

Protocol | Quantum Mechanics

Quantum Mechanics of Light and the Atom

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Bring a laptop computer to lab this week.

Introduction

Watch the [introduction and theory video](https://youtu.be/t18vNFcUuFo)  [\(https://youtu.be/t18vNFcUuFo\)](https://youtu.be/t18vNFcUuFo) for this experiment.

Objects at atomic or sub-atomic scales do not behave like the macroscopic objects of our everyday experience. Rather than being governed by the physical laws of classical mechanics, very small entities are governed by quantum mechanics. At its heart, quantum mechanics starts from the idea that all objects have both particle-like properties such as position and velocity *and* wave-like properties encoded in a wave function. Trying to interpret one set of properties in terms of the other leads to very non-intuitive conclusions, such as “particles can only take on particular energy values” or “waves collapse into particles upon measurement.” Ultimately, quantum-mechanical entities are neither particles nor waves, although they have properties related to both concepts.

Although quantum mechanics may seem very abstract and theoretical due to the small scales involved, it does have very important practical implications in chemistry. Atoms, molecules, and light are all small enough to be governed by quantum mechanics. As such, the interaction between light and matter is a fundamentally quantum-mechanical phenomenon. Even a question as simple as “why do objects have color?” requires quantum mechanics to be answered in detail. In this experiment, we will investigate several macroscopic manifestations of the quantum nature of light and atoms.

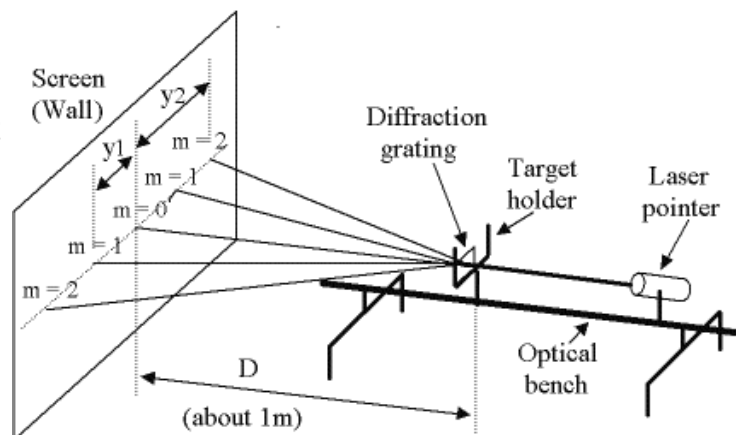
Light as a Wave Phenomenon

Light was classically viewed as a wave due to its tendency to diffract through small openings and refract in different media. According to the classical picture, light is an oscillating wave of electric and magnetic fields. The electric and magnetic fields oscillate at right angles to one another as the wave travels through space. This oscillation explains a variety of optical phenomena as well as the ability of light to cause charged particles such as electrons to move back and forth. A light wave is characterized classically by its *intensity*, *frequency* ν (units of time^{-1}), and *wavelength* λ (units of length). Intensity reflects the amplitude of oscillation of the light wave. Frequency and wavelength are inversely related to each other as their product is equal to a constant, the *speed of light* $c = \lambda\nu$.

In this experiment, we will observe the *diffraction* of light through a grating, a classic wave property. When a light wave encounters a small opening whose width is on the same order as the wavelength

of the light wave, the opening acts as a source for a new circular light wave. A diffraction grating contains regularly spaced grooves that act like these openings. Thus, when light passes through a diffraction grating, a large number of circular waves are generated that overlap and interfere with one another. The result is a regular pattern of repeating spots on the other side of the diffraction grating. A screen or board can be used to detect these spots.

For a laser light source with small radius, we define the *angle of diffraction* θ as the angle formed by the un-diffracted central spot, the point on the diffraction grating where the laser light strikes, and the diffracted spot closest to the central line. This angle is related to the wavelength of the laser light λ and the distance d between grooves in the grating. The beauty of this relation is that we can use macroscopic measurements of distances (y_1 and D) to draw a conclusion about a very small microscopic distance d .



