CBE 310 Molecular Concepts and Applications

09 03 2014

Schrödinger Equation

For Today: 1) Summarize the experiments that lead up to the development of QM

2) Derive Schrödinger's Equation

3) Talk about some formal math relating to how we will be dealing with quantum mechanical equations.

Reading: Finish Chapter 1 of Quantum Chemistry Book, Chapter 8 of P-Chem book
start Chapter 2 of Quantum Chemistry Book

Blackbody Radiation

Kirchhoff

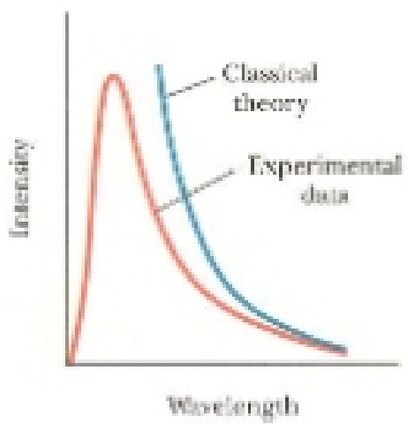
Boltzmann

$$P^* = \varepsilon\sigma T^4$$

Rayleigh

$$\rho(\lambda) = \frac{8\pi kT}{\lambda^4}$$

1) Counts oscillators based on Maxwell's laws
2) Applies Equipartition of Enegy



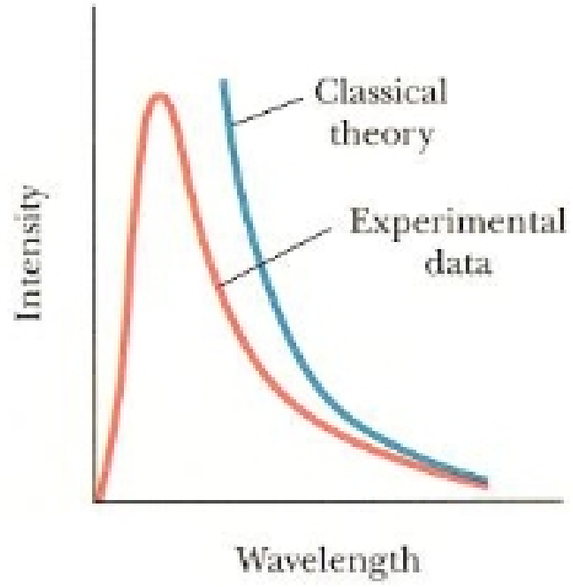
Max Planck

Says that the energy of the oscillators that give rise to the radiation have quantized (discrete, incremental) as opposed to a continuous energy distribution. When he calculates this new energy function and combines it with Rayleigh's calculation, his result fits the data

Energy = hν

Spectrum of Blackbody Radiation

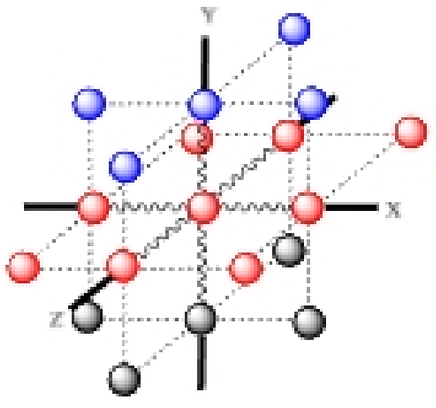
$$\rho(\lambda) = \frac{8\pi kT}{\lambda^4}$$



The classical explanation fails,

$$\rho(\nu) = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{h\nu/kT} - 1}$$

Idea that energy is quantized leads to a solution.



$$\frac{dU}{dT} = 3R\left(\frac{\theta_E}{T}\right)^2\left(\frac{e^{\theta_E/2T}}{e^{\theta_E/T} - 1}\right)^2$$

This same idea leads to a solution of a different problem