Solid State Physics
Lecture 35

Energy Levels in a Periodic Array of Quantum Wells

After discussing Bloch Theorem, let us see let us try to find out the Energy Levels of Electrons in a Periodic Array of Quantum Wells. So, that is a possible a simple kind of potential for which we have in quantum mechanics course learn the solution, we know what kind of wave function we have for the potential wells. So, we will try to work this out to understand what exactly happens if we put an electron in a periodic potential and in order to do this we will first take something very simple in hand and then we will further simplify it to understand the idea and we will apply Bloch theorem to find out some reasonable solution to this problem. (Refer Slide Time: 01:24)

So, how do we find out the energy levels for a periodic array of quantum wells, let us draw the picture first, say we have this kind of a quantum well this kind of a barrier, again a quantum well and a barrier and the well, a barrier, a well and this keeps on extending on both sides it does not end anywhere. Now, let us consider this as the x-axis this is x and let us consider this as the potential axis V(x) and if we put x = 0 here, then here x = -w that is the width of the well is w, here x = b the width of the barrier is b, here x = b + w and so on the potential is 0 here and this V_0 here. So, the lattice constant for this kind of an arrangement would be a = w + b this is the lattice constant a is the lattice constant. Now, if we consider an electron within the unit cell then the unit cell ranges between $-w < x < b$. So, within the unit cell we have the well region this region that is $-w < x < 0$ let us call it region 1 and then there is the region $0 < x < b$ this is the barrier region and let us call this barrier region as region 2. So, we know the general solution for wave function in region 1 and region 2 from our quantum mechanics courses and if we have an electron or any quantum particle with $E > 0, but < V_0$ we will have an oscillatory solution in region 1 and an exponentially decaying solution in region 2 this kind of a solution will be there. So, the solution for wave function for region 1 can be expressed as $\psi_I(x) = Ae^{iqx} + Be^{-iqx}$ this is for the region $-w < x < 0$ and q which is a function of the energy $q(E) = \sqrt{\frac{2mE}{\hbar^2}}$. In region 2 that is the barrier region where the energy of the electron is less than the barrier here we would not have e^i kind of a thing which is the signature of an oscillatory solution. We will have rather exponentially decaying solution $\psi_I I(x) = Ce^{\beta x} + De^{-\beta x}$ this kind of a solution we will have. This is in the region $0 < x < b$ and here this β which is a function of energy may be expressed as $\beta(E) = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$. So, we have learned this in the quantum mechanics course we have just written the solution the general solution here and let us see what it means. So, this quantity q(E) this is the propagation wave number in the well and $\beta(E)$ this refers to the barrier A B C D these are arbitrary constants so far. (Refer Slide Time: 08:18)

We consider $E < V_0$ and so the arbitrary constants must be chosen in such a way that the boundary conditions are satisfied. What are the boundary conditions, we must have continuity of the wave function and the continuity of the first order derivative of the wave function in space, so that the wave function is differentiable to at least the second order. So, those are the boundary conditions that has to be obeyed which is which has to be observed at x = 0. Which means we have the boundary conditions $\psi_I(0) = \psi_I I(0)$ and $\frac{d\psi_I}{dx}|_{x=0} = \frac{d\psi_I I}{dx}|_{x=0}$, is there another non trivial point? Yes, there are other non trivial points to be considered for a periodic boundary condition we will consider that this point here that is this x = b and this point here that is this x = -w these are equivalent. Because they are equivalent we will also have $\psi_I I(b) = e^{ika}\psi_I(-w)$. (Refer Slide Time: 10:24)

So, this factor e^{ika} comes from the expression of the Bloch theorem. (Refer Slide Time: 10:26)

