Note Title 16-09-2009

Quantum Chemistry

Lecturer

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Tutors

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Academic Orientation

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1. * You are no longer in high school.*

2. Expect to have material discussed at / two to three/ times the pace of high school. Above that, we aim for greater command of the material, esp. the ability to apply what you have learned to new situations.

3. You cannot be "taught" everything in the classroom. * It is / your/ responsibility to learn the material. * Most of this learning must take place *outside* the classroom.

Academic Orientation (contd.)

4. The instructor's job is primarily to provide a framework to guide you in your learning of the concepts and methods that comprise the material of the course.
5. You are expected to read the textbook for comprehension. The textbook is not a novel, so the reading must often be careful.
6. Read the appropriate section(s) of the book before the material is presented in lecture.
7. Exams will consist largely of fresh problems falling within the material that is being tested.

Thermal Radiation

Iron rod $\xrightarrow{\text{heat}}$ dull red → bright red

→ bluish white

"Optical Pyrometer"

Three commandments

1. Thou shalt be in your seats "on time"
2. Thou shalt keep your eyes & ears open in class
3. Thou shalt keep your cellular telephone in "non-sounding" mode

$\rho(\nu) \propto R_T(\nu)$ Power $R_T(\nu)$

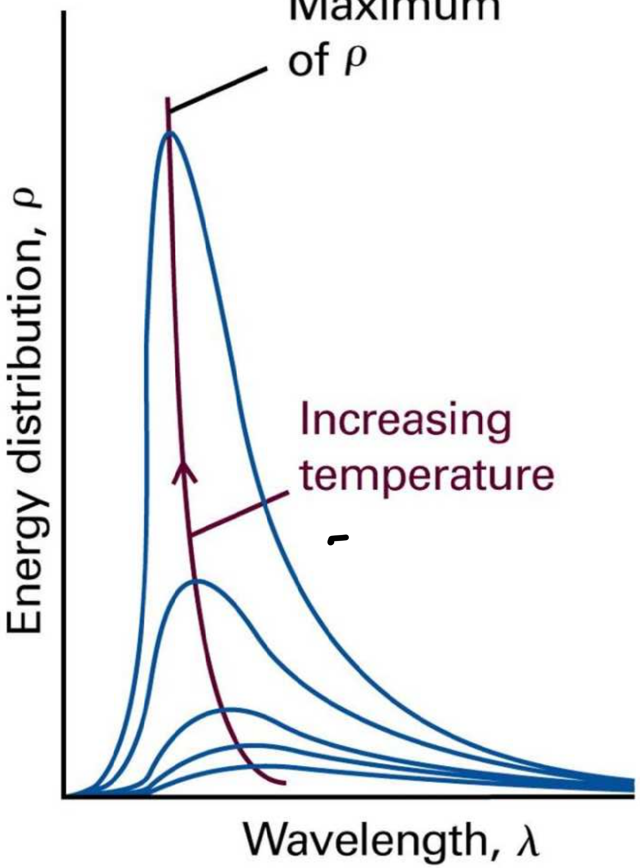


Figure 8-3
Atkins Physical Chemistry, Eighth Edition

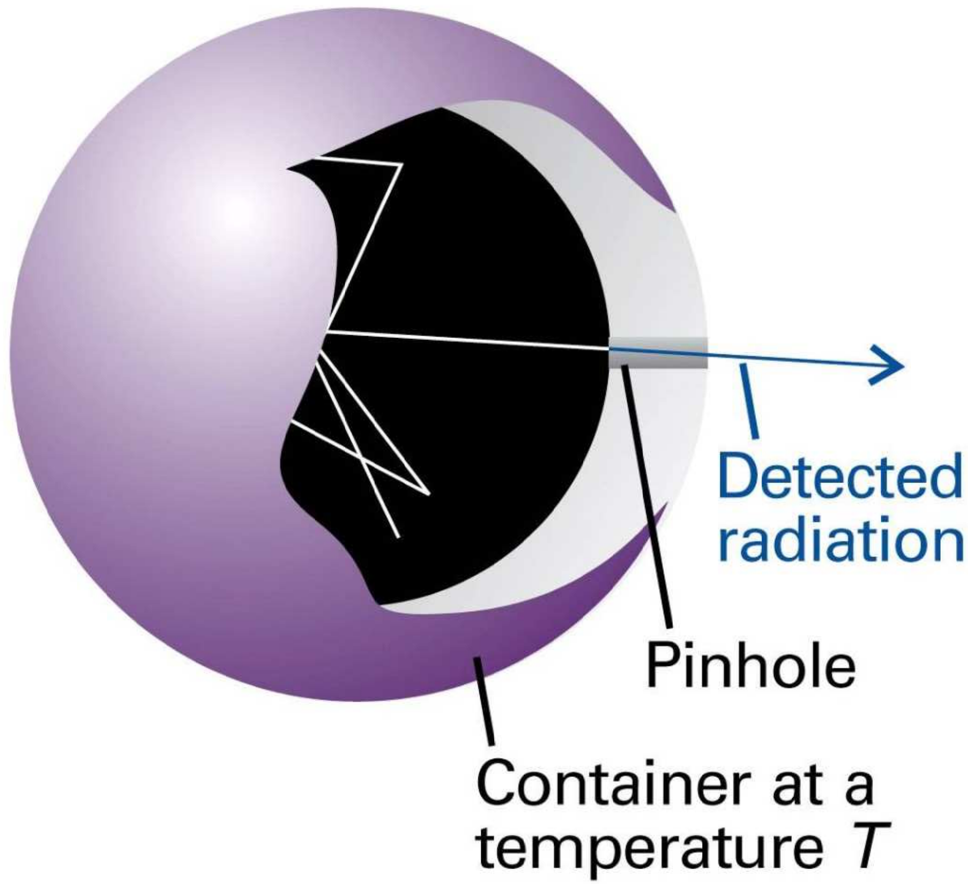


Figure 8-4
Atkins Physical Chemistry, Eighth Edition

Rayleigh - Jeans

1) # of modes in the range ν and $\nu + d\nu$

2) Average energy / mode

$$\rho(\nu)\, d\nu = \frac{8\pi\nu^2}{c^3} \times kT\, d\nu$$

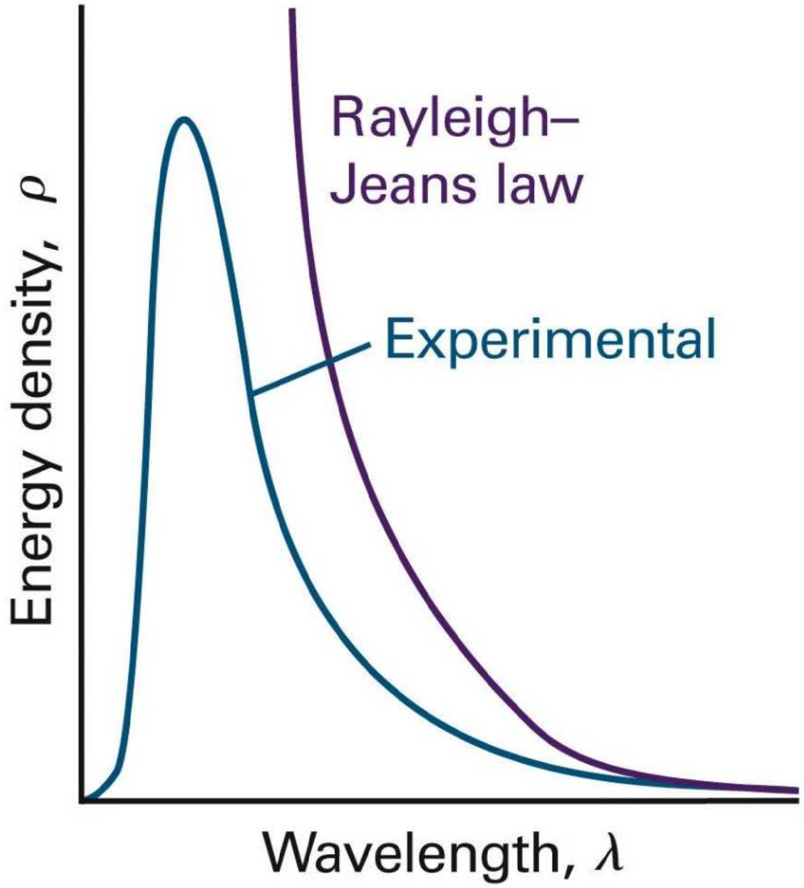


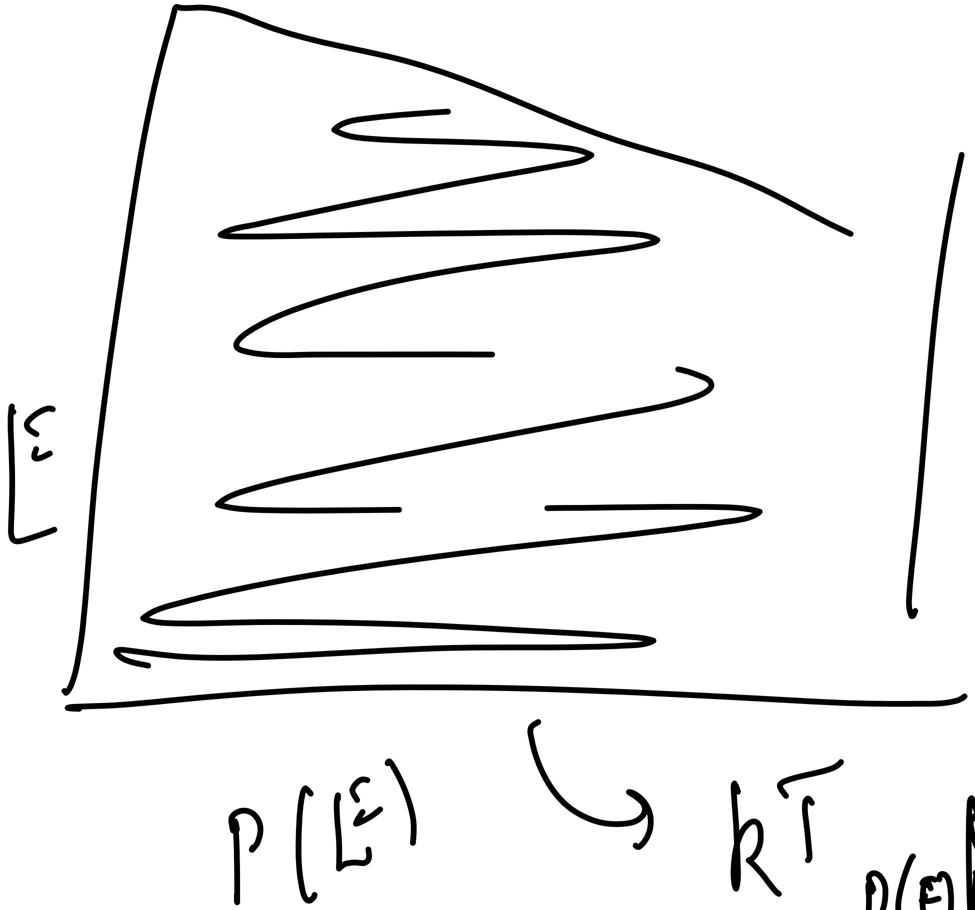
Figure 8-6
Atkins Physical Chemistry, Eighth Edition

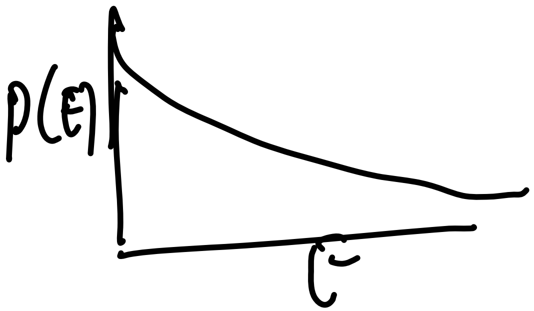
"Ultraviolet catastrophe"

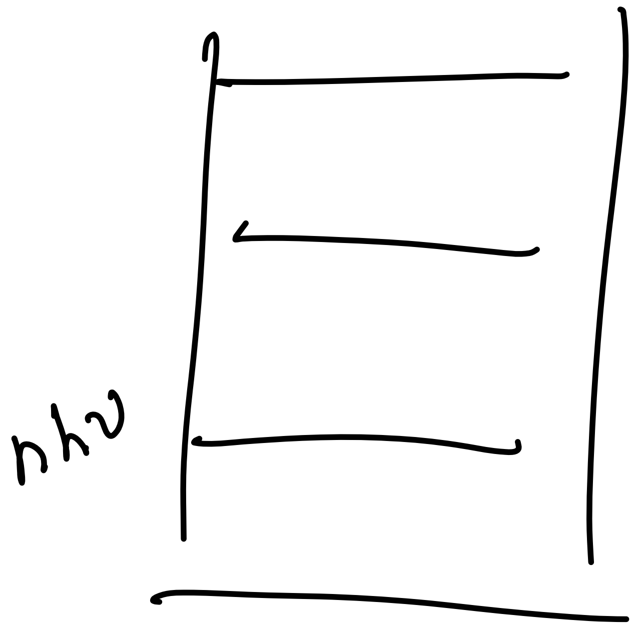
Planck

$0h\nu, 1h\nu, 2h\nu \ldots$

$nh\nu$


E
p(E)
kT


p(E)
E


nhν

$$\int \rho(\nu)\, d\nu = \int \frac{8\pi \nu^2}{c^3} \frac{h\nu}{e^{h\nu/kT} - 1} d\nu$$

