Spectroscopy Lab: Group 2

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I. INTRODUCTION

Spectroscopy is a useful tool in many applications to better understand light and its emission and absorption lines. Spectroscopy has been around for centuries but has only recently been used to analyze quantum mechanics quantities. Spectrometers work by shining light through an object such as a prism and then refocusing the light to measure across a wide array of wavelengths. In quantum mechanics, the light is pointed towards a quantum well or quantum dots, and the emission and absorption spectra can provide information on the energy required to excite electrons between the conduction and valence bands of the shell. It is a very similar process to the quantized energy levels seen in atoms, where electrons need photons of a specific wavelength to excite to the next state. Quantum dots have many biophysical applications including medicine delivery and bioimaging; they are also useful in solar cells. The information that spectroscopy provides is not only about the energy that is required to make the jump but also about the probabilities. The more intense the peaks can be, the higher likelihood that these jumps are being made. This lab consists of two different experiments, one to measure the size of the quantum dots that come in two shapes, spherical and ellipsoidal, and to measure the width of the quantum wells in a sample with four finite potential cases. These experiments were carried out by firing different light sources, such as UV and a Halogen lamp at the samples and measuring their intensity and wavelength.

II. THEORETICAL BACKGROUND

A. Quantum Dots

Quantum dots are semiconductor nanocrystals with special conduction properties and in this particular case, they are composed of a core, shell, and polymer coating. The shell is made of ZnS in this experiment, and the core is CdSe. As UV light enters the quantum dot the shell will absorb the light and the electron will make the jump from the valence band to the conduction band leaving a hole. The electron will then settle into the core of CdSe and can release the energy it once absorbed by emitting light. A diagram depicting these three transitions can be seen in Figure 1.

In this lab, quantum dots have two distinct shapes a spheroid and an ellipsoid. The can, however, be approximated as a three-dimensional particle in a box. The sphere is represented by a cube with side lengths, a, and the ellipsoid is represented by a rectangular prism with side lengths $b, b, 2.2b$. By treating this approximation as a particle in a box and using equations from the finite potential well, the information can be carried over to a three-dimensional version with the energy of the system given by the equation,

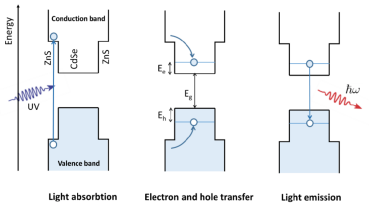

FIG. 1: The figure shows the layout for the theoretical setup consisting of the conducting and valence bands and the movement of the electrons through them as light is either absorbed or emitted. The graph shows energy as a function of position x [1].

$$E_\alpha(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2m_\alpha^*}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right). \quad (1)$$

L denotes the dimensions of the box in three dimensions, x,y, and z and m_α^* is the effective mass, with $m_e^* = 0.13m_e$, where m_e is the mass of an electron, and $m_h^* = 0.45m_e$. E_α can describe either E_h, which is the energy of the hole ground state, or E_e, which is the energy of the electron ground state. Their relationship can be seen in Figure 1, where E_g is the band gap energy. These terms are related by the equation,

$$\hbar\omega = E_g + E_e + E_h, \quad (2)$$

where ω is the angular frequency of the emitted light[2].

B. Quantum Wells

The quantum well experiment follows a very similar approach only now the setup is shown in the graph in Figure 2. The wells are created by using two different materials, GaInP and GaAs, and the thickness of each of the wells is given by L_I, L_{II}, L_{III}, and L_{IV} respectively.

The equation to relate the energy is relatively similar to the quantum dots and is given by

$$\hbar\omega = E_g^{GaAs} + E_e + E_h, \quad (3)$$

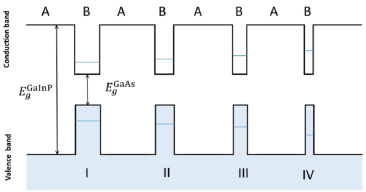

FIG. 2: The figure shows the layout for the theoretical setup consisting of the conducting and valence bands for four different quantum wells of varying thicknesses [1].

