

MODULE 4: All things Quantum

“Quantum mechanics makes absolutely no sense” – Roger Penrose, Mathematician

LEARNING OBJECTIVES

1. Learn the basics of quantum mechanics
2. Explore how quantum mechanics relates to materials science (specifically through band gaps and quantum dots)

BACKGROUND

Before we get into it, what is quantum mechanics? Quantum mechanics is a field of study in physics that describes the physical properties of the universe at small scales (such as atoms, electrons, and particles). In terms of size, think nano (or even smaller).

1. Wave and Particles

To really understand the difference between **waves** and **particles**, we have to start at the very beginning. For a long time, physicists believed that light was a wave. Well in the 1800s, they realized that light acted both like particles and waves (this is known as wave-particle duality, a concept we will get into later). How did they determine this, you may ask? To start, have you heard of the phenomena known as **blackbody radiation** or a **blackbody**? This is a theoretical object that absorbs all light without reflecting any back, like the color black. It also can radiate energy, but not all energy of a blackbody has the same intensity. You can predict the energy coming from a **blackbody** based on its temperature. When physicists came up with an equation to calculate this intensity, assuming that light was a wave, there was a big problem. [1]

Physicists realized that they may have been incorrect in their assumptions. The **Rayleigh-Jeans Law** predicted that a higher frequency of radiation (or a shorter wavelength) would have a higher intensity. Figure 1 shows the predictions from the Rayleigh-Jeans law [1]. This matched experimental information really well... up to a certain point. Physicists saw that once the frequency of light reached the ultraviolet zone or higher, the **Rayleigh-Jeans Law** did not fit the experimental results. What did physicists see instead? At a certain frequency, the light emitted by the **blackbody** would be the most intense, but the intensity would decrease as the frequency increased, as shown by the Planck Law curve in Figure 1. This peak remained as physicists continued their experiments. It was not supposed to be this way! Physicists expected to see an exponential increase of intensity as frequency also increased. At the root of it, **Rayleigh-Jeans Law** predicted that you would find infinite power. Unfortunately, this totally contradicts the **Law of Conservation of Energy**. The contradiction of the **Law of Conservation of Energy** (when using classical physics) is known as the **ultraviolet catastrophe**.

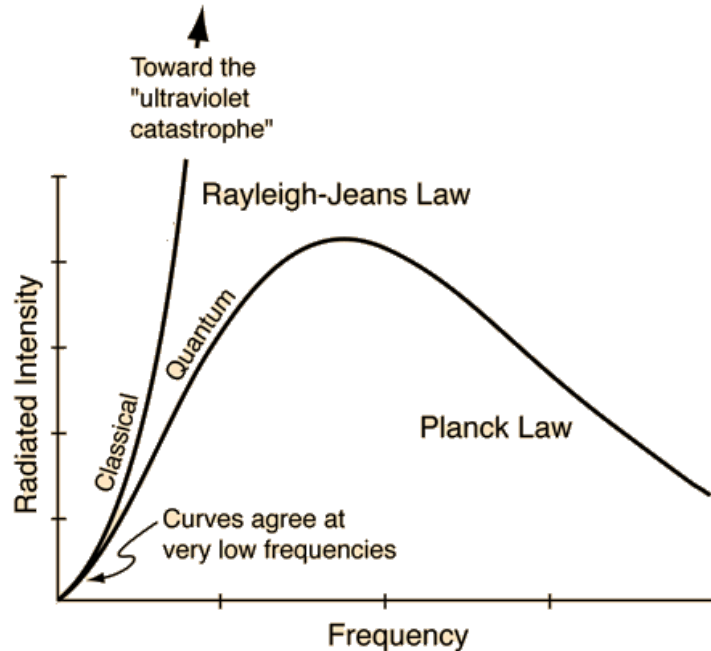


Figure 1. Comparison of Rayleigh-Jeans Law (Classical Physics) and Planck's Law (Quantum Mechanics) [2].

So, how did physicists make sense of this? In 1900, German physicist Max Planck came up with an equation that can be considered one of the founding equations of **quantum mechanics**. [1] He predicted that electromagnetic energy takes the form of tiny discrete packets known as **quanta**. At a certain point, you cannot divide energy into anything smaller than these **quanta**. The energy of each quanta, E , is given by the frequency of the light (ν) multiplied by a constant. This constant was later known as **Planck's constant** ($h = 6.626 \times 10^{-34} \frac{m^2 kg}{s}$). **Planck's Law** can be written as

$$E = h \times \nu . \quad (1)$$

When you predict the intensity of **blackbody radiation** and take **Planck's Law** into account, you end up with an equation that fits the experimental results perfectly. This resolves the **ultraviolet catastrophe!**

But, Planck's Law caused physicists to rethink the way they saw the world... [1] Before, physicists thought energy could be any size, but they found out there was a limit for dividing energy into smaller amounts. It was not until Albert Einstein's scientific achievements that physicists could work this out.