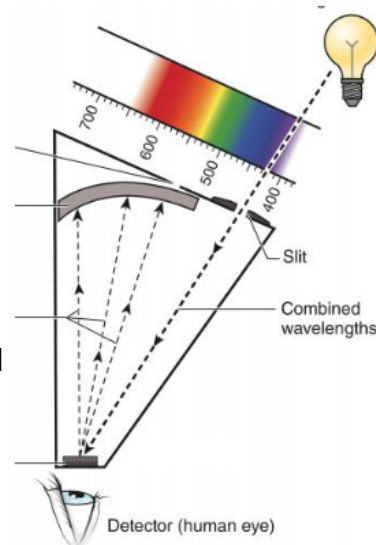
$$\frac{\lambda}{d} = \sin \theta = \frac{y_1}{\sqrt{y_1^2 + D^2}}$$

Diffraction is useful in general for determining microscopic distances. For example, light in the x-ray region of the electromagnetic spectrum is of the right wavelength to diffract appreciably when passed through a crystal. Angles formed by the diffracted light enable the determination of bonding distances and orientations within the crystal. Diffraction is also useful for separating a light beam containing multiple wavelengths into its “pure” wavelength components. The angle of diffraction depends on the wavelength of light, so passing a mixture of different wavelengths through a diffraction grating spreads out the different wavelengths in space. This is the basis of the *spectroscope*, a handheld device containing a diffraction grating used to measure the wavelengths in an incoming light beam.

The input light beam comes through a slit on the left-hand side of the device. The beam travels through a grating and the separated light is reflected onto a wavelength scale. We will use a handheld spectroscopy to measure the wavelengths of light emitted by excited atoms (see below).

Light as a Stream of Particles

The observation that light can cause the ejection of electrons from a metal surface (the photoelectric effect) forced a re-evaluation of the idea of light as a wave. The kinetic energy of ejected electrons depends on the frequency of the light but not on its intensity, which contradicts the classical wave theory of light. Furthermore, below a minimum frequency



that depends on the metal, the ejection of electrons was not observed (also not consistent with the classical model). A simple explanation for the photoelectric effect, first articulated by Einstein, started from the idea that light consists of particles with energy E proportional to their frequency ν . Such particles are called *photons*.

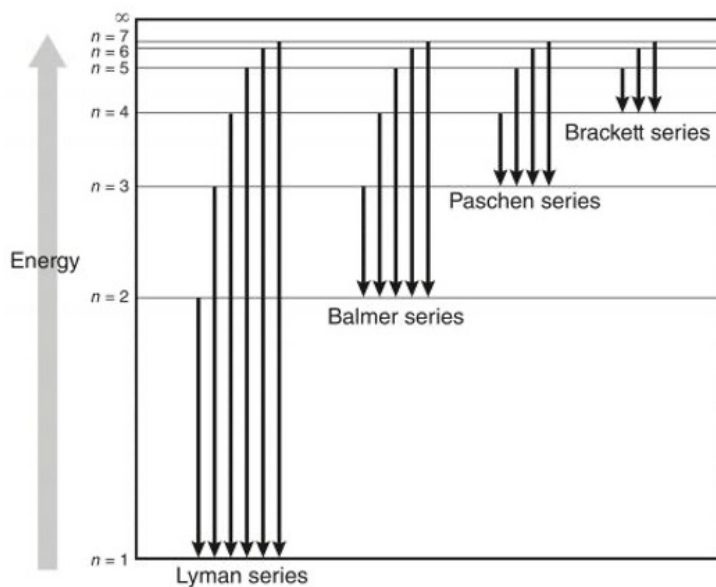
$$E = h\nu = \frac{hc}{\lambda}$$

In the end, quantum theory landed on the notion that light has both particle-like and wave-like properties. The ideal perspective to take depends on the phenomenon under investigation. In this experiment, we will make some observations that suggest light is a wave and others that suggest light behaves like a stream of photons.

