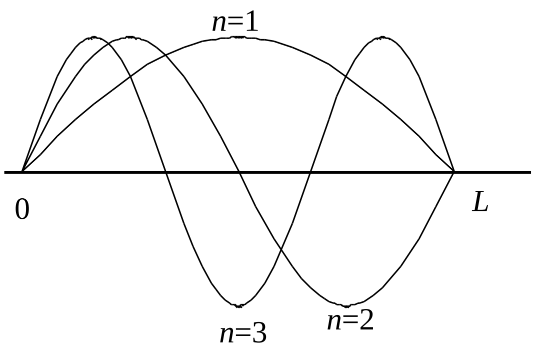
1290: Shape of electron distribution on an atom and atomic orbitals

(Note that the electron distribution when an electron enters an atomic orbital is expressed as a function of the distance *r* from the nucleus)

Key words: (electron) distribution function; square of wave function; isoradial distribution; the distances from the nucleus in the maximum distribution and in the average distribution of electrons are different

There are two differences between the electron distribution and the shape of atomic orbitals. The electron distribution function ($P(r)$, where r is position) is expressed as the square of the wave function (ψ) (ψ^2, or $\psi^*\psi$ if ψ is a complex function). For the one-dimensional wave function quoted in the "Shapes of Atomic Orbitals" section (**1280**), it looks like the diagram below. Since it is the square of the wave function, the electron distribution is sharper than the amplitude intensity of the wave function. $\psi^*\psi dx$ is the probability of an electron being found between x and $x+dx$.

Wavefunction : $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$



Distribution function : $P(x) = \psi(x)\psi(x) = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)$

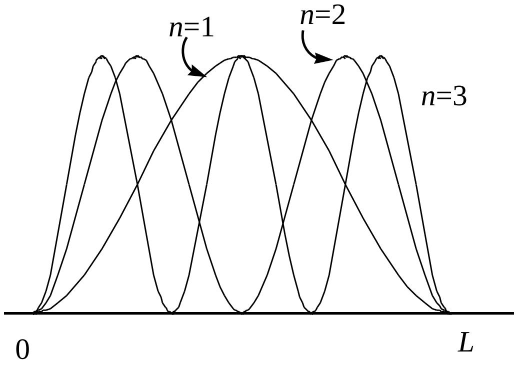


Figure 1. Electron distribution based on one-dimensional wave function

Another difference needs special attention when considering the radial distribution of electrons. The radial distribution is the distribution of electrons as a function of distance (*r*) from the nucleus. The probability of an electron being found is the probability of finding an electron in a volume that is $4\pi r^2$ multiplied by dr, which is the surface area of a sphere at r. This probability is calculated by multiplying it by the probability of electron distribution in space, $\psi^*\psi$, giving $4\pi r^2\psi^*\psi \mathrm{d}r$, and $\pi r^2\psi^*\psi$ is the radial distribution function.

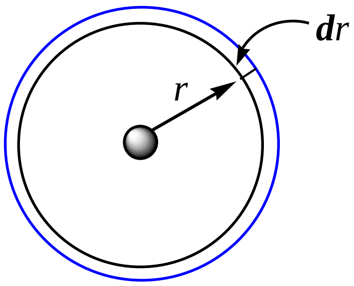


Figure 2. The radial distribution function is a function that expresses the probability that an electron will enter a gap at distances between r and $r+dr$ from the nucleus. The volume of the gap is $4\pi r^2 \mathrm{d}r$, and the probability of an electron being present is expressed as $4\pi r^2\psi^*\psi \mathrm{d}r$. $4\pi r^2\psi^*\psi$ is the radial distribution function

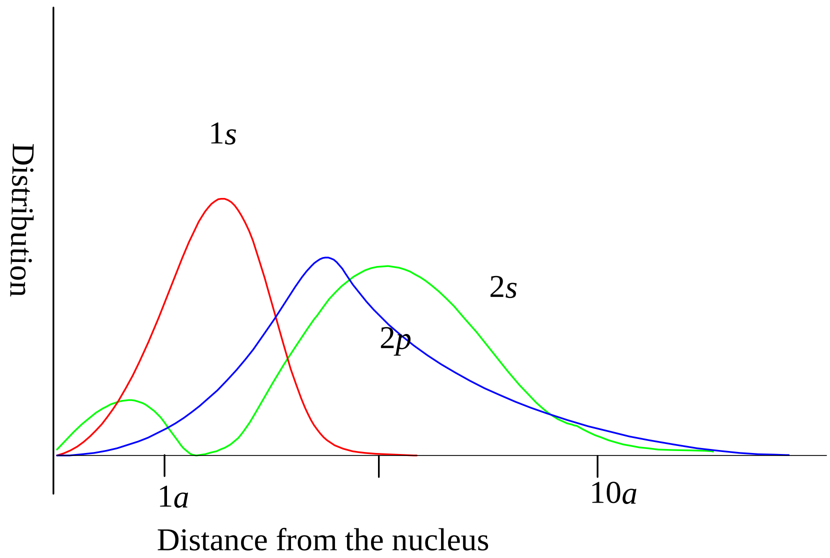


Figure 3. Approximate radial distribution of electrons. In the figure above, *a* is the Bohr radius (0.521947 Å). When shown by the radial distribution function, the electrons do not exist on the nucleus. Note that some of the electrons that enter the 2*s* atomic orbital are inside the 1*s* atomic orbital.

Let us find the maximum distribution position r of electrons in the $1s$ atomic orbital of a hydrogen atom. The $1s$ orbital of a hydrogen atom is (see **1280**),

$$\psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a}\right)^{3/2} e^{-\rho} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a}\right)^{3/2} e^{-\frac{1}{a}r}$$

Distribution function is,

$$P(r) = 4\pi r^2 \psi_{1s}\psi_{1s} = \frac{4}{a^3} r^2 e^{-\frac{2}{a}r}$$

If you differentiate this with respect to r, you will get extreme values at r=0 and r=a.

[Average distance from nucleus to electrons]

As stated in **1280**, the average distance from the nucleus to the electrons is given by the formula,

$$\bar{r} = \frac{a\,n^2}{z}\left\{\frac{3}{2} - \frac{l(l+1)}{2n^2}\right\}$$

Using this formula, if there is an electron in the 1s atomic orbital, the average distance from the nucleus to the electron is $a \times 1.5$, which is different from the maximum distribution position (a).