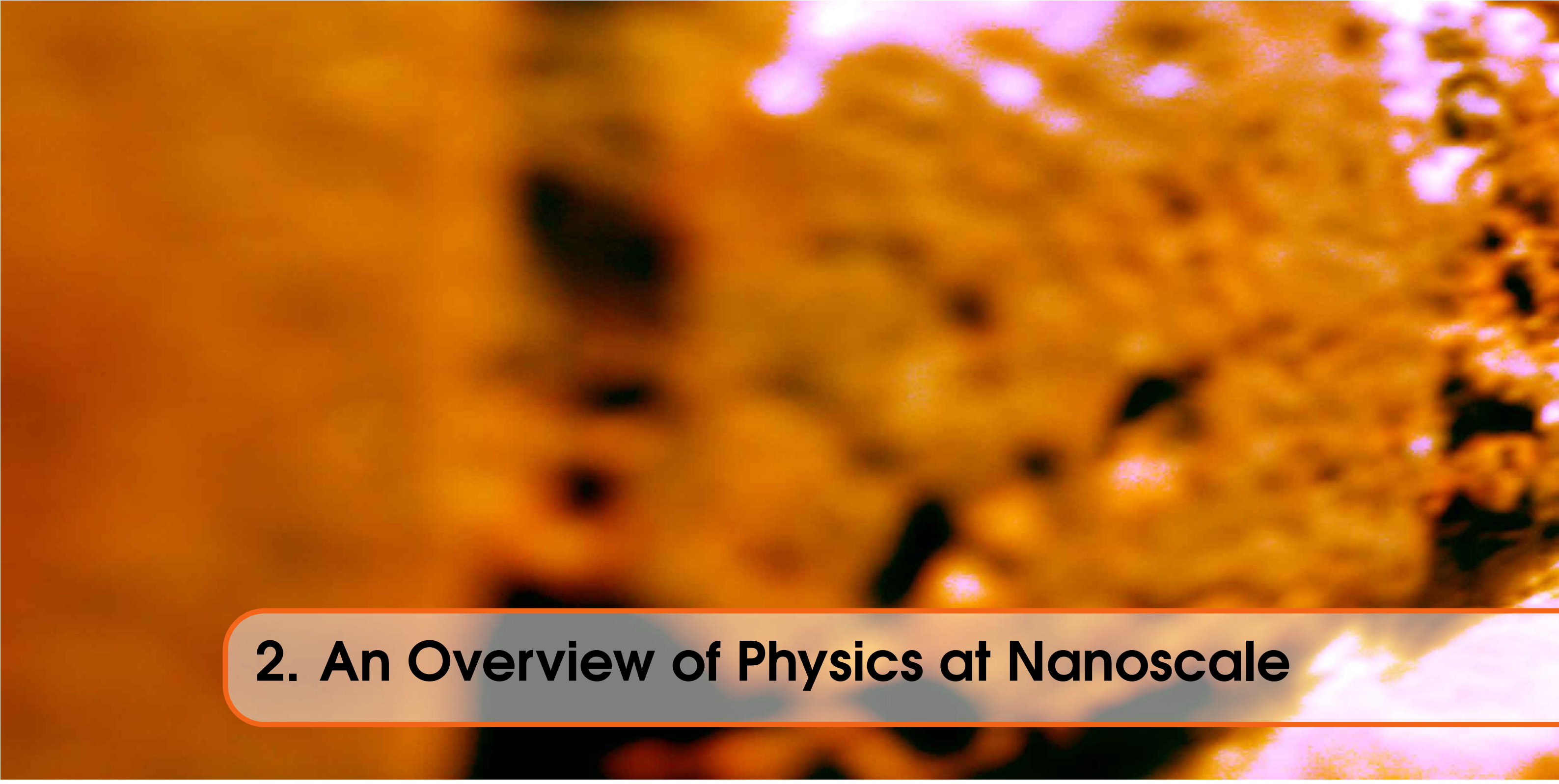

2. An Overview of Physics at Nanoscale

In previous chapter we have seen that we use different physical theories to model the physics at different length scales of the nature. Here, we will see how the wave nature of matter becomes significant at relevant length scales. In this chapter we will take a look at the basics of quantum mechanics. Using the principles from quantum mechanics we will construct a model for solids. We will also review basics of the electromagnetic theory that is relevant to nanotechnology.

