

5.12: Electron Density and Potential Energy

When we turn our attention from the potential energy of charged macroscopic particles which have a definite location in space to microscopic particles like the electron, we immediately encounter a difficulty. The electron in an atom is not a fixed distance from the nucleus but is “smeared out” in space in a wave pattern over a large range of distances. Nevertheless it is still meaningful to talk about the potential energy of such an electron cloud. Consider the 1s electron illustrated by the dot-density diagram in [Figure 1 of Electron Waves in the Hydrogen Atom](#), for example. If the electron were actually positioned at one of these dots momentarily, it would have a definite potential energy at that moment. If we now add up the potential energy for each dot and divide by the number of dots, we obtain an average potential energy, which is a good approximation to the potential energy of the electron cloud. The more dots we have, the closer such an approximation is to the exact answer.

In practice we can often decide which of two electron clouds has the higher potential energy by looking at them. In [Figure 1 from the Orbitals section](#), for example, it is easy to see that the potential energy of an electron in a 1s orbital is lower than that of a 2s electron. An electron in a 1s orbital is almost always closer than 200 pm to the nucleus, while in a 2s orbital it is usually farther away. In the same way we have no difficulty in estimating that a 3s electron is on average farther from the nucleus and hence higher in potential energy than a 2s electron. It is also easy to see that electron clouds which differ only in their orientation in space must have the *same* potential energy. An example would be the $2p_x$, $2p_y$, and $2p_z$ clouds.

When we compare orbitals with different basic shapes, mere inspection of the dot-density diagrams is often insufficient to tell us about the relative potential energies. It is not apparent from [Figure 1 in Orbitals](#), for instance, whether the 2s or 2p orbital has the higher potential energy. Actually both have the same energy in a hydrogen atom, though not in other atoms. In the same way the 3s, the three 3p, and the five 3d orbitals are all found to have the same energy in the hydrogen atom.

Although dot-density diagrams are very informative about the potential energy of an electron in an orbital, they tell us nothing at all about its kinetic energy. It is impossible, for example, to decide from [Figure 5.6](#) whether the electron in a 1s orbital is moving faster on the whole than an electron in a 2s orbital, or even whether it is moving at all! Fortunately it turns out that this difficulty is unimportant. The *total* energy (kinetic + potential) of an electron in an atom or a molecule is always one-half its potential energy. Thus, for example, when an electron is shifted from a 1s to a 2s orbital, its potential energy increases by 3.27 aJ. At the same time the electron slows down and its kinetic energy drops by half this quantity, namely, 1.635 aJ. The net result is that the total energy (kinetic + potential) increases by exactly half the increase in potential energy alone; i.e., it increases by 1.635 aJ. A similar statement can be made for *any* change inflicted on any electron in any atomic or molecular system. This result is known as the **virial theorem**. Because of this theorem we can, if we want, ignore the kinetic energy of an electron and concentrate exclusively on its potential energy.

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