Atomic and Molecular Electrons as Waves and/or Particles

Unlike light, the constituents of atoms and molecules were classically viewed as particles. However, observations of the energies of electrons within atoms demanded a re-evaluation of this idea as well. Electrons bound in atoms followed constrained dynamics in a manner reminiscent of the standing waves of a plucked string. The wave-like properties of an electron are captured by its *wave function* or *orbital* ψ , a mathematical function that encodes the probability of finding the electron “particle” at each point in space. Because of the wave-like nature of the electron, we cannot in general locate it at a specific position: it is “smeared” over all space in a probabilistic way. However, orbitals are constrained by the structure of the atom in such a way that only *specific, discrete* values of electronic energy are allowed. In this experiment, we will observe firsthand that atomic orbitals are associated with discrete energy levels.

Using observations of the light emitted by excited hydrogen atoms, we will measure the orbital energies of the electron in the hydrogen atom relative to the $n = 2$ level, where n is the *principal quantum number*. The electron in an excited hydrogen atom emits visible light at one of four very precise wavelengths as it relaxes from $n = 6, 5, 4$, or 3 to the $n = 2$ level; these wavelengths form a group called the Balmer series. Each wavelength is associated with a *transition* of the electron between two principal quantum numbers n_i and n_f . For a transition involving emission of a photon n_f is less than n_i , and for the Balmer series $n_f = 2$. By fitting wavelength measurements to a mathematical model, we will gain insight into how the energy of the electron in the hydrogen atom depends on n and we will make a prediction concerning the electronic energy when $n = 1$.



Note that we can associate each transition with a change in energy ΔE . The wavelength of light observed when an emissive transition occurs reflects ΔE and the definition of the energy of the photon.

$$\Delta E = E(n_f) - E(n_i) = -\frac{hc}{\lambda}$$

Thus, we can use a measured wavelength to determine the energy gap associated with a transition between electronic energy levels. The negative sign appears because for an emissive transition $E(n_f)$ is less than $E(n_i)$, but wavelength is necessarily positive.

Safety and Materials

In this experiment, we will work with lasers and atomic gas-discharge lamps, both of which present some rather unconventional hazards. Lasers are high-intensity light sources that can damage the eyes, so make sure to avoid looking directly at the beam or pointing it at someone else. (Generally, you should leave the lasers set up as they are in the lab and just turn them on and off as needed.) The atomic gas-discharge lamps use a very high voltage to excite and ionize atoms; as the atoms relax back to the ground state, they emit photons. The very high voltages of these devices present a serious electrical hazard—only switch the lamps on and off as needed. High current flows also cause the lamps to get very hot, so take care when operating them. Stand a safe distance back from the lamp when recording a spectrum using the handheld spectroscope.

Relevant Experimental Techniques

[Working with a Handheld Spectroscope](https://www.youtube.com/watch?v=LOV52BYfAeU&list=PLykBd3LSjfsSRFat96li9c1WhwBbqIGPd&index=8)  (<https://www.youtube.com/watch?v=LOV52BYfAeU&list=PLykBd3LSjfsSRFat96li9c1WhwBbqIGPd&index=8>)



Procedures

A. Diffraction: Light as a Wave

1. At the front of your lab room you will find red ($\lambda = 633 \text{ nm}$) and green ($\lambda = 532 \text{ nm}$) laser pointers and a diffraction grating. Set up the grating and lasers so that the dry erase board in your lab room acts as a “detector” for laser light that passes through the diffraction grating.
2. With help from your lab partner, turn on the red laser and ensure its light passes through the grating. Measure and record the distance D from the grating to the central un-diffracted spot of laser light and the distance y_1 between the central spot and the first diffracted spot (see the diagram in the Introduction).
3. Repeat these measurements twice more so that you have three measurements each of D and y_1 .

4. Repeat steps A-2 and A-3 for the green laser. *Before turning on the laser*, make a prediction concerning the angle of diffraction of green laser light relative to red laser light. Do you expect the spots to be closer together or farther apart? Discuss with your lab partner.

