General Chemistry I
Tutorial 03

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Outline

Wave Functions

Remark 1.1

For a microscopic system, all of its physical properties can be determined by a **wave function** *given by* $\Psi(x, y, z, t)$*, where* Ψ *is a function of both space (x,y,z) and time t.*

Probability of finding particles in a specified volume is proportional to $\psi\psi^*$,i.e.

$$\mathrm{d}\boldsymbol{p} = \psi\psi^*\mathrm{d}\tau$$

$$\int \psi\psi^*\mathrm{d}\tau = 1$$

Remark 1.2

To make a wave function acceptable, stringent conditions should be satisfied:

- *Must not be infinite over a finite region.*
- *Must be single-valued.*
- *Must be continuous.*
- *Must have continuous first derivatives.*

Schrödinger Equation for Standing Waves

The time-independent Schrödinger equation for a particle of mass m moving with energy E in a system that does not change with time:

$$\hat{H}\psi = E\psi$$

$$(-\frac{\hbar^2}{2m}\nabla^2 + \hat{V})\psi = E\psi$$

Where $\nabla^2 = \frac{\partial^2}{\partial x^2}$ for 1D, $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ for 2D and $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ for 3D systems.

1D Standing Wave

Consider a particle in a box in which a particle of mass m is confined to a region of one-dimensional space between two impenetrable walls. The potential energy is zero inside the box but rises abruptly to infinity at the walls located at $x = 0$ and $x = L$.

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x \leq 0 \text{ and } x \geq L \end{cases}$$

By solving Schrödinger equation:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n}{L}x\right) \qquad E_n = \frac{n^2h^2}{8mL^2}$$

number of nodes = **n-1**

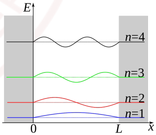

Figure 1: Energy diagram for particle in a box

Shape of 2D Orbitals

Node is the place whenever wave function is zero.
Angular quantum number l can change from 0 to (n-1).
Angular quantum number determines the shape of orbitals.

Remark 1.3

- *Number of nodes = n-1*
- *Number of* **angular** *nodes = l*
- *Number of* **radialz** *nodes = n-l-1*

Remark 1.4

Radial nodes always have ring-shaped look.
Angular nodes always appear like flat or curved plane.

Quiz 3.1

The power of a beam of green laser at $\lambda = 532$ nm is 0.100W. (1 W = 1 J$\cdot s^{-1}$) How many photons are emitted per second?

Quiz 3.2

What are the principle quantum number n, angular quantum number l, and symbol (e.g., 2s) for the waves in Figure3 and Figure4?

(a) In Figure 3, n =__________, l =__________, symbol = __________.

(b) In Figure 4, n =__________, l =__________, symbol =__________.

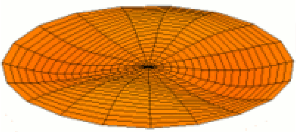

Figure 3

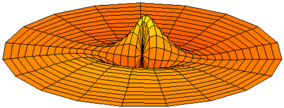

Figure 4

PS2.1

Photons of wavelength 315 nm or less are needed to eject electrons from a surface of electrically neutral cadmium.

(a) What is the energy barrier (in electron volts, eV) that electrons must overcome to leave an uncharged piece of cadmium?

(b) What is the maximum kinetic energy of electrons ejected from a piece of cadmium by photons of wavelength 200 nm?

(c) Suppose the electrons described in (b) were used in a diffraction experiment. What would be their wavelength?

PS2.2

Express the velocity of the electron in the Bohr model for fundamental constants (m_e, e, h, ε_0), the nuclear charge Z, and the quantum number n. Evaluate the velocity of an electron in the ground states of He^+ ion and U^{91+}. Compare these velocities with the speed of light c. As the velocity of an object approaches the speed of light, relativistic effects become important. In which kinds of atoms do you expect relativistic effects to be greatest?

PS2.3

Although the Bohr model does not apply to atoms or ions with more than one electron, it works reasonably well for the n = 2 to n = 1 transition (denoted K_α in physics) for most metal elements.

(a) Derive the formula for calculating the K_α emission wavelength from the atomic number Z and physical constants.

(b) Physicist Henry Moseley discovered in 1913 that the experimental K_α wavelength depends on Z-1 instead of Z. What will be the metal that emits a K_α X-ray of 1.54 Å wavelength?

PS2.4

It has been suggested that spacecraft could be powered by the pressure exerted by sunlight striking a sail. The force exerted on a surface is the momentum p transferred to the surface per second. Assume that photons of 6000 Å light strike the sail perpendicularly. How many must be reflected per second by 1 cm^2 of surface to produce a pressure of 10^{-6} atm?

PS2.5

It is interesting to speculate on the properties of a universe with different values for the fundamental constants.

(a) In a universe in which Planck's constant had the value $h = 1$ J·s, what would be the de Broglie wavelength of a 145g baseball moving at a speed of 20 m$\cdot$ s^{-1}?

(b) Suppose the velocity of the ball from part (a) is known to lie between 19 and 21 m$\cdot$ s^{-1}. What is the smallest distance within which it can be known to lie?

(c) Suppose that in this universe the mass of the electron is 1 g and the charge on the electron is 1 C. Calculate the Bohr radius of the hydrogen atom in this universe.