts.org/@api/dek...jpg?revision=1, CC BY-NC-SA 3.0)

The spin quantum number is understood most easily when you view the electron as a particle rotating around its own axis. A counter-clockwise rotation would be associated with $s = +1/2$, a clockwise rotation would be associated with $s = -1/2$. The rotation produces a magnetic field with the direction of the field lines depending on the direction of rotation.

Dr. Kai Landskron ([Lehigh University](#)). If you like this textbook, please consider to make a donation to support the author's research at Lehigh University: [Click Here to Donate](#).

This page titled [1.2.2: The Schrodinger Equation](#) is shared under a [CC BY-SA 4.0](#) license and was authored, remixed, and/or curated by [Kai Landskron](#).

- [1.2: The quantum-mechanical model of the atom](#) by Kai Landskron is licensed CC BY 4.0.