

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

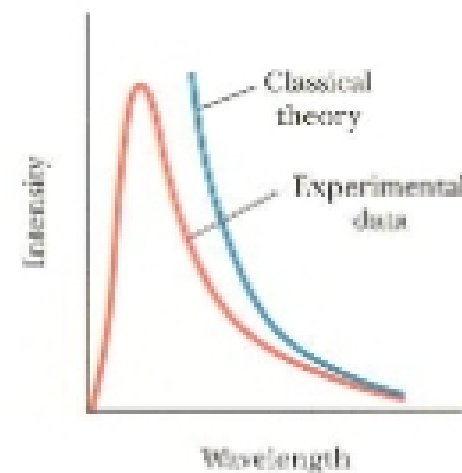
$$P^* = \epsilon \sigma T^4$$

Rayleigh



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

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



Max Planck

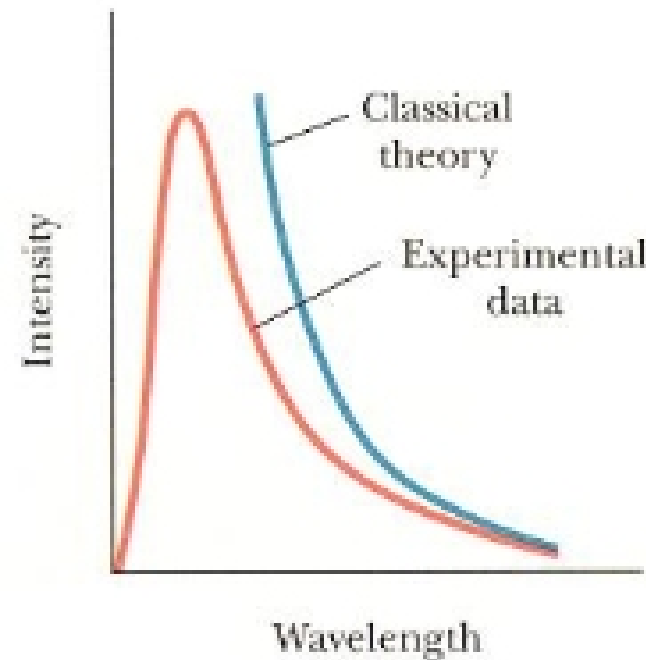


Says that the energy of the oscillators that give rise to the radiation have quantized (discrete, incremental) as opposed to a continuous energy distribution. When he calculates this new energy function and combines it with Rayleigh's calculation, his result fits the data

$$\text{Energy} = h\nu$$

Spectrum of Blackbody Radiation

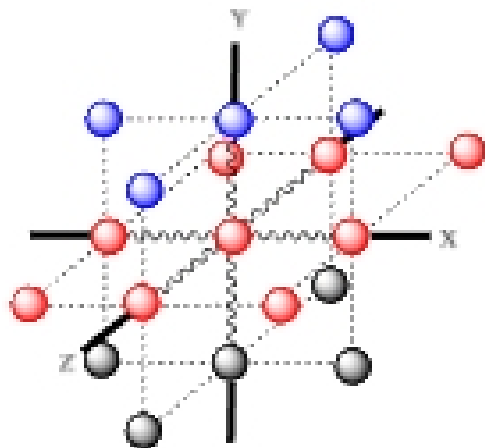
$$\rho(\lambda) = \frac{8\pi kT}{\lambda^4}$$



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