B. The Photoelectric Effect: Light as a Stream of Particles

1. Access and run a simulation of the photoelectric effect here:
<https://phet.colorado.edu/en/simulation/photoelectric> 
(<https://phet.colorado.edu/en/simulation/photoelectric>). A recent version of [Java](https://java.com/en/) 
(<https://java.com/en/>) is required.
2. From the *Target* dropdown menu, select a metal and record your choice. Use the *Intensity* slider to set the intensity of light impinging on the metal to 75%. **Note:** you and your lab partner should choose different metals and pool your data before leaving the lab.
3. Determine the maximum wavelength of light (the threshold wavelength) required for ejection of electrons from the metal. To do this, move the *Wavelength* slider all the way to the right into the infrared and carefully decrease the wavelength of light until you observe non-zero current. Record the threshold wavelength of your chosen metal to the closest nanometer.
4. The metal is layered on top of a capacitor that is connected to a battery. The battery can be adjusted to apply a *stopping voltage* that prevents ejected electrons from reaching the opposite plate by attracting them back to the metal. The absolute value of the *minimum* (in magnitude) stopping voltage in Volts is equal to the maximum kinetic energy of ejected electrons in electron-Volts (eV).
5. For eight wavelengths *shorter* than the threshold wavelength covering a range of at least 150 nm (100 nm for platinum), measure and record the minimum stopping voltage. To do this, first select the wavelength of light and then carefully adjust the battery voltage until you *just* observe zero current. Record the wavelength and stopping voltage, keeping in mind that the *absolute value* of the stopping voltage is equal to the maximum kinetic energy of ejected electrons.
6. You now have a data set that relates the wavelength of light impinging on the metal and the maximum kinetic energy (KE) of emitted electrons (the absolute value of stopping voltage simply written with units of eV). This data is nonlinear. Why do you think this is? How could you transform the data to make it appear linear? Consider the particulate or photon model of light.

C. Measurement of the Emission Spectrum of an Incandescent Bulb and the Hydrogen Atom

1. **Partner I** should operate the spectroscope in this part of the experiment and **Partner II** should record wavelengths. Wear gloves when handling the spectroscope and if desired, disinfect it with ethanol spray.
2. Obtain a blue handheld spectroscope and identify the eyepiece, slit for incoming light, and wavelength scale. The top of the device lists some important wavelengths with their

associated elements; make sure to hold the device so that the top points up.

3. Use the fluorescent lights overhead to practice measuring wavelengths. The mercury in these lamps has a characteristic green line at 546 nm. If necessary, slide the scale slightly to calibrate it, so that the green line appears at exactly 546 nm.
4. On the benches in your lab room, you will find an incandescent light bulb and a series of atomic discharge lamps. Align the spectroscope slit with the incandescent bulb and record wavelength *ranges* for the following colors: red, orange, yellow, green, blue, and violet. There is some subjectivity here; estimate to the closest 10 nm.
5. Point the spectroscope at the **hydrogen** atomic discharge lamp, which glows light purple. Carefully align the input slit with the lamp tube, so that you see bright lines appearing on the wavelength scale. Red, blue-green, and deep blue lines should appear. You likely will not see a deep violet line at 410 nm; make sure to record this line as well. With help from your lab partner, record the wavelengths of light emitted by excited hydrogen atoms.

D. Observation of the Emission Spectra of Other Elements

1. **Partner II** should operate the spectroscope in this part of the experiment and **Partner I** should record wavelengths. Wear gloves when handling the spectroscope and if desired, disinfect it with ethanol spray.
2. Repeat step C-4 for two other elements of your choosing. Available elements in atomic discharge lamps include **neon**, **mercury**, and **helium**. When you see large numbers of lines clustered close together, record wavelength ranges and an approximate number of lines within each range.

Group Modeling

Discuss the data with the other students at your bench. Using hydrogen, work through the calculations to obtain energy values for 4 energy levels above the valence electron shell (the Data Workup section also describes the process for hydrogen which has a valence shell of $n=1$.) When determining which wavelength corresponds to a particular energy gap between energy levels, refer to the electromagnetic spectrum for relative energy values of each color observed. A larger energy should correspond to a larger energy gap!

Consider the formula below considering that the value of the constant factor (R) used to incorporate Rydberg's and Planck's constants is 2.179×10^{-18} J.

