Semiconductor Device Modeling
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Lecture – 28
Energy band diagrams

In the previous lecture, we have begun the discussion on energy band diagram, which is a very important tool in the analysis of semiconductor devices. We have mention 2 types of energy band diagram, which are complementary to each other. One is the Ex diagram, which tells you the allowed energy levels of electrons as a function of distance within a device.

Now, this diagram; the Ex diagram helps you to analyse the distribution of electron concentrations, hole concentrations, electron current density, hole current density, electric field and potential within a device. On the other hand, the Ek diagram, where you represent the allowed energies as a function of the wave vector, which reflects the crystal momentum of the electron.

The Ek diagram helps you to estimate the effective mass, the group velocity of the electron and the crystal momentum and this Ek diagram is useful to analyse an interaction of an electron or a hole with other carriers, impurities, phonons and photons. We gave a qualitative model of the energy band diagram, in which there were 2 approaches. On approach that is the Bloch approach develops the allowed bands of energies in a crystal for electrons from the single energy levels of electron in an isolated atom.

On the other hand, the Brillouin approach develops the forbidden energy bands for electrons in a crystal from a continuous band of energies associated with a free electron.

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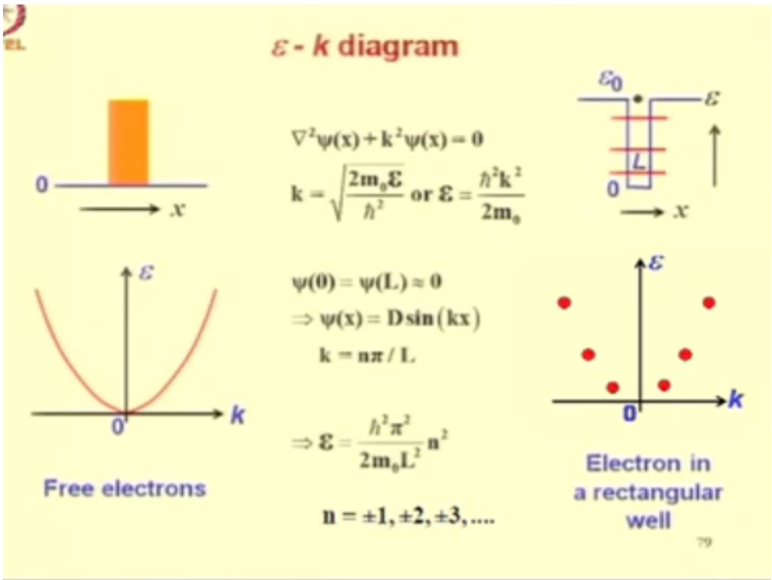

ε - k diagram

$$\nabla^2\psi(x) + k^2\psi(x) = 0$$

$$k = \sqrt{\frac{2m_0\mathcal{E}}{\hbar^2}} \text{ or } \mathcal{E} = \frac{\hbar^2 k^2}{2m_0}$$

$$\psi(0) = \psi(L) \approx 0$$

$$\Rightarrow \psi(x) = D\sin(kx)$$

$$k = n\pi / L$$

$$\Rightarrow \mathcal{E} = \frac{\hbar^2\pi^2}{2m_0L^2}n^2$$

$$n = \pm 1, \pm 2, \pm 3, \ldots.$$

Free electrons

Electron in a rectangular well

Then, we began a discussion of the quantitative model of the energy band diagram, first we took up the Ek diagram. Now, for the Ek diagram, we consider the rectangular potential well and this Ek diagram is what we are going to develop further in this lecture. Now, here is the rectangular potential parabola. The allowed energy levels shown here, where it so the boundary conditions psi = 0, the wave function at x = 0 that is at the left end of the well.

And the wave function at the right end of the well here, were both approximately 0, because the height of the potential barrier was really large and because of the boundary conditions you get and this discretisation leads you to the discretisation of the energy. As a limiting case of L tends to infinity, you get the picture for free electrons, which are a parabola for E as function of k, in which all energies allowed.

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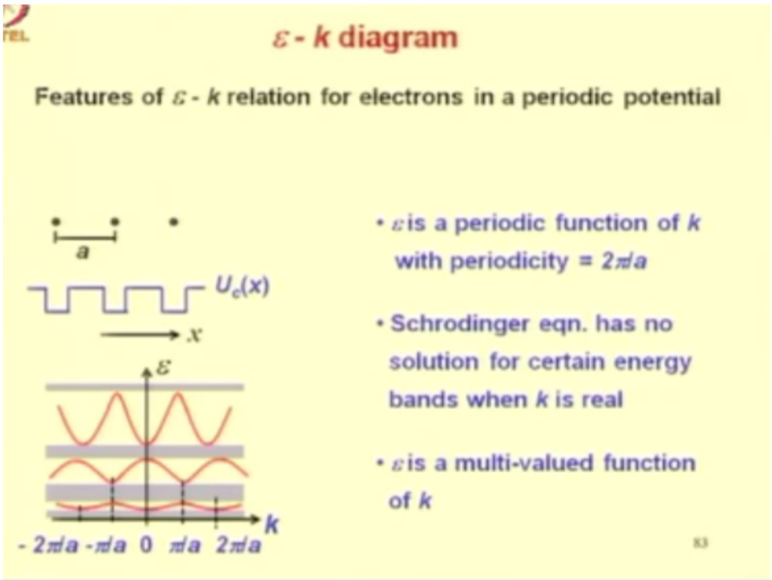