\# of modes

energy / mode

$$= \sigma T^4$$

Stefan-Boltzmann

Wien's displacement law

$$\lambda_{max} T = \text{constant}$$

$$\rho(\nu)\, d\nu \longrightarrow \rho(\lambda)\, d\lambda$$

"COBE"

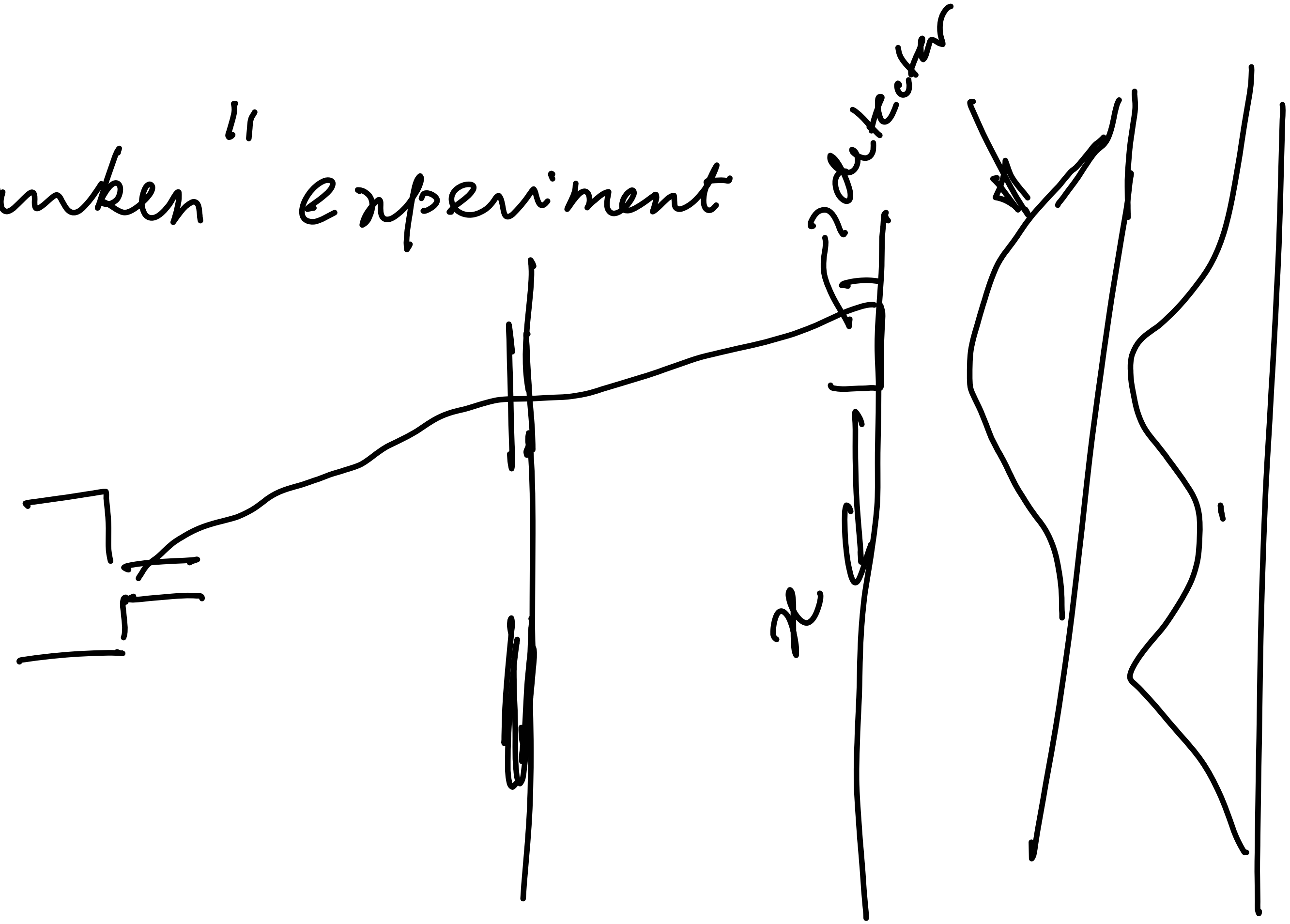
Quantization of oscillator energies

Atoms → Particles → { atomic Spectrum

Light → Wave { Photoelectric

"Gedanken" experiment

1)



Wave - particle duality

Photons - Maxwell

Schrödinger equation

Postulates of Quantum Mechanics

1) Particle in a box
2) Harmonic oscillator
3) Rigid rotor
4) Hydrogen atom
5) Bonds in molecules