Formula for the energy of electron transitions:

$$\Delta E = -\frac{hc}{\lambda} = -R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Measured energy differences between levels:

$\Delta E = -hc/\lambda$ where, Planck's constant, $h = 6.626 \times 10^{-34}$ J*s, the speed of light, $c = 2.99 \times 10^8$ m/s, and wavelength, λ is in units of meters.

Expected energy differences between levels:

$\Delta E = -R (1/n_f^2 - 1/n_i^2)$ where, Rydberg's constant, $R = 2.179 \times 10^{-18}$ J, n_f refers to the first energy level above the valence shell (i.e. 2) and n_i refers to each energy level above it (3,4,5,6) in order of smallest to largest energy difference from the lowest level (2).

Discuss and generate a model using the white board to represent the energy levels in the atom of interest and the movement of electrons between them upon the release of photons of light. Your model can be a graph of some sort, an atomic drawing with labeled energy gaps and electrons, a Jablonski-style diagram similar to the background section, or any other model your group prefers to visualize your explanation. If there is time, discuss your model with other groups and make revisions before drawing it in your lab notebooks.

Post-lab Calculations and Data Workup

Use the [data workup spreadsheet \(https://gatech.instructure.com/courses/334258/files/42101059?wrap=1\)](https://gatech.instructure.com/courses/334258/files/42101059?wrap=1) [↓ \(https://gatech.instructure.com/courses/334258/files/42101059/download?download_frd=1\)](https://gatech.instructure.com/courses/334258/files/42101059/download?download_frd=1) to work with your data while following the instructions below.

Part A. Tabulate your measured spacings between spots and distance from the diffraction grating to the wall (Table 1) and calculate the microscopic spacing d between grooves in the diffraction grating for each set of measurements in micrometers (μm). Consider whether your results for the two lasers are consistent with one another.

Part B. Tabulate your metal, threshold wavelength, and wavelength-kinetic energy (KE) data (Table 0-1). Note that the kinetic energy of ejected electrons in eV is simply equal to the stopping voltage in V. Transform the wavelength-KE data so that a plot of the transformed data appears to be linear. (*Hint:* consider the relationship between the *frequency* of impinging light and the kinetic energy of ejected electrons.) Plot the transformed data (Figure 1) using carefully labeled axes with units. Make sure to plot the independent variable on the x-axis and the dependent variable on the y-axis. Add a line of best fit with equation and correlation coefficient R^2 . Include two the metals you have measurements for on the same graph and compare the slopes and intercepts of the lines.


The slopes are related to an important physical constant with great relevance to quantum chemistry. Identify the constant, and using the average of the two slopes and $c = 2.998 \times 10^8$ m/s, calculate its value based on your data.

Part C. The energy of the $n = 2$ level of the hydrogen atom is -3.40 eV. Using this value along with your four measured wavelengths for hydrogen, determine the energies of the next four energy levels: $n = 3, 4, 5$, and 6 , adding these to the Hydrogenic Energy Level column (Table 0-2). Make use of the idea that $\Delta E = -hc/\lambda$ for emissive transitions and the fact that as ΔE increases n_i must increase, because $n_f = 2$ for all the transitions we observed.

For the hydrogen atom (and *only* the hydrogen atom!) there is a simple theoretical relationship between the principal quantum number n of the electron and its energy E .

$$E \propto \frac{1}{n^2}$$

Using your calculations so far, plot the energy E (in eV) of each hydrogenic energy level as a function of $1/n^2$ for $n = 2$ through 6 (Figure 2). Add a line of best fit to the plot with equation and correlation coefficient R^2 . Use the equation of this line to predict the energy of the electron in the ground state of the hydrogen atom, for which $n = 1$.

Part D. As part of the post-lab assignment for this experiment, you will create digital images of the spectra you observed for elements other than hydrogen. To convert your measured wavelengths to spectral images (Figures 3 and 4), download and unzip [this file](https://gatech.instructure.com/courses/334258/files/42101079?wrap=1) (<https://gatech.instructure.com/courses/334258/files/42101079?wrap=1>)  (https://gatech.instructure.com/courses/334258/files/42101079/download?download_frd=1) and open index.html in a web browser.