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- ε is a periodic function of k with periodicity = 2π/a
- Schrodinger eqn. has no solution for certain energy bands when k is real
- ε is a multi-valued function of k

In today’s lecture, we want to develop the Ek diagram for electron in a periodic crystal potential starting with the solution of the Schrodinger equation. Now, let us look at the features of the Ek relation for electrons in a periodic potential one by one. This is the approximate form of the periodic potential. The first feature of the Ek diagram of electron in a crystal is that E is a periodic function of k with periodicity 2 pi/ a.

You can see this here, so Ek relation is a periodically varying function and the period is 2pi/a. so, you can see from here that this end to this end here is one period or from 0 to 2 pi/ a is one period, okay. Now, how do we explain this feature? We will see that; first let us list all the features, the second feature are that the Schrodinger equation has no solution for certain energy bands, when k is real.

Now, these bands are shown here in grey colour, okay, so they are the forbidden energy bands. So, for these energies the Schrodinger equation has no solution. Finally, E is multivalued functions of k, so you see for any value of k. you have several values of energy; multiple values of energy, okay. So, these are the 3 features, which we need to explain on the basis of Schrodinger equation, solved for a periodic crystal potential.

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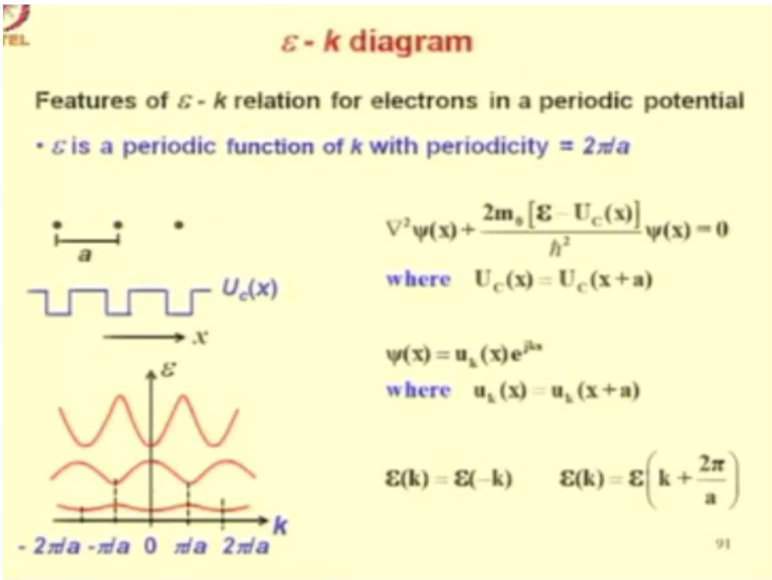

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- ε is a periodic function of k with periodicity = $2\pi/a$

$$\nabla^2\psi(x) + \frac{2m_e[\mathcal{E} - U_c(x)]}{\hbar^2}\psi(x) = 0$$

where $U_c(x) = U_c(x+a)$

$$\psi(x) = u_k(x)e^{jkx}$$

where $u_k(x) = u_k(x+a)$

$$\mathcal{E}(k) = \mathcal{E}(-k) \qquad \mathcal{E}(k) = \mathcal{E}\left(k + \frac{2\pi}{a}\right)$$

Let us look at the first feature; E is the periodic function of k with periodicity 2pi/ a. Now, this is the Schrodinger equation for electrons in a crystal, Ucx is the periodic potential. The property of Ucx is that it is periodic with period a, which is the distance between the atoms. So, Uc of x = Uc of x+a. Now, there is a theorem called Bloch theorem, which says that if the potential is periodic as considered here, then the wave function, which is the solution of the Schrodinger equation is of this form.

U of x; here the suffix k indicates that this U contains k as a parameter, so U of x * e power jkx. Now, for a free electron, you recall that the solution was just e power jkx, okay. So, here what is happening is; the periodic potential is multiplying this e power jkx with an envelope function, which also is periodic with the period a, like the crystal potential. Now, this is the important result that we simply import from the Bloch theorem.

