

Quantum Chemistry 1.1 - Blackbody Radiation

This discussion will focus on blackbody radiation and the origins of early quantum theory. Let's begin by understanding a black body, which is an object that is heated up and emits radiation at all frequencies.

The theory predicts that as the frequency of light increases, the amount of radiation also increases with the square of the frequency. This posed a problem, which was subsequently solved by Max Planck in the year 1900, through the introduction of quantum theory.

Planck proposed that the energy levels inside the black box cannot have any possible level, as classical theory suggests, but rather there exists a quantized set of values. He derived a formula for the density of the radiation at a given temperature, which is represented as:

$$8\pi(h/c)^3 f^3 / (e^{hf/kT} - 1)$$

where h is Planck's constant, c is the speed of light, f is the frequency, k is the Boltzmann constant, and T is the temperature.

Here are a few examples of this formula:

- At a frequency of 1 Hz and temperature of 1000 K, the density of radiation is 0.023 Wm⁻³Hz⁻¹.**
- At a frequency of 10¹⁴ Hz and temperature of 300 K, the density of radiation is 2.06 x 10⁻³ Wm⁻³Hz⁻¹.**

Quantum Chemistry 1.2 - Photoelectric Effect

The Photoelectric Effect

The photoelectric effect is a phenomenon where ultraviolet (UV) light ejects electrons from a metal surface. This effect was solved by a quantum hypothesis, providing an example of a quantum solution to a classical physics problem.

Classical Theory

Classical theory predicted that the frequency of the UV light would not affect the kinetic energy or speed of the ejected electrons. Changing the frequency of the light from red to green to blue would not change the electrons that are ejected from the surface.

Quantum Theory

Quantum theory, on the other hand, predicts that the kinetic energy of the ejected electrons is not dependent on the intensity of the light. This means that changing the intensity of the UV light will not change the speed of the ejected electrons.

Quantum Chemistry 1.5 - Bohr Hydrogen Model

2: Energy

Bohr Hydrogen Model - Energy



$\left(\text{Coulomb Force} \right) = \left(\text{Centrifugal Force} \right)$
 $\frac{e^2}{4\pi\epsilon_0 r^2} = \frac{m_e v^2}{r}$
 $\ell = mvr = n\hbar \quad n \in \mathbb{Z}$
 $r = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} = 0.529 \text{ \AA} \quad \text{"Bohr radius"}$

$E = T + V = \frac{1}{2} m_e v^2 - \frac{e^2}{4\pi\epsilon_0 r}$
 $\frac{e^2}{8\pi\epsilon_0 r} = \frac{m_e v^2}{2} \quad \frac{1}{2} m_e v^2 = \frac{e^2}{8\pi\epsilon_0 r}$
 $E = \frac{-e^2}{8\pi\epsilon_0 r} = \frac{-e^2}{8\pi\epsilon_0} \left(\frac{m_e e^2}{4\pi\epsilon_0 \hbar^2 n^2} \right)$
 $E = \frac{-m_e e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left(\frac{1}{n^2} \right)$

$\Delta E = E_{n_2} - E_{n_1} = h\nu = hc\tilde{\nu} = \frac{m_e e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$
 $\nu = \frac{c}{\lambda} \quad \tilde{\nu} = \frac{1}{\lambda}$
 $\tilde{\nu} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_2 > n_1, \quad n_1, n_2 \in \mathbb{Z}$
 $R_H = \frac{m_e e^4}{8\epsilon_0^2 h^3} \quad (R_\infty)$
 $R_H = 109,737.3 \text{ cm}^{-1}$

accurate w/in 0.05% of experiment
 $m_p \neq \infty \quad m_e \rightarrow \mu = \left(\frac{1}{m_e} + \frac{1}{m_p} \right)^{-1} = \frac{m_e m_p}{m_e + m_p}$
 $m_e = 1.672 \cdot 10^{-27} \text{ kg}$
 $m_p = 1.674 \cdot 10^{-27} \cdot 10^{-31} \text{ kg}$
 $\mu = 0.9995 m_e$
 $R_H \rightarrow \mu$
 $R_1 = 109,676 \text{ cm}^{-1}$
 w/in 0.001% error $(109677.6 \text{ cm}^{-1})$

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Quantum Chemistry 2.1 - Classical Wave Equation

This is an introduction to the classical wave equation, also known as a second-order partial differential equation. It involves second derivatives and partial derivatives, and is an equation in which we need to solve using the derivatives of a function for the function itself.

Below is the solution to the separation of variables for the general classical wave equation in one dimension. In the next video, we will apply this specifically to the case of a one-dimensional vibrating string. The solution to each of those is going to be sines and cosines.

General Solution:

Solution to the wave equation: $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$

Solution to the separation of variables: $u(x,t) = X(x)T(t)$

By substitution, we arrive at two ODEs: $X''(x) + kX(x) = 0$ and $T''(t) + c^2 kT(t) = 0$

The solution to each ODE is: $X(x) = A\sin(kx) + B\cos(kx)$ and $T(t) = C\sin(ct) + D\cos(ct)$

Therefore, the general solution to the wave equation is: $u(x,t) = (A\sin(kx) + B\cos(kx))(C\sin(ct) + D\cos(ct))$

The solution involves sines and cosines, which is taught in an ordinary differential equations course to solve this particular equation.