where $E_g^{GaAs} = 1.52eV$ and the larger band gap (shown in Figure 2) $E_g^{GaInP} = 1.96eV$. This creates a potential well of height V_0, whose value is shown in the equation,

$$V_0 = \frac{E_g^{GaInP} - E_g^{GaAs}}{2} = 0.22eV. \tag{4}$$

Finite wells are notoriously difficult to solve and usually require numerical solutions, however, in this case the relationship between the energies is enough. After solving the Schrödinger equation and finding the wave equations, the remaining coefficients can be matched to find an equation that determines the allowed energies. For this case, the equation is given by,

$$tan\left(\frac{L}{2}\sqrt{\frac{2m_\alpha^*}{\hbar^2}E_\alpha}\right) = \sqrt{\frac{V_0 - E_\alpha}{E_\alpha}}. \tag{5}$$

In the case of quantum wells, $m_e^* = 0.067m_e$ and $m_h^* = 0.48m_e$. The width of the well, L, can now be graphically found by finding the point of intersection for the hole ground state and the electron ground state [2].

III. METHODS

As stated, the main focus of this experiment was on investigating the energies of bound states of electrons in two different types of samples. That is, a sample containing Quantum Dots, and the other containing Quantum Wells. The method employed was based on measuring the absorption and emission spectra of each sample. The utilization of quantum dots that fluoresce in two colors, green and orange, was made use of in the lab. The dots, which consisted of an innermost composition of Cadmium selenide (CdSe) and a Zinc sulfide (ZnS) shell, were capable of luminescence in these colors. The absorption spectra were measured by utilizing a Halogen lamp, which was employed to irradiate the sample. Prior to measuring the sample spectra, a reference spectrum was measured using a solvent vial (containing no Quantum Dots) placed in the light path. Subsequently, a vial containing suspended Quantum Dots was inserted into the light path, and spectra were measured. Additionally, to observe what ratio is absorbed, the obtained spectra were then subtracted from the reference spectra, and normalized by the reference spectrum: $\left(\frac{I_d - I_s}{I_d}\right)$. To obtain the emission spectra, the sample was irradiated with a UV LED torch, and the resulting spectra were measured. The wavelengths obtained from the emission spectra were utilized to calculate the dimensions of the Quantum Dots. This setup is depicted in Figure 3.

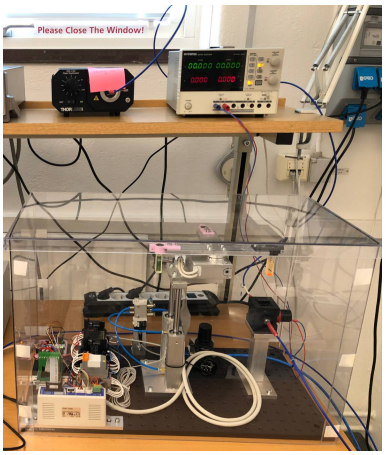

FIG. 3: The figure shows the layout for the Quantum Dots experiment setup consisting of a halogen lamp, a sample holder, a spectrometer, and the Sample containing Cuvettes.

The setup used for the Quantum Wells experiment consisted of a laser source, a mirror to control the direction of the laser light to increase the accuracy of the obtained data, and a spectrometer whose data was visualized and studied using computer software connected to this measuring instrument. With regard to the Quantum Wells, the sample was irradiated with UV-light, and the resulting emission spectrum was measured in this study. The relevant frequencies of the emitted light were deduced from the spectrum, and the ground state energies were determined by numerically solving the bound state equation. The widths of the four quantum wells were estimated in this study by utilizing the measured frequencies and the results obtained from the aforementioned equations. This setup is depicted in Figure 4.

Visualization of the spectral peaks as well as technical adjustments to both settings was made possible by using software specifically programmed for this purpose. Numerical analysis and graph generation were conducted using Excel.

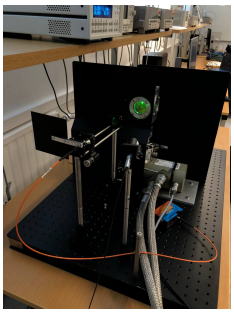

FIG. 4: The figure shows the layout for the Quantum Wells experiment setup consisting of a laser source, a spectrometer connected to a computer, a mirror to adjust the direction of the laser beam, and a Cryostat.

