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Luigi Pagani

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Particle in a Square Box

Let's assume $\psi(\vec{r}) = 0$, outside the box. For symmetry reasons, we can factor the wave function: $\psi(\vec{r}) = X(x)Y(y)Z(z)$.:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]X(x)Y(y)Z(z) = EX(x)Y(y)Z(z)$$

We can assume that inside the box the potential is null.

$$\frac{-\hbar^2}{2m}\left[Y(y)Z(z)\frac{d^2 X(x)}{dx^2} + X(x)Z(z)\frac{d^2 Y(y)}{dy^2} + X(x)Y(y)\frac{d^2 Z(z)}{dz^2}\right] = EX(x)Y(y)Z(z)$$

$$\frac{-\hbar^2}{2m}\left[\frac{1}{X(x)}\frac{d^2 X(x)}{dx^2} + \frac{1}{Y(y)}\frac{d^2 Y(y)}{dy^2} + \frac{1}{Z(z)}\frac{d^2 Z(z)}{dz^2}\right] = E$$

We can split this equation, on the three coordinates:

$$\frac{\hbar^2}{2m}\frac{d^2 X(x)}{dx^2} + E_x X(x) = 0$$

$$\frac{\hbar^2}{2m}\frac{d^2 Y(y)}{dy^2} + E_y Y(y) = 0$$

$$\frac{\hbar^2}{2m}\frac{d^2 Z(z)}{dz^2} + E_z Z(z) = 0$$

$$E = E_x + E_y + E_z$$

The general solution, imposing the boundaries condition that $\psi(x) = \psi(L) = 0$ for the x case is:

$$X(x) = A sin(kx)$$

where $k = \frac{\pi}{L}n$, $n \in \mathbb{N}$. With this solution we get the following eigenvalue:

$$\implies E_x = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 \hbar^2}{2L^2 m}n_x^2 = \frac{h^2}{8L^2 m}$$

The total energy is thus:

$$E = \frac{h^2}{8L^2 m}(n_x^2 + n_y^2 + n_z^2), \quad n_x, n_y, n_z \in \mathbb{N}$$

To calculate the zero-point (ground state) energy of a particle in a 3-dimensional box with sides of length $L = 1$ m, we use the energy equation derived for a particle in a 3D box:

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

where:

- h is Planck's constant ($6.62607015 \times 10^{-34} \, \text{m}^2\text{kg/s}$),

- m is the mass of the particle (in this case, the mass of a methane molecule we calculated previously as $2.66 \times 10^{-26} \, \text{kg}$),

- L is the length of each side of the box (1 m in this case), n_x, n_y, and n_z are quantum numbers corresponding to the three dimensions, which can take on positive integer values.

For the ground state energy, we consider the lowest possible energy state, where $n_x = n_y = n_z = 1$ (the lowest non-zero integer values possible for the quantum numbers). Let's perform this calculation.

The zero-point (ground state) energy of a particle (in this case, a methane molecule) in a 3-dimensional box of length $L = 1 \, \text{m}$ is approximately $6.18 \times 10^{-42} \, \text{J}$.

Hydrogen Energy Levels

To determine the energy of orbitals in atomic hydrogen and the energy required for excitation between different orbitals, we'll use the formula for the energy levels in a hydrogen atom, which is given by:

$$E_n = -\frac{R_H}{n^2}$$

where E_n is the energy of the electron in the nth energy level, and R_H is the Rydberg constant for hydrogen, approximately 2.18×10^{-18} joules.

The energy required for excitation from an initial state n_i to a final state n_f is simply the difference in the energies of the two states:

$$\Delta E = E_{n_f} - E_{n_i} = -\frac{R_H}{n_f^2} + \frac{R_H}{n_i^2}$$

Let's calculate some examples using Python, such as the energy levels for $n = 1, 2, 3$ (the first three energy levels), and the energy required for excitation from the ground state ($n = 1$) to the first excited state ($n = 2$) and to the second excited state ($n = 3$).

