1230：Energy value of an electron in a 1Å^3 box

(The conclusion of this section can be obtained by solving the Schrödinger equation)

Key words: Schrödinger equation; wave function; quantum numbers; ground state; excited state; electron kinetic energy

The "behavior" and energy of an electron trapped in space can be calculated by solving the Schrödinger equation below (details will be omitted here).

$$E\psi(x,y,z) = \frac{-\hbar^2}{2m}\nabla^2\psi(x,y,z)$$

By solving this equation, we obtain the energy (E) and the wave function (ψ), which represents the motion of the electrons (this expression is inaccurate, but please understand it as such for now). Since there are no charges on the nucleus or other objects that would generate potential energy, the E obtained is kinetic energy.

The (kinetic) energy of an electron in a cube with side length L is,

$$E(n_x, n_y, n_z) = \left(n_x^2 + n_y^2 + n_z^2\right)\frac{h^2}{8mL^2}$$

where m is the mass of an electron, and n_x, n_y, and n_z are called quantum numbers, each independently taking the natural numbers 1, 2, 3, ... When $n_x = n_y = n_z = 1$, this is the lowest energy state. This state is called the ground state, and all states other than the ground state have higher energy than the ground state, and are called excited states.

If we calculate the ground state energy with L = 1 Å, an electron confined to 1 Å^3 has an energy of approximately 10^4 kJ/mol (10,080 kJ/mol).

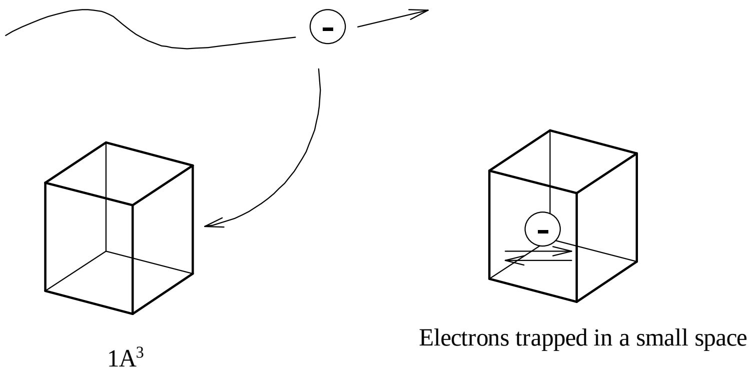

Figure 1. A large amount of energy is required to confine a "freely moving" electron into a box of 1 Å^3. Electrons confined in a small space have a large amount of kinetic energy.

From the above equation, we can see that the kinetic energy of the electron decreases when the length of one side of the cube, L, is increased. Electrons in a small space have a lot of energy, and to reduce that energy, electrons tend to spread out as much as possible.