IV. RESULTS

A. Quantum Dots

The intensity values for the quantum dot samples were collected from the two vials and subsequently subtracted from the reference spectra vial, seen in Figure 5, which contained no quantum dots, resulting in the graphs of Figures 6 and 7. The peak wavelength corresponding with the color of the sample were then found to be $528nm$ and $593\,nm$ from the green and orange samples respectively. These two data points can be seen on their appropriate graphs in orange. Unfortunately, we did not measure data for the emission spectra of the two quantum dot samples, but if we had done so we would expect graphs with a noticeable peak at the corresponding peak wavelength. For the Green Quantum Dot emission spectrum we would expect a peak at wavelength $528\,nm$ and for the Orange Quantum Dot Emission spectrum we would expect a peak at wavelength $593\,nm$ (as seen in Figures 6 and 7 respectively).

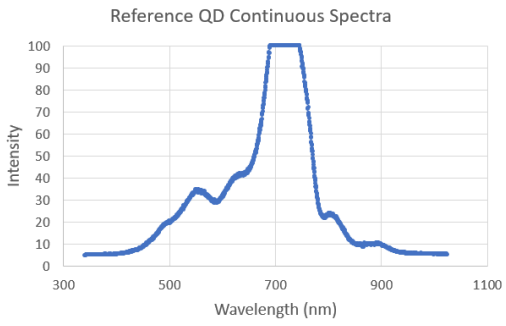

FIG. 5: The figure above displays the results from measuring the reference spectra, which contained no quantum dots. This graph was utilized along with the absorption graphs of the sample spectra to result in Figures 6 and 7.

Equation 1 can be utilized to find an equation that can relate the wavelength of the sample to the side lengths of the Quantum Dot cube, a, and rectangular prism, b.

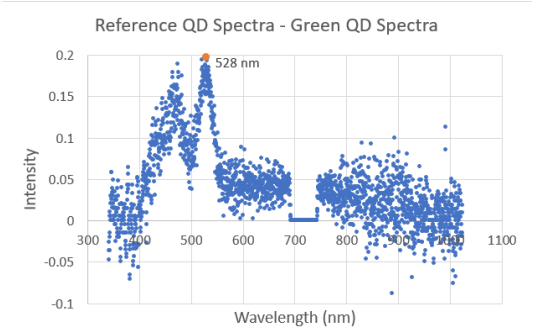

FIG. 6: The figure above displays the intensity values of the green quantum dot sample subtracted from the reference spectrum which has no quantum dots. The peak wavelength value chosen for the analyzation step is shown in orange with a label.

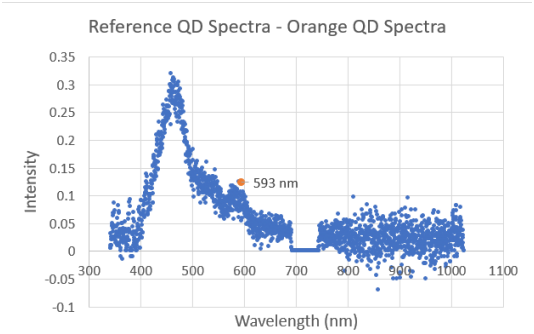

FIG. 7: The figure above displays the intensity values of the orange quantum dot sample subtracted from the reference spectrum which has no quantum dots. The peak wavelength value chosen for the analyzation step is shown in orange with a label.

This equation can be manipulated to solve for the side value of either a or b, which are represented in the values of L. All of the values of n are found to be one, the values of L in the equation correspond to the sides of the according shape, and the relationship $\hbar = h/2\pi$ was applied to change from rotational frequency ω to linear frequency f. The resulting equations are

$$a = \sqrt{\frac{3\hbar^2\pi^2}{2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right)\frac{1}{(\hbar\omega - E_g)}}, \tag{6}$$

for a and

$$b = \sqrt{\frac{2.2\hbar^2\pi^2}{2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right)\frac{1}{(\hbar\omega - E_g)}}, \tag{7}$$

for b. The found vales for a and b are $a = 4.29\,nm$ and $b = 1.99\,nm$, which both fall within the expected order of $10^0\,nm$.

