

Introduction to Semiconductor Devices
Dr Naresh Kumar Emani
Department of Electrical Engineering
Indian Institute of Technology – Hyderabad

Lecture - 02
Classical Vs Quantum Mechanics

This document is intended to accompany the lecture videos of the course “Introduction to Semiconductor Devices” offered by Dr. Naresh Emani on the NPTEL platform. It has been our effort to remove ambiguities and make the document readable. However, there may be some inadvertent errors. The reader is advised to refer to the original lecture video if he/she needs any clarification.

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The slide features a periodic table with the following elements highlighted in yellow:

III	IV	V
5 B	6 C	7 N
13 Al	14 Si	15 P
31 Ga	32 Ge	33 As
49 In	50 Sn	51 Sb

Handwritten notes on the right side of the slide include:

- III - V
- Ga-As
- 3 - 5, $8/2$ rule
- In-As
- GaP
- Group II - VI
- Cd-Te

Below the periodic table, there are two bullet points:

- Elemental Semiconductors – Single species of Group IV atoms
 - Silicon, Germanium, Carbon (sp^3 hybridized)
- Compound Semiconductor – More than one atomic species (Group III-V)
 - GaAs, InP, InSb, AlAs, InAlAs, etc

The slide also includes the NPTEL logo in the top right corner and a video feed of the lecturer in the bottom right corner.

In the previous lecture we have seen the broad classification of materials into insulators, semiconductors and metals. We also noted the distinction between elemental and compound semiconductors. But we did not explain why semiconductors exhibit their characteristic property of ‘adjustable’ conductivity.

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Classical Mechanics	Quantum Mechanics
Motion of objects described by deterministic dynamic variables like position, velocity and energy	A particle is assigned wave function – a complex number is assigned to each point in space and at each moment $\Psi(x, t) = \sin(kx) e^{i\omega t}$
Measurement outcomes are <u>predictable</u>	Measurement outcomes are <u>probabilistic</u>
Describes the macroscopic world accurately	Describes microscopic systems (de Broglie wavelength scale) accurately

To understand that, we will have to understand a little bit of quantum mechanics. Whenever I say quantum mechanics, a lot of engineering students feel are scared since they are not familiar. Quantum mechanics can seem little difficult, but it is not that difficult once you understand the fundamental principles. And if we want to understand semiconductor devices thoroughly, it is essential to have some basic knowledge of quantum mechanics.

After all, if you look at today's devices, the MOSFETs that have been fabricated, like say, in Intel or TSMC fabs (00:54) today, they are fabricated using what is called a 7 nano-meter technology. So, that means the dimensions of the devices are in the nano-meter scale. So, when you go to the nano-meter scale, it is essential to apply the laws of quantum mechanics. Without that, you cannot explain the properties.

So, for the rest of the lecture, I will just introduce a few basic concepts in quantum mechanics, please bear with me and it will become clearer why these are important. Before we get into the details, why should we study quantum mechanics? Why not simple classical mechanics - the age-old laws that Newton gave us in 1600s? (01:32) Well, Newton's laws work at the macroscopic scale.

For example, if I want to compute the trajectory of a car, let us say I know the position and velocity of a car, and I know how much force is applied, then I can compute how much distance it travels. Or I can take the example of planets, if I know the force that is acting on the planet, and I know the position and the speed with which it is moving, I can compute the orbit of the planet precisely.

So, these are all laws of classical mechanics. And one of the important features of classical mechanics is that the measurement outcomes are predictable, by which we mean that if you know the initial conditions and we know the force, we can compute the trajectory entirely predictably. There is no error or a probability associated with the calculation. Classical mechanics works very well for the macroscopic world.

But the moment you try to go into the microscopic dimensions, on a nanometer scale classical mechanics does not capture the behavior. How much is a nanometer? If you take a strand of human hair, the diameter of that strand would be a few microns. Micron is 1,000th of a millimetre. So, one single strand of human hair is a few microns, and 1 nanometer is 1000 times smaller than that.

So, imagine in the modern nm-scale MOSFET we are really going into the atomic dimensions, and the classical mechanics does not work anymore. We need a probabilistic description known as quantum mechanics. What we do in quantum mechanics is instead of talking about a particle, say an electron, we will talk of a wave function associated with an electron.

Wave function is simply a quantity which has spatial and time dependence, say it is a function of position(x) and time(t). It could be a function like $\sin(kx)$, and I could also add a time dependence ($\exp(i\omega t)$). This is a simple wave function that essentially tells you the probability of finding the particle at a position and at a particular time. The movement of the particle is captured by position and time evolution of the wave function.

The evolution of wave function, *i.e.*, how the particle moves, is determined by the Schrodinger equation. Schrodinger equation is essentially an analogue of the Newton's second law. Once you know the wave function at a particular position and a particular time, the evolution of the wave function can be calculated using the Schrodinger equation.

An important aspect that is to be noted is that the measurement outcomes in quantum mechanics are probabilistic. By this we mean that we cannot accurately, with 100% certainty, know that the electron is going to be at this position. We can only say that electron will have about 90% probability of being in position x and 10% probability of finding it somewhere else. This is called the probabilistic description.