The energies for the first three levels of atomic hydrogen are as follows:

- For $n = 1$ (ground state): $E_1 = -2.18 \times 10^{-18}$ J - For $n = 2$: $E_2 = -5.45 \times 10^{-19}$ J - For $n = 3$: $E_3 = -2.42 \times 10^{-19}$ J

The energy required for excitation from the ground state to the first excited state ($n = 1$ to $n = 2$) is $\Delta E_{1 \to 2} = 1.635 \times 10^{-18}$ J, and from the ground state to the second excited state ($n = 1$ to $n = 3$) is $\Delta E_{1 \to 3} = 1.938 \times 10^{-18}$ J.

These results demonstrate that as the principal quantum number n increases, the energy levels get closer together, which is a characteristic of the hydrogen atom's energy spectrum. The general formula for the energy required for excitation between any two levels n_i and n_f is:

$$\Delta E = -\frac{R_H}{n_f^2} + \frac{R_H}{n_i^2}$$

This formula shows that the energy difference between levels decreases as n increases, reflecting the fact that the energy levels of the hydrogen atom converge towards zero as n approaches infinity.
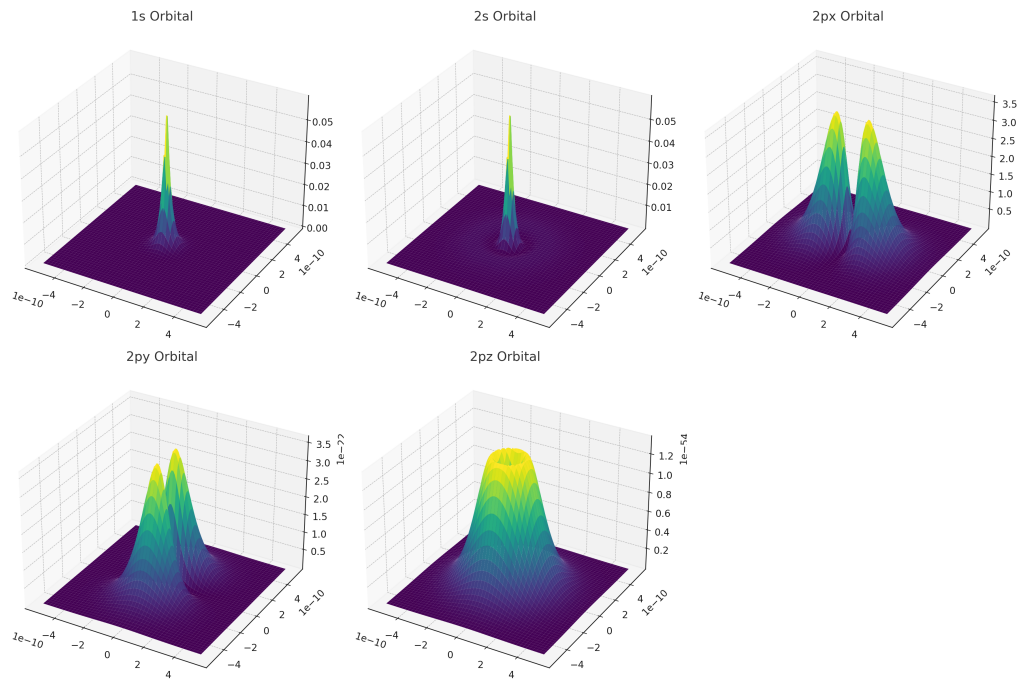
Hydrogen Orbitals

Figure 1: Visualization of Hydrogen Atom Orbitals: This set of 3D plots illustrates the probability densities of the 1s, 2s, 2px, 2py, and 2pz orbitals of the hydrogen atom, using the real Bohr radius for scale. Each plot captures the unique spatial distribution of electron probability within the respective orbital, showcasing the spherical symmetry of the 1s and 2s orbitals, the dumbbell shapes of the 2px and 2py orbitals along their respective axes, and the projected representation of the 2pz orbital.