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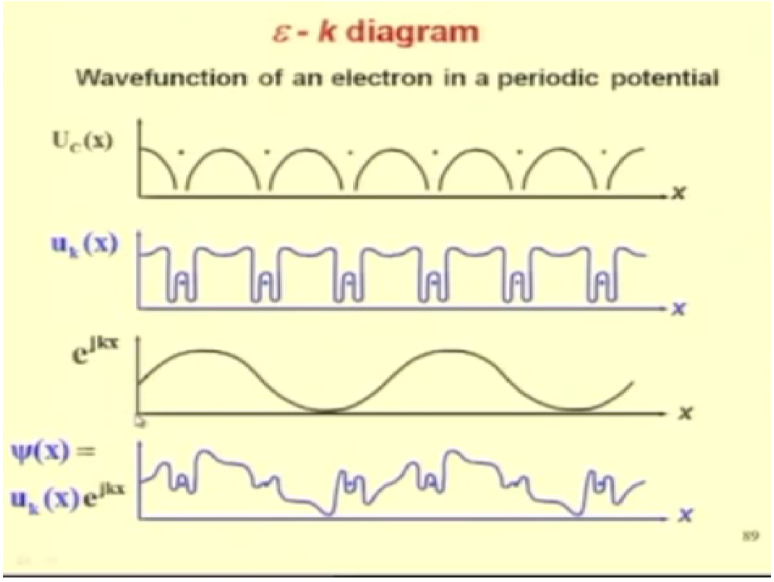

ε - k diagram

Wavefunction of an electron in a periodic potential

Now, based on this important result for the wave function, psi of x, how do we show that E is the periodic function of k with periodicity 2pi/a? Now, while we do that let us first look at some graphs of the wave functions psi x, the envelope function or the Bloch function Ux with the suffix k and e power jkx and so on. Now, here is an example, these calculations are done numerically and I have picked them up from a figure available in Lindstroms book.

So, if Ucx is periodic having a shape, I shown here, then U of x has the shape something like this. The points here indicate the location of the atoms in the crystal, e power jkx on the other hand is like a sinusoidally varying function. You can take either the real part or the imaginary part. Now, when you multiply these 2; U of x and e power jkx, you get the wave function, now you see that the wave function is fairly complex, okay.

This wave function is obtained by multiplying this function and this function. So, this gives you some idea of the various functions that are there in the solution of the Schrodinger equation for periodic potential. Now, let us move on to show how E is a periodic function of k? Now, the first point to note is that the Ek relation is even that is E of k = E of –k. Now, this is straight forward.

Because if an electron is moving in the positive x direction or moving in the negative x direction that is from right to left, it sees the same form of crystal potential and therefore the energy is associated with these 2 movement should be the same, that is essentially what is said by this particular relation, okay. So, the k vector here indicates movement in the positive x direction, whereas –k indicates movement in the negative x direction.

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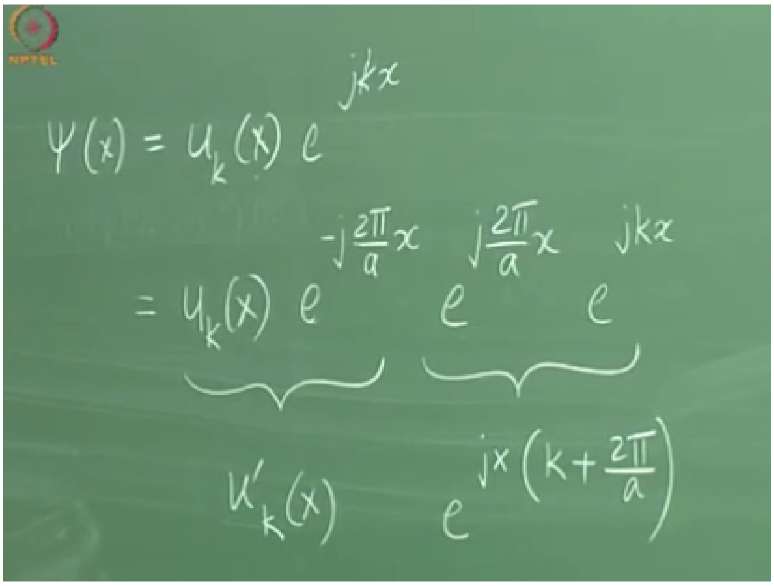

Now, we will establish that E of k = E of k+2 pi/ a, based on this particular wave function solution given by the Bloch theorem. So, psi of x = Uk of x * e power jkx. Now, since Uk of x is periodic with the period a, let us multiply this right hand side and divide by a function e power j * 2 pi/ a * x, so I am going to multiply by e power – j 2pi/ ax and e power j 2 pi/ ax. Note that the product of these 2 is 1.

Now, since x is periodic with the period a; and this function also is periodic with the function; with periodicity a, you can see that here when you put x = a, it becomes 2 pi, when you put x= 2a, it becomes 4 pi. So, you know that for integral multiples of 2 pi, this quantity will be the same, it will be unity. Therefore, I can clubbed these 2 and write this as another periodic function, okay, which has the periodicity a, multiplied by this part appears as e power jx * k+2 pi /a.

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