# Spectroscopy – Physics & the Life Sciences

### **1** Broad Scientific Objectives

- Use theoretical predictions to determine, and
- Posit original questions that are falsifiable.

### Specific Objectives & Experimental Setup

- Verify a fundamental example in the quantum theory of matter
- Use spectroscopy to answer three questions, two of which you will form yourselves.

### Quantum Mechanics

Depending on your TA, you will be assigned one of the following two tasks:

- 1. The Hydrogen Atom & Atomic Spectra
- 2. Thermal Properties & Spectroscopic ignatures

#### Discrete Atomic Spectra

The hydrogen atom, consisting of one proton and one electron, is the starting point of anyone interested in quantum mechanics and quantum chemistry. Our task is to reproduce the Rydberg constant based on the spectrum of hydrogen gas.

The allowed energy values in the hydrogen atom looks obey the relationship  $E_n = \frac{-13.6eV}{n^2}$  for an electron in the *n*th orbital, where the 0eV scale is set to the difference between the electron being bound to the nucleus or not – negative energies imply a bound state. Then, the difference in energy between two bound states is  $\Delta E = -13.6eV\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$ , when the electron goes from an orbital  $n_1$  to  $n_2$ . Even before a formal theory of quantum mechanics was established, the discrete spectrum of hydrogen was known. The Swedish physicist Johannes Rydberg proposed the following relationship between the observed spectrum of hydrogen and positive integers  $n_1$ ,  $n_2$  and the observed wavelengths  $\lambda$ :

$$\frac{1}{\lambda} = R\Big(\frac{1}{{n_2}^2} - \frac{1}{{n_1}^2}\Big),$$

where R is the Rydberg constant.

Collect a sample hydrogen atom spectrum, and calculate the Rydberg constant (and uncertainty!) from the data.

Collect a sample of the Neon spectrum. What similarities are there? What differences? Does it seem reasonable to have a Rydberg-like formula for Neon? Why or why not?

#### Thermal Properties & the IR-spectrum

Vibrational states, quantum states describing molecular vibrations, also give some information spectroscopically. In recitation, we have explored models of diatomic molecules that involve a spring-like force between the nuclei with discrete (quantized) amplitudes/energies. The springs model with quantized amplitudes give a convenient qualitative picture of the physics. Wein's law states that a blackbody (a perfect emitter/absorber of radiation) will have a peak in its emission spectrum according to

$$\lambda_{max}T = b$$

where  $\lambda_{max}$  is the wavelength of peak emission, T is the temperature in Kelvin, and b is Wein's displacement constant, with value  $2.8978 \times 10^{-3}m \cdot K$ . For objects about 300K, this peak occurs in the far infrared. While Wein's original derivation did not use quantum mechanics, Max Planck re-derived Wein's law using the assumption of E = hf that then led Einstein to describe the photoelectric effect, one of the initial experiments leading to quantum mechanics.

Using Wein's law, utilize your spectrometer to determine the effective temperature of three objects in the room, along with uncertainties calculated by the Full-Width at Half-Max approach.

### Using Spectroscopy to Probe the World Around Us

Once you have the quantized nature of matter, use spectroscopy to probe practical (fun) questions about the objects around you. Your task is to answer 3 questions by using spectroscopy. The first question is common to everyone in lab to help start this process.

#### What makes White Light White?

Examine at least 3 white light sources spectroscopically. What qualitative predictions do you have about the spectra and how similar/different they will be? After measuring the spectra (and doing any relevant data manipulation), how accurate were your predictions? If any of your spectra look drastically different, explain what this says about the materials that generate the light, and in particular, what can you say about the mechanisms to generate the light.

#### Two Original Questions & Spectrographic Data

Once you have examined white light sources, create two original questions that can be answered with spectroscopy. For each question, pose the question along with any biological significance, a hypothesis and reasoning for what you believe will happen, and how you will test it using the tools available in lab..

Note, that these have to be original questions, not just asking the same question twice, e.g. you can't reuse the same question, once for red light and one for blue.

## **Expectations of Data Analysis**

A standard method of error analysis for spectra is called Full-Width at Half-Maximum (FWHM), which has convenient values for Gaussian & Lorentzian distributions. The uncertainty of a peak is given in part by the full width at half maximum, plus any uncertainties from other sources. When determining the Rydberg constant or temperatures of objects for the quantum mechanics portion of the lab, you are expected to perform uncertainty analysis of those objects.

## **References & Acknowledgments**

This lab is adapted from a Nexus Physics lab from the University of Maryland, originally developed by K. Morre, J. Giannini, K. Nordstrom, and W. Losert:

UMD Nexus PhyiscsLab: Analyzing light spectra and exploring implications for living systems.

Wein's Displacement Law & constant value taken from the Wikipedia article on Wein's Law.