2.1 New Physics Towards "Nano"

> "After dinner, the weather being warm, we went into the garden and drank thea, under the shade of some apple trees...he told me, he was just in the same situation, as when formerly, the notion of gravitation came into his mind. It was occasion'd by the fall of an apple, as he sat in contemplative mood. Why should that apple always descend perpendicularly to the ground, thought he to himself..."

This excerpt is taken from William Stukeley's *Memoirs of Sir Isaac Newton's Life* book on the famous apple story. A falling apple had inspired Newton to think about a set of rules that keep the moon up in the orbit of the Earth while that makes an apple fall from a tree. How far can we stretch this thinking? Would it be possible to apply the Newtonian physics to galaxies or atoms? Interestingly enough the Newtonian mechanics can explain many of the observed phenomena in nature very well. Yet, when we start investigating phenomena that directly arise from the atomistic properties of matter we will start seeing the quantum effects. Indeed, at the end of 19th century, in a speech Lord Kelvin had given, he stated that there are two significant problems of physics which one of them was relevant to the quantum mechanics while the other was to the theory of relativity before these theories were around.

Figure 2.1 gives the visible spectrum of the light that reaches to the Earth surface from the Sun. There are missing lines in the spectrum due to absorption of the elements in the atmosphere of the Sun as well as the Earth. More interestingly these missing lines come in discrete form. They have a very specific wavelength as well as width. Indeed, this is one of the first hints towards the quantum nature of the atomistic physics. The observation of the spectral lines dates back to early 19th century.

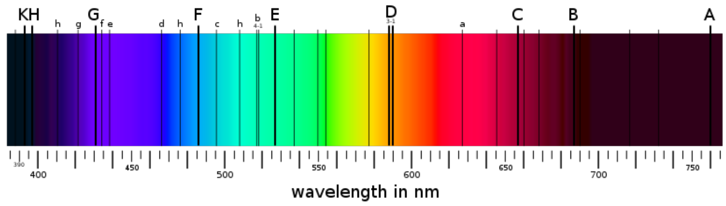

Figure 2.1: Chart shows the solar spectrum also known as the Fraunhofer spectrum.The missing lines correspond to the discrete energy levels of the elements absorbing the light at specific energies.(Courtesy of Wikipedia)

Another significant mystery in the Newtonian physics was the spectrum emitted by a heated black body. A black body is an hypothetical object that absorbs all the incident radiation, thus it heats up and re-emits radiation at a different wavelength. The problem was, when the problem solved taking energy as a continuous parameter, emitted power increases exponentially towards shorter wavelengths. The solution came in 1900 by Max Planck, a German physicist. He first found the formula that explains the observed spectrum. With the agreeing formula in hand, he realized that the energy needs to be "quantized". This quantization, resulted in the correct explanation for the black body radiation and also for the first time the Planck's constant appeared in a formula to spark the beginning of the quantum mechanics. Five years later, another significant contribution to