This form this form gives that kind of an expression and the other condition for the derivative would be $\frac{d\psi_I I}{dx}|_{x=b} = e^{ika}\frac{d\psi_I}{dx}|_{x=-w}$. The condition here on this line imposes the continuity of the wave function and its derivative at x = 0 and the second condition that is this one here that comes from the periodic boundary condition the phase factor e^{ika} is required by the Bloch theorem as we have discussed. So, now these conditions lead to the constraints or the equations on of the arbitrary constants that we have from these conditions we find

$$A + B = C + D$$

we get A plus sorry

$$A \times iq - B \times iq = C\beta - D\beta$$

$$Ce^{\beta b} + De^{-\beta b} = e^{ika}\left[A\, e^{-iqw} + Be^{iqw}\right]$$

and finally,

$$C\beta e^{\beta b} - D\beta e^{-\beta b} = e^{ika}[timesAiqe^{-iqw} - Biqee^{-iqw}]$$

. So, we have a set of four equations with four unknowns in here and in order to have non trivial solution for all the unknowns we must have the determinant of the coefficients of A B C D to be equal to 0 that is the condition for solving linear set of linear equations. (Refer Slide Time: 14:28)

So, we must have the coefficients that is $\begin{vmatrix} 1 & 1 & -1 & -1 \\ iq & -iq & -\beta & \beta \\ -e^{ika-iqw} & -e^{ika+iqw} & e^{\beta b} & e^{-\beta b} \\ -iqe^{ika-iqw} & iqe^{ika-iqw} & \beta e^{\beta b} & -\beta e^{-\beta b} \end{vmatrix}$ = 0, in order to have a non trivial solution to the set of equations. And if we set this determinant to 0 we will arrive at the following condition $\frac{\beta^2-q^2}{2q\beta}\sinh\left(\beta b\right)\sin\left(qw\right)+\cosh\left(\beta b\right)\cos\left(qw\right) = \cos ka$ this kind of a condition we arrive at. Now, if we make a simplification; that means, we change the form of this barrier a little bit without really changing the problem too much just for simplicity we make the following simplification we let we make the width of the potential barrier approach 0; that means, $b \to 0$ and we have a periodic sequence of δ like Dirac delta like potential barriers where $b \to 0$, but $V_0 b$ this is a constant; that means, $\int \delta = V_0 b$. So, these are the constraints that we apply on the problem on the pattern of the potential barrier. So, with this we obtain a simplified solution which is $P\frac{\sin qa}{qa} + \cos qa = \cos ka$. What is P in here, $P = \frac{mV_0 ba}{\hbar^2}$ and this is a dimensionless parameter it of course, depends on the materials properties the V_0 is there, a is there these are the material dependent quantities. (Refer Slide Time: 19:37)

Now, if we try to plot this equation and obtain a graphical solution to this equation what do we get. Let us plot a quantity $F(qa) = P\frac{\sin qa}{qa} + \cos qa$. So, we are plotting F(qa), F as a function of (qa) in the y axis and in the x axis we are plotting qa what kind of graph shall we get we will get something like this which will keep on going. Now, let us consider something interesting here this quantity has to be equal to $\cos ka$ which ranges between -1 to +1 say -1 is here and +1 is here. Then the acceptable solution acceptable values of F(a) that makes sense is confined within this region which leads to a gap here there is no acceptable solution a gap in this region there is no acceptable solution, a gap here, a gap here and so on. So, if we move higher on (qa) there would be smaller gaps and once after certain value there would be no gap the gap will not exist anymore, but at lower values of (qa) there are gaps in this spectrum. And we can see that if P this value of P becomes 0 then we will have perfect free electron and if $P \to \infty$ if P is very large then we will have a very narrow band in here very narrow region where acceptable energies are possible beyond that it is not acceptable. And in general for moderate values of P the energy spectrum would be gapped not every energy would be acceptable for the energy of the electron under consideration which is subject to a periodic potential. So, when we have the electron in a periodic potential like this, it will not have any arbitrary energy it cannot have any arbitrary energy rather there are certain energies that are forbidden. This is what we learn from this mathematics this kind of simple model that we have considered, certain energies are forbidden this actually gives the idea of band gap and this model is known as the Kronig-Penney model.