2. Photons and Photoelectric Effect

In 1921, Albert Einstein won the Nobel Prize in Physics, can you guess for what? He had argued that light energy travels in packets that are now called **photons**. This would essentially make light act like a particle. This seemed to contradict earlier experiments which suggested that light acted like a wave. Like any good scientist, Einstein proved what he was suggesting by conducting an experiment involving the **photoelectric effect**. The **photoelectric effect** describes

what happens when you shine a beam of light on a metal plate. **Figure 2.** describes how the experiment for the **photoelectric effect** works. Electrons leave the plate as the light hits it. The electrons leave and hit a collector creating a current. Einstein determined that if he studied the way the electrons left the plate, then physicists could learn about the properties of light. In both particle and wave theories of light predict that light knocks electrons off the metal plate, but each theory has different predictions about what and how this happens. [3]

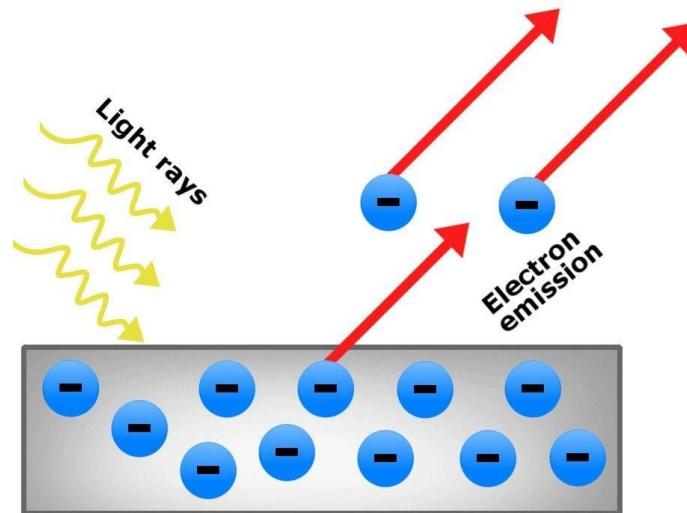


Figure 2. The photoelectric effect of light experiment [4].

The electromagnetic wave theory says that when a light wave hits an electron it exerts a force on the electron that ejects it from the metal. According to this theory when you increase the intensity of the light you increase the strength of the electric field hitting the electrons, which increases the number of electrons that are being ejected from the plate. Consequently, the electrons have a higher speed as they leave the metal plate which results in a higher **kinetic energy** (this is the **kinetic energy** of the fastest electron as it leaves the plate. In wave theory though, the frequency of the light should not make a difference, ONLY the intensity. [1]

On the other hand, **particle theory**, says the electrons get ejected from the metal when they are hit by individual **photons**. The **photon** transfers its energy to the electron, which then leaves the metal. This destroys the **photon** in the process. There is a minimum amount of energy that the **photon** needs to transfer in order for the electron to leave the metal plate. This is known as the **work function** (w_0). If the **photon** has less energy than the **work function** then the electron will not leave the metal plate. If the **photon** has more energy than the **work function** then some of the **photon's** energy will be transferred to the electron to be used to leave the metal plate and use as **kinetic energy**. [1]

Analysis of the photoelectric experiment showed that the energy of the ejected electrons was proportional to the frequency of light. This showed that whatever was knocking the electrons out had an energy proportional to light frequency. This fit in well with **Planck's Law** that light in the **blackbody radiation** experiment could exist only in discrete bundles with energy. **Photon** energy ($E = h \times \nu$) explains the experiment and shows that light behaves like particles. [3]

So, physicists could conclude that **photons** really exist! Light was found to travel in discrete packets and behaves like a particle.

3. Wave-particle duality

Now that we've discussed the difference between waves and particles, let's talk about the **wave-particle duality**. As the name of this concept would suggest, the **wave-particle duality** is just the idea that in quantum mechanics that every particle or quantum entity can be described either as a particle or a wave. This duality can be specifically with light. Early scientists debated whether or not light was composed of particles or waves. Which do you think light is? It may not be as simple as you might initially think. If you were to focus on different types of phenomena (like reflection, refraction, interference, diffraction, and polarization) observed with light, then a strong case can be made for thinking that light acts more like a wave. This is what most physicists believed in the 19th century (that light could be fully described by a wave). But... they were wrong. [3]

Louis de Brogile questioned if the “**wave-particle duality**” could be applied to everything! Applying the **wave-particle duality** to matter led to the development of a way to analyze the behavior of tiny particles more accurately than before. de Brogile's reasoning was that if light could behave like both a particle and a wave, then matter should be able to do it too. This was found to be true when considering light's momentum ($p = \frac{h}{\lambda}$, p is momentum, h is **Planck's constant**, and λ is wavelength). In other words, you should be able to determine any type of matter's wavelength as long as you know its momentum. The **photoelectric effect** and the **double-slit experiment** suggested a particle nature for light. It was later found that electrons also exhibit this **wave-particle duality** and many other things such as atoms, molecules and any type of matter. [5]

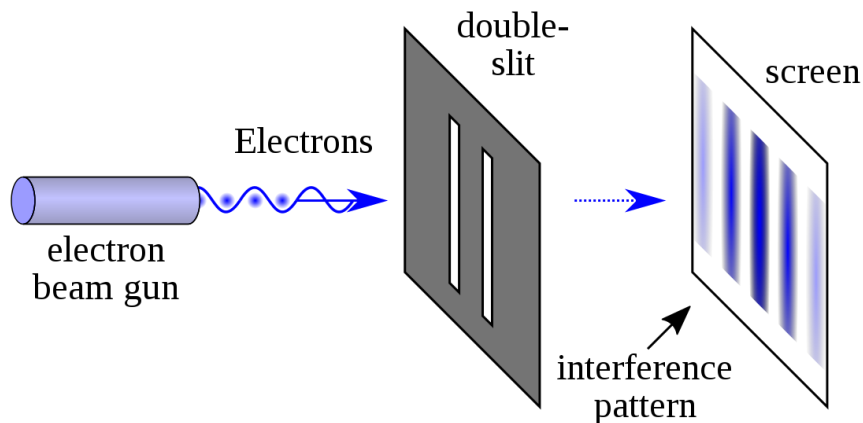


Figure 3. Experimental set-up of the double slit experiment [6].

4. Schrodinger's Equation and Probability Density Function

Probability is a huge factor in determining how waves and particles behave at a quantum level. When quantum mechanics looks at the wave nature of matter, it's mostly concerned with the probability that particles, like electrons or even atoms or molecules will be in certain places at certain times. That probability is predicted by the wave function. An equation that relates some of the properties that relate to a quantum mechanical system like an electron or atom. This is known as **Schrödinger's equation**. It was created by Erwin Schrödinger in the 1920s. It is

useful because it can be used to predict the probability of a particle at any given space. This is known as the **probability density function**. [5]

Think of the electron clouds that you have learned about in chemistry, like the s, p_{0-1} , p_0 , p_1 , d_{-1} , d_0 , d_1 orbitals, etc. The different electron orbitals are shown in Figure 4. These models of atoms show the probability of finding electrons in the space surrounding the nucleus. They are a graphical representation of the **probability density function**, meaning that the shapes of the clouds are calculated using **Schrödinger's equation**. One of the most intense debates in quantum mechanics is about what it actually means for a particle to have **probability density function**. [5]

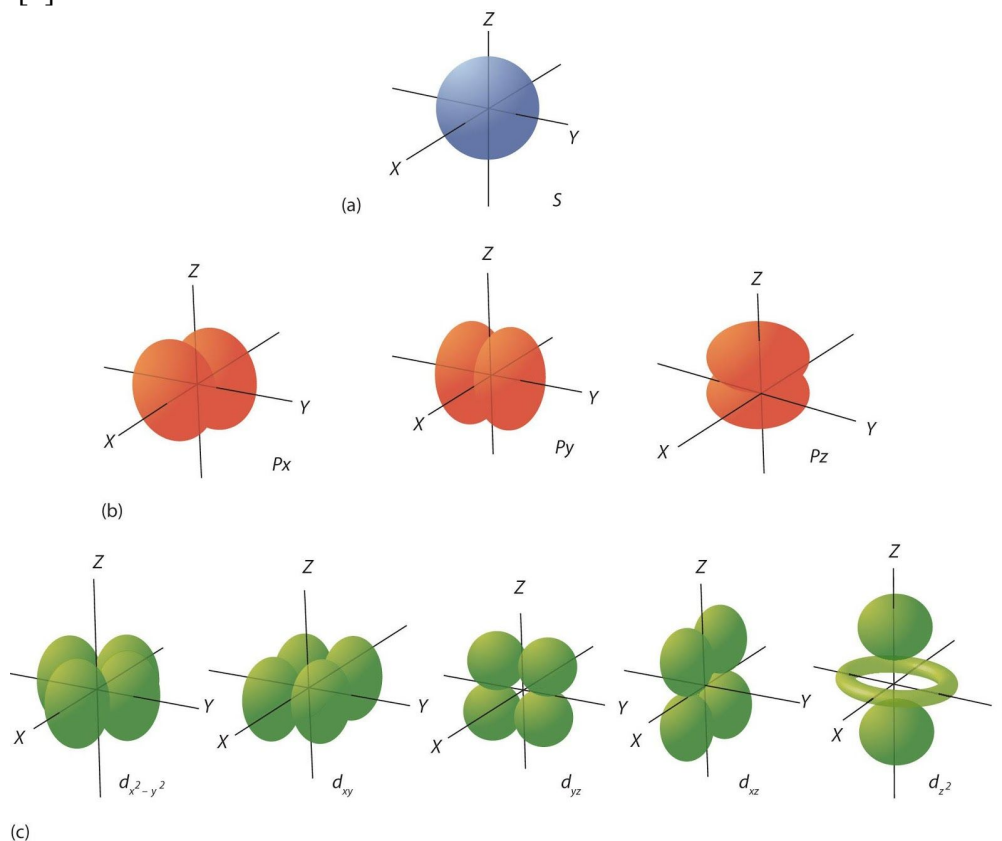


Figure 4. Electron Orbitals (s (blue), p (red), and d (green) orbitals), look how many places an electron could be [7].

Have you ever heard of the cat in the box? Well if not, this famous thought experiment is known as “Schrödinger’s cat” and is used to explain the theory of particle in a box and **quantum superposition**.

Quantum superposition is the idea that a particle can be in more than one state at a time [5]. Schrödinger wrote that if you place a cat and something that could kill a cat (like a radioactive atom) in a box and sealed it, you would not know if the cat was dead or alive until you opened the box, so that until the box was opened, the cat was in a way both “dead and alive”. So the question he posed was: at the end of the hour, is the cat dead or alive? According to the Copenhagen Interpretation which is used to explain what is happening to the smallest part of an

atom without looking at it, a particle could be 50% likely to be in one place at one time, or 50% likely to be in one place at another time. However, the only way to be 100% sure of where a particle is, is to observe it.

So now let's apply this to if you were to have an electron in a box, the electron's **probability density function** tells you that at any given moment there's a certain probability that the electron will be in various locations in the box. If you were to open the box to check where the electron is you'd see that the electron would be in only one specific spot. Once you observe and measure the electron in some way then it's only in one spot because you observed it to be there (which forces the electron to be in one spot). [5]

5. Heisenberg Uncertainty Principle

Even if you do measure this electron, there will still be some uncertainty in that measurement. This is known as the **Heisenberg Uncertainty Principle**. The principle states that no matter how good your measuring instrument is, you can only know the position and momentum of a particle like an electron in the box, up to a certain level of precision. After that, you could get a better measurement of your electron's position, but you'd have a much less precise measure of its momentum. You could get a better measurement of the electron's momentum, but then you'd have to lose some knowledge of its position. (Because of the wave, particle nature). Physicists did the next best thing, by describing things like electrons with what is known as a **wave packet** (a collection of waves all added together). Using **Schrödinger's equation** to calculate different waves that describe a quantum mechanical system and adding all those waves together, you can then get an idea of the electron's position. There will still be some uncertainty when it comes to the electron's momentum. In other words, there is a limit to how precisely you can measure position and momentum combined. There will always be an uncertainty which is equivalent to $\frac{h}{4\pi}$. [5]

This may not seem like a big deal, but when dealing with really small things (like atoms or electrons) this can be a HUGE problem! You can't always know an electron's position as precisely as you'd hope, because then you'll have a less precise measurement of its momentum. Even though this is the case, quantum mechanics is still the best way to describe the behavior of very tiny things.

6. Band Theory of Solids

A **band gap** is the distance between the valence band of electrons and the conduction band. The **band gap** represents the minimum energy that is required to "excite" an electron up to a state in the conduction band where it can participate in **conduction**. [8] The **band gap** is an energy range in a solid where no electron state exists. The **band gap** generally refers to the energy difference between the top of the valence band and the bottom of the conduction band. It is the amount of energy required to free an outer shell electron from its orbit about the nucleus. Generally, the smaller the size of the crystal, the larger the **band gap**. [9] The size and existence of **band gaps** allows us to visualize the difference between **conductors**, **semiconductors**, and **insulators**. [8]

In a **conductor**, electric current can flow freely, in an **insulator** it cannot [10]. Metals are **conductors**. There is no **band gap** between their valence and conduction bands, since they overlap. There is a continuous availability of electrons in these closely spaced orbitals. [11] A

conductor implies that the outer electrons of the atoms are loosely bound and free to move through the material.

Knowing what a **conductor** is, can you predict the behavior of an insulator? Well, in **insulators**, the **band gap** between the valence band and the conduction band is so large that electrons cannot make the energy jump from the valence band to the conduction band [10]. Most atoms hold on to their electrons tightly which makes a lot of materials **insulators**. In addition, solid materials are classified as **insulators** because they offer very large resistance to the flow of electric current. [11]

Now, let's talk about the in-between, do you know what a material is called when there is a small energy gap? These are known as **semiconductors**. In **semiconductors**, electrons can make the jump to the conduction band, but not with ease compared to conductors. There are two types of **semiconductors**: **intrinsic** and **extrinsic**. What's the difference between **intrinsic** and **extrinsic semiconductors**? An **intrinsic semiconductor** can be considered a pure **semiconductor**. Whenever an electron jumped into the conduction band, a hole would be generated in the valence band. So whenever an electron had jumped to the conduction band, there would be an equal number of holes in the valence band. [11]

For **extrinsic semiconductors**, a process known as **doping** is done in order to control the **band gap** by adding small impurities to the material. **Doping** can change the electrical conductivity of the material and the material's efficiency. Unlike for **intrinsic semiconductors**, in **extrinsic semiconductors** the number of holes will not equal the number of electrons that have jumped from the valence band to the conduction band. There are two kinds of **extrinsic semiconductors**, **p-type** (positive charge) and **n-type** (negative charge). [11]

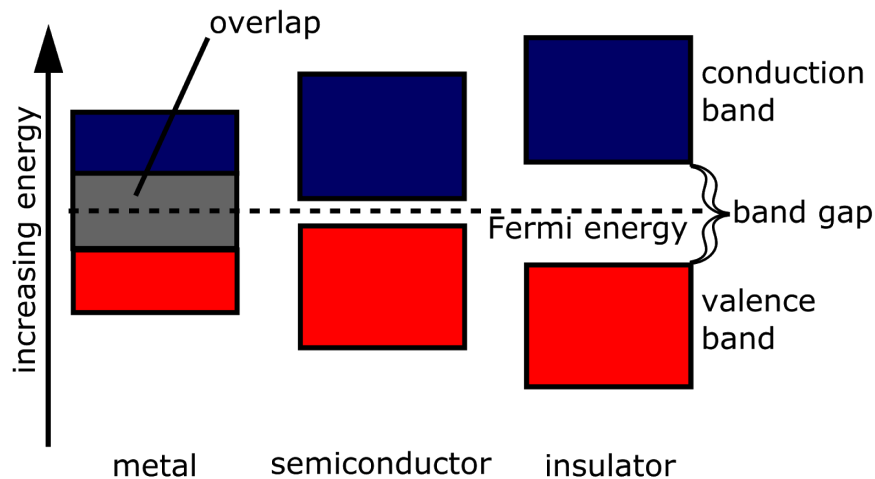


Figure 5. Band theory of solids (of a metal, semiconductor, and insulator) [8].

An important parameter in the band theory of solid is the **Fermi level**. The position of the **Fermi level** with the relation to the conduction band is a crucial factor in determining electrical properties. [12] The **Fermi level** is the term used to describe the electron energy levels at absolute zero temperature. As you may recall, electrons cannot exist in identical energy states due to the Pauli exclusion principle. At absolute zero, electrons pack into the lowest available energy states to build up rows of electron energy states. The concept of **Fermi energy** is a

crucial concept for the understanding the electrical and thermal properties of solids. The **Fermi level** in **doped semiconductors** is shifted by the impurities, which can be seen based on their **band gaps**. [13]

7. Quantum Dots

Quantum dots are small crystals which are small semiconductor particles that can contain one electron and one “hole” (the absence of an electron). These electrons and holes act like small particles which can move freely inside the semiconductor, but cannot get out (think of the particle in the box scenario). [9] They are nanosized semiconductor crystals composed of several tens to a few thousand atoms. **Quantum dots** can also be considered “artificial atoms”, since they exhibit discrete electronic states as seen in atoms and molecules [14].

By carefully observing quantum dots with different sizes, we can see the effect of changing the size of the box on the energy levels of the system. **Quantum dots** are nanoscale semiconductors whose conducting characteristics are closely related to the size and shape of the individual crystal. Relating back to **band theory of solids**, as the nanocrystal size decreases, the energy of the first excited state increases, and more energy is released when the crystal returns to its resting state. [9]

Because of the makeup of **quantum dots**, they have very unique electrical and optical properties. Since **quantum dots** have such unique properties, they have many different applications in many fields such as solar cells, LEDs, transistors, displays, laser diodes, quantum computing, and medical imaging. [14] For example, in fluorescent dye applications, this equates to higher frequencies of light emitted after excitation of the dot as the crystal size grows smaller, which results in a color shift from red to blue in the light emitted [9]. Why do I bring up colors you ask? This has to do with the experimental nanoHUB resource, “Turning Fruit Juice into Graphene Quantum Dots” which is what these four modules were built from to be the wrap-up concluding activity to tie-in all the concepts and topics we have learned.

REFERENCES

- [1] Lerner, Alyssa, Dr. Shini Somara. (2017). “Quantum Mechanics- Part 1: Crash Course Physics #43,” *Crash Course*.
- [2] Vongehr, Sascha. (2013). “Observer Dependence of Hawking Radiation Doubts Boltzmann Brains,” *Science 2.0*.
- [3] Nave, R. “Wave-Particle Duality,” *HyperPhysics*.
- [4] Ashish. (2019). “What is the Photoelectric Effect,” *ScienceABC*.
- [5] Lerner, Alyssa, Dr. Shini Somara. (2017). “Quantum Mechanics- Part 2: Crash Course Physics #44,” *Crash Course*.
- [6] Wikipedia. (2020). “Double-slit experiment,” *Wikipedia*.
- [7] Ball, David. (2011). “8.2 Quantum Numbers for Electron,” *Beginning Chemistry*.
- [8] Hanania, Jordan, Kailyn Stenhouse, Jason Donev. (2015). “Band gap,” *University of Calgary, Energy Education*.
- [9] Palmer, Joyce. (2011). “Quantum Dots Real-World Particles in a Box,” *NNIN Nanotechnology Education*.
- [10] Nave, R. “Conductors and Insulators,” *HyperPhysics*.
- [11] Blair, Sierra, Jim Clark. (2019). “6.8B: Band Theory of Metals and Insulators,” *LibreTexts*.

[12] Nave, R. “Band Theory of Solids,” *HyperPhysics*.

[13] Nave, R. “Fermi Level,” *HyperPhysics*.

[14] Kumar, D. Sumanth, B. Jai Kumar, H.M. Mahesh. (2018). “Chapter 3- Quantum Nanostructures (QDs): An Overview,” *Synthesis of Inorganic Nanomaterials (Woodhead Publishing)*.

ACTIVITY

Learning through Simulations II

Level of Difficulty: Advanced

<https://nanohub.org/tools/qdot>

For this activity, we will be playing predict and guess the energy level using the nanoHUB simulation “Quantum Dot Lab”, which can be found here: <https://nanohub.org/tools/qdot>. In addition, using this simulation. For this simulation, we will be running the original parameters that exist for the simulation.

Pre-Simulation Question: Draw a prediction of what you think the quantum dot will look like for the following energy levels: 1, 3, and 7.

Procedure:

1. Launch the nanoHUB website and the simulation: <https://nanohub.org/tools/qdot>
2. You will be taken to an introduction and welcome page to the module (Figure 1). You do not need to interact with this page except to go to the next page “Structure”.
3. On the next page, “Structure”, you can adjust the number of states for the quantum dot, but we will leave it as **8**. This page also allows you to change the shape you would like to view the quantum dot as, again we will leave it as a **cuboid** (if you are interested in seeing different shapes of the quantum dot you can play around with this if you would like). (Figure 2) You will not need to adjust any of the other parameters that exist on the “Structure” page (such as x-dimension, lattice constant, etc.)

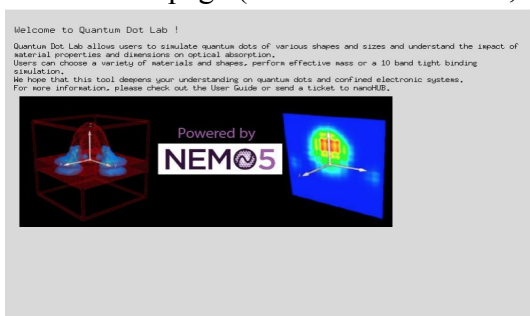


Figure 1. Step 2

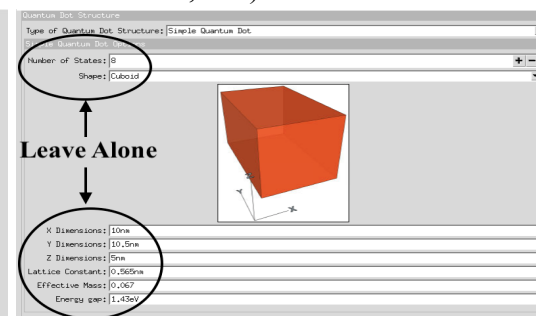


Figure 2. Step 3

4. The next page is the “Optical” page, nothing needs to be changed on this page (leave all parameters alone). For further learning, we suggest adjusting temperature to 273 K (steady state), but this is not necessary for this activity. (Figure 3)

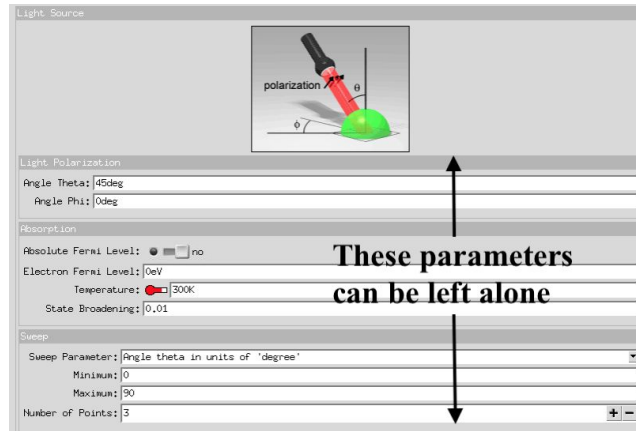


Figure 3. Step 4

5. You will then run the simulation. Figure 4, shows you what the resulting simulation should look like.
6. Using the “play” button at the bottom of the simulation (Figure 5) you can see and change the energy level that is being displayed.
7. To slow down the simulation to see the energy levels more clearly, adjust the options (which can be seen in Figure 5) to slow down the simulation when you press “play”.
8. Draw the energy levels from the simulation (all eight of them). We recommend using the “pause” button (where the “play” button is) to see all the energy levels.

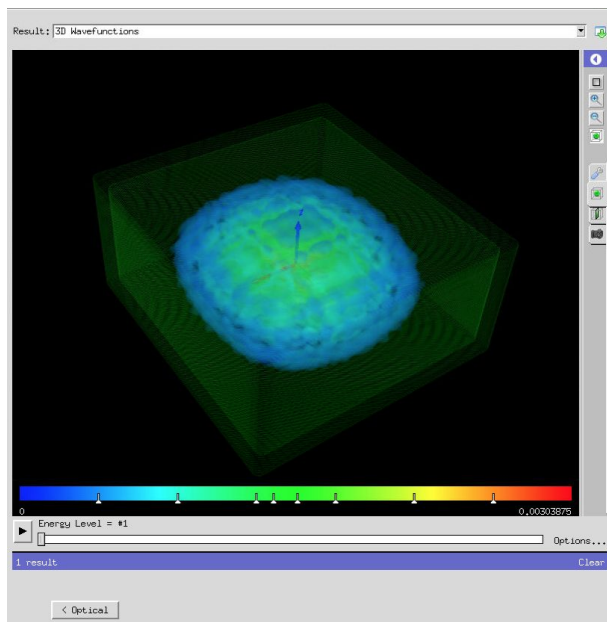


Figure 4. Step 5

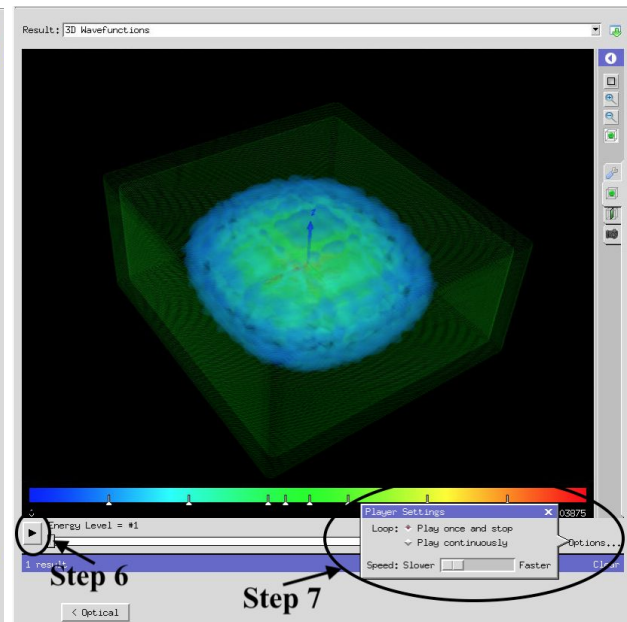


Figure 5. Step 6-7

Questions:

1. Compared to your pre-lab drawings of energy levels: 1, 3, and 7, how does this compare what you saw in the simulation for these energy levels?

2. In terms of symmetry, what assumptions can you make about quantum dots (regardless of energy level)?
3. Based on your understanding of quantum dots and what you have seen using this simulation tool, predict the shape of the quantum dot at an energy level of 12. Why do you think this? Use the simulation tool to confirm your assumptions.

Relating back to **band theory of solids**, as the nanocrystal size decreases, the energy of the first excited state increases, and more energy is released when the crystal returns to its resting state.

ADDITIONAL RESOURCES

Interactive Media for Learning (Particle in a Box/ Psi and Delta): <http://learnqm.gatech.edu/>

Additional Quantum Dots Lab Activity: <https://www.nci.net/node/5335>

CONCLUSION

In this module, all things quantum mechanics was explored. From waves and particles to applying quantum mechanics to semiconductors and quantum dots. This last module is meant to be the capstone of the four modules to lead up to the experimental resource “Turning Fruit Juice into Graphene Quantum Dots” on nanoHUB.

Key Takeaway: Quantum mechanics can be applicable in so many different ways (especially to materials science- think semiconductors, conductors, and insulators), but the concepts can be complicated to understand.

*“I think I can safely say that nobody understands quantum mechanics”
– Richard Feynman, Physicist*

APPENDIX

Let’s talk about waves and the electromagnetic spectrum a little bit more in case more background is needed to understand the learning objectives of this module.

The electromagnetic spectrum is a group of radiations. Radiation is energy (the ability to do work) that travels and spreads out as it travels. There are different types of radiation such as radio, microwave, infrared, visible light, ultraviolet (UV), x-rays, and gamma rays.

Electromagnetic radiation can be described as photons (like we described in the BACKGROUND of this module). Figure 1 shows the range of the electromagnetic spectrum.

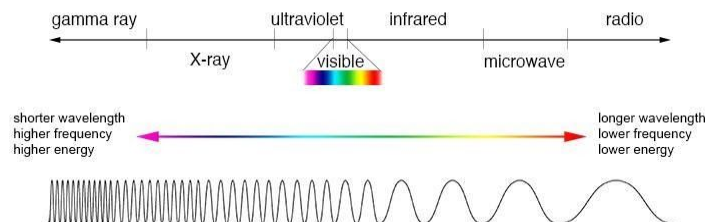


Figure 1. Electromagnetic spectrum [1].

In comparison, the electromagnetic spectrum can be expressed in terms of energy, wavelength, or frequency. To understand these three concepts, characteristics of a wave must be known. Amplitude, period, wavelength, frequency. Frequency describes the number of waves that pass a

fixed place in a given amount of time [2]. Usually frequency is measured in the hertz unit (Hz), is the number of waves that pass by per second [2].

Like mentioned in the BACKGROUND, wavelength can be related to energy and frequency ($E = h \times f$). In general, the shorter the wavelength, the higher the frequency which related to the energy of the photons. The visible spectrum is the portion of the electromagnetic spectrum that is visible to the human eye. The human eye can see wavelengths of about 380 nm to 750 nm. Colors that can be produced by visible light of a single wavelength are referred to as the spectral colors (red, blue, yellow, etc.). Each of these colors have a range of corresponding wavelengths.

There are some wave characteristics that are necessary to relate wavelength to frequency and energy. Figure 2 shows the parts of a wave. Like in MODULE's 1 and 3, important wave characteristics will be listed.

- **Crest:** highest point of the wave
- **Trough:** lowest point of the wave
- **Wavelength:** distance from one crest/trough to the next (normally described in meters (m))
- **Wave height:** height from trough to crest (also described in meters)
- **Amplitude:** distance from the center of the wave to the bottom of the trough
- **Wave period:** time for one full wavelength to pass a given point or points

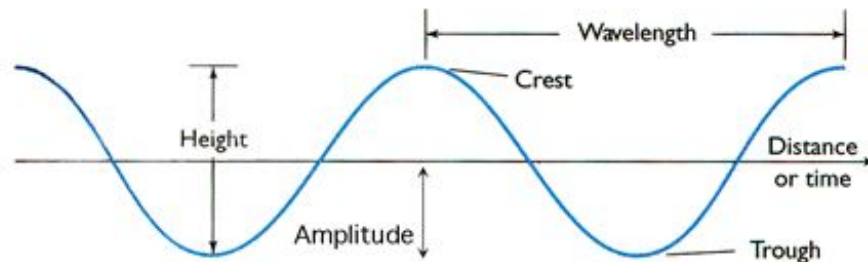


Figure 2. Characteristics of a wave [3].

[1] Smale, Alan. (2013). "The Electromagnetic Spectrum," *Goddard Space Flight Center- NASA*.

[2] Forbus, Kenneth. (2020). "What is frequency," *Qualitative Reasoning Group- Northwestern University*.

[3] James, Samantha, Roland Stull. (2019). "Wave Characteristics," *UBC ATSC 113- Weather for Sailing, Flying & Snow Sports*.