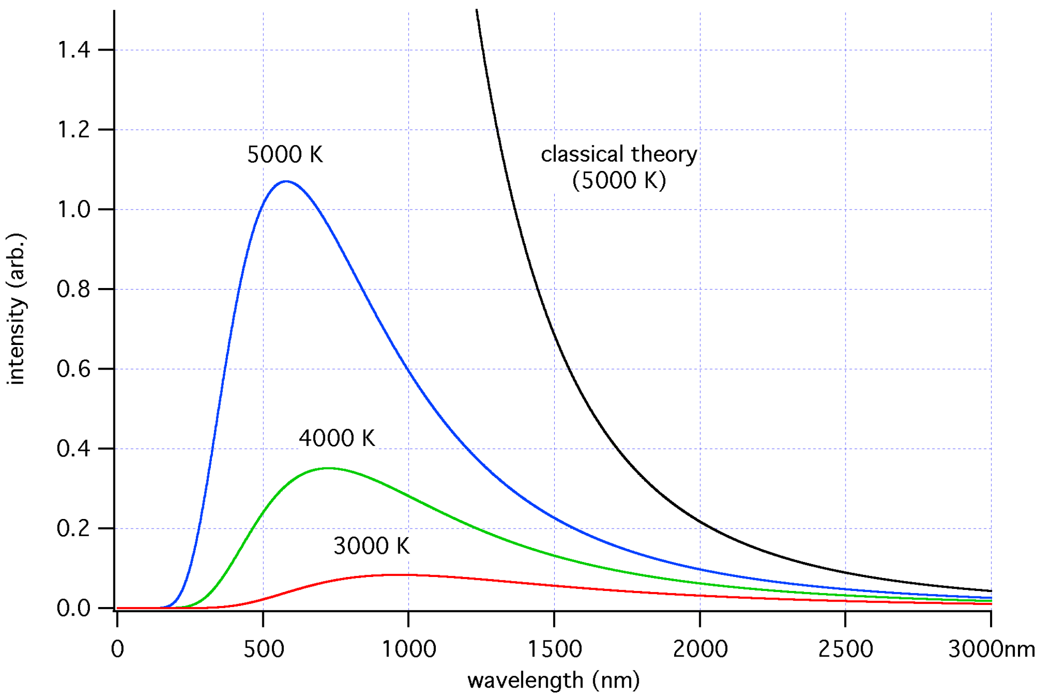

Figure 2.2: Blackbody radiation at various temperature compared to the prediction of the classical theory (Courtesy of Wikipedia).

the quantum theory came from Albert Einstein in 1905. After Maxwell's equations (1860's) there was no doubt that the light was an electromagnetic wave from a theoretical stand point. However, when the wave picture applied to the photoelectric effect, the momentum delivered to the metal surface was simply not enough to knock out any electrons. Einstein, explained this problem by quantizing the light, this time. This is the first glimpse of the wave-particle duality! Under certain conditions it seems like the light behaves like a wave and in some others it behaves like a particle!

2.1.1 Wave Nature of Matter

Now we will fast forward in the history of quantum mechanics by about a 20 years to understand the wave nature of matter. An experiment performed by Davisson and Germer demonstrated that electrons behave as a wave.

de Broglie Relation and Davisson-Germer Experiment

An old PhD student Lois de Broglie, came up with an hypothesis that applies Planck's and Einstein's ideas to matter. He claimed that matter just like light, may have a wave nature and its wavelength can be written as

$$\lambda = \frac{h}{mv} \tag{2.1}$$

where h is the Planck's constant, m is the mass and v is the velocity of the matter. This relation, as we will see later on, is consistent with Bohr's atomic model and explains a major assumption in that model. Around similar dates Davisson and Germer was working on electron scattering from a nickel surface and in a meeting they realized that the data they get can be explained by the de Broglie's hypothesis. From the diffraction data they extracted that for their 54 eV electrons the Bragg's law give 0.165 nm while the de Broglie wavelength is 0.167 nm, in close agreement.

Yet it is difficult to comprehend what this wave-like nature of matter is as in our classical worlds it has no counterpart. It is important to understand that this wave behavior is not a property in ordinary three-dimensional space, but is in an abstract configuration space. There are real consequences to it though! To be able to comprehend it further, we need to take a deeper look in the the mathematical structure of the quantum theory.

2.1.2 Probability Density

In physical systems, dynamics are determined by the relevant energies and time evolution of the system under these energies. It turns out that in quantum mechanics a quantity called the **wave function** evolves with the energy of the system and |**wave fundtion**|^2 gives the probability density. The wave function gives a description of the quantum system.

Notation 2.1. *Wave Function*

1. *Let's denote the wave function with* $\Psi(x,t)$*;*
2. *Thus the probability density will be* $|\Psi(x,t)|^2$.

Probability density is a function of spatial position and time and by integrating this density over relevant quantities we can find the probability of finding the value of the parameter that we are interested in a given range of values. At this point I am aware that this explanation might sound a little too abstract to the reader. Here, I will give a classical example to elucidate the concept of probability density a bit more.

■ **Example 2.1** Let's assume we drop a pebble from an height of h. Assuming that the gravitational acceleration g is constant throughout h, find the probability density of position of the pebble.

Solution Time dependent position of the pebble will be given by $x(t) = h - \frac{1}{2}gt^2$ and the speed is $v(t) = \dfrac{dx}{dt} = gt$. When the pebble hits the ground, the total time of $T = \sqrt{\frac{2h}{g}}$ will be