The next important aspect that we need to discuss is the length scale at which quantum mechanics needs to be applied. We have previously said it is applicable to microscopic systems, but what is the exact length when quantum description is necessary? This is given by the de Broglie wavelength, which we will discuss next.

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de Broglie's hypothesis

Louis de Broglie hypothesized that matter exhibits wave-like behavior

$$\lambda_B = \frac{h}{p}$$

λ_B - De Broglie Wavelength
 h - Planck's constant
 p - Momentum

$L = n\lambda$

$\lambda > L$

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The de Broglie relation is one of the foundational principles of quantum mechanics. Back in 1924, a French physicist named Louis de Broglie hypothesised that matter exhibits wave like behaviour. It is somewhat counterintuitive to us, because we are used to thinking of matter as particles *i.e.*, a ball, an electron or a proton.

But it turns out that they also have a wave like character which can be described by a probability wave. So, if you have a classical particle that is moving from position 1 to position 2. Instead of saying that, I will represent that in the wave description using a probability wave. The probability wave has a maximum amplitude at position 1 and then after certain time, it has a maximum amplitude for position 2.

So, de Broglie said that the wavelength of matter wave(λ) is given by the Planck's constant(h) divided by the momentum of the electron(p).

$$\lambda_B = \frac{h}{p}$$

How does this help us? Well, you might remember studying about a string tied between 2 rigid supports. What happens when I pluck the string tightly tied between 2 rigid supports? It

oscillates at certain discrete frequencies. You will notice the same effect when we pluck a guitar string.

The discrete wavelengths (or equivalently discrete frequencies) which are supported are those for which the distance between supports (L) is equal to $n\lambda$. This means that the length is an integral multiple of the wavelength.

For example, here you have a red line whose wavelength is exactly equal to L . This mode is supported by the system. Whereas the blue line, which has a wavelength longer than L , cannot be supported since the wavelength is not an integral multiple of L . Something similar happens in atoms (in a microscopic scale) as we will see next.

At the beginning of 19th century physicists started studying how light is emitted from heated gases. For example, they observed emission from heated Sodium vapour. It turns out that the emission is not any random wavelength, but a particular wavelength determined by Sodium gas. And by measuring the wavelength of the emitted light from hot gases, they could predict the gaseous species present in the vapour.

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The slide is titled "de Broglie's hypothesis" and features the NPTEL logo in the top right corner. It contains the following text and diagrams:

- Text: "Louis de Broglie hypothesized that matter exhibits wave-like behavior".
- Equation:
$$\lambda_B = \frac{h}{p}$$
 with definitions: λ_B - De Broglie Wavelength, h - Planck's constant, p - Momentum.
- Text: "The energy levels occupied electron orbiting the nucleus are 'quantized'. This is explained by the principles of Quantum Mechanics."
- Diagram: A diagram of an electron orbiting a nucleus. The orbit is shown as a circular path with a central nucleus. A red wave is drawn along the path, and a blue wave is also shown. A dimension L is indicated for the path length. Below the diagram, the equation $2\pi r = n\lambda_B$ is written, with a handwritten note " $f \propto 1/\lambda_B$ ".

The scientists were puzzled by this phenomenon since it could not be explained by classical mechanics. The Bohr's model was proposed to explain these observations. The basic hypothesis was that an electron which is going around the nucleus cannot take any random orbit. Rather it must occupy certain discrete orbits for which the circumference of the orbit ($2\pi r$) is an integral multiple of the wavelength – the de Broglie wavelength.

Here you can see 2 orbits whose circumference is 6 and 4 times the wavelength. Essentially, you see that the circumference of the orbit is an integral multiple of wavelength. Only these orbits are supported. This concept was very useful I mentioned the discrete emission lines from hot gases such as Lyman, Balmer series and so on that you might have studied in plus 2. How much is the de Broglie wavelength?

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Let us look at an example problem which requires us to calculate the de Broglie wavelength given the velocity of an electron as 10^5 m/s . So, what is the de Broglie wavelength?

The de Broglie wavelength is $\lambda_B = \frac{h}{p}$. The first step is to compute the momentum(p) which is simply mass times velocity. So, the mass of electron is $9.1 \times 10^{-31} \text{ kg}$. The velocity is 10^5 m/sec . The momentum will be $9.1 \times 10^{-26} \text{ kg m/sec}$.

The de Broglie wavelength will be simply $\frac{h}{p} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-26}} = 7.3 \times 10^{-9} \text{ m}$. So, what this is telling us is that de Broglie wavelength is a very small number on the scale of a few nm .

So, we do not have to worry about quantum behaviour when the length scales are much larger than λ_B . If you are talking about, let's say the movement of a car on a highway which is kilometres long we do not have to apply quantum mechanics at all. But if you are talking about propagation of electron in a semiconductor, like in a modern MOSFET whose channel length is about 10's of nm , then we do have to apply quantum mechanics.

I also would like to write the de Broglie relation in a slightly different form from $p = \frac{h}{\lambda}$. We can rewrite this by multiplying and dividing by 2π . We get $p = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k$, where \hbar or \hbar ($\frac{h}{2\pi} = \hbar$) is a fundamental constant and $\frac{2\pi}{\lambda} = k$ is the wavevector. $p = \hbar k$ is an important expression which we will use again later, and I want you to remember this expression. In the next lecture let us start applying Schrodinger equation.