B. Quantum Well

The Quantum Well data was collected from the experimental set up after properly setting the machine with the appropriate parameters. Once the appropriate values were collected, the integration time was automatically set with Figure 8 being the result. The four peak wavelengths corresponding to the four different quantum wells were then collected and used for further analyzation. These four values are $650\,nm$, $680\,nm$, $711\,nm$, and $732\,nm$ and can all be seen on Figure 8 in orange.

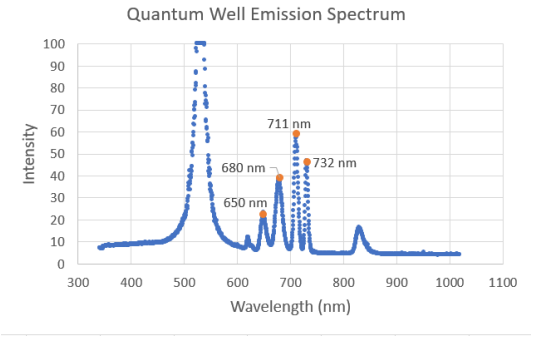

FIG. 8: The figure above displays the results from the quantum well experiment with the four peaks that have wavelength values and orange dots associated with them represent the four quantum wells as seen in Figure 2. The other three peaks come from reflected green light, the GaInP transition, and an unshown transition between a large width of GaAs material to the right of the quantum wells in Figure 2.

After these four values were collected a python script that calculates and plots Equation 5 was utilized to find the four corresponding L values. The Python script works by calculating and plotting the right hand side, the left hand side where $\alpha = e$, and the left hand side where $\alpha = h$ of Equation 5. The sum of the intersection between the right hand side equation and the two left hand side equations is equal to the total energy released by the electron subtracted by E_g^{GaAs} as shown in Equation 3.

Finally, by varying the L value until the added intersections equal the energy value of the calculated electron, $\hbar\omega$, the proper L value can be found for each wavelength of light collected. These four values can be found in Table I which contains said L values along with their associated wavelength. These values are all reasonable and well within the expected range of values for the diameters of the quantum wells.

V. DISCUSSION

The spectroscopy experiment aimed to investigate the properties of quantum dots and quantum wells. In the quantum dot experiment, the intensity values for the green and orange quantum dot samples were collected, and the peak wavelengths for each were found to be $528nm$ and $592nm$, respectively. These peak wavelengths were then used to determine the side lengths of the quantum dot cube and rectangular prism. The calculated values for a and b were $4\,nm$ and $1\,nm$, respectively, which fell within the expected order of magnitude. Therefore, the experiment was successful in determining the size of the quantum dots.

L Values for Each Wavelength				
Wavelength	$650\,nm$	$680\,nm$	$711\,nm$	$732\,nm$
L Value	$0.629\,nm$	$1.30\,nm$	$2.16\,nm$	$2.94\,nm$

TABLE I: The table showcases the various L values found from the peak wavelengths in Figure 8. The four L values are associated with their corresponding wavelength values from Figure 8 and were calculated using the procedure described in Section IV B.

In the quantum well experiment, four peak wavelengths were found to be $649\,nm$, $679\,nm$, $711\,nm$, and $731\,nm$. These values were then used to calculate the L values of the quantum wells using a Python script that utilized Equation 5. The calculated L values were $0.62\,nm$, $1.3\,nm$, $2.1\,nm$, and $2.9\,nm$, which were reasonable and well within the expected range of values for the diameters of the quantum wells. Therefore, the experiment was successful in determining the diameter of the quantum wells.

Overall, the experiment was deemed to be successful in achieving its objectives of investigating the properties of quantum dots and quantum wells. The experiment's results provided valuable insight into the size of quantum dots and the diameter of quantum wells, which can have significant implications for the development of advanced electronic devices. In general, these results can be used to further our understanding of the behavior of quantum structures and their potential applications in various fields.

VI. ACKNOWLEDGMENTS

All three group members set up and performed the experiment. Natalie wrote the introduction and theoretical background; Alex wrote the results; Iman wrote the methods and discussion.

[1] Lab Manual Spectroscopy Lab
https://canvas.education.lu.se/courses/22074/files/3655950?module_item_id=865817

[2] Spectroscopy Lab Powerpoint https://canvas.education.lu.se/courses/22074/files/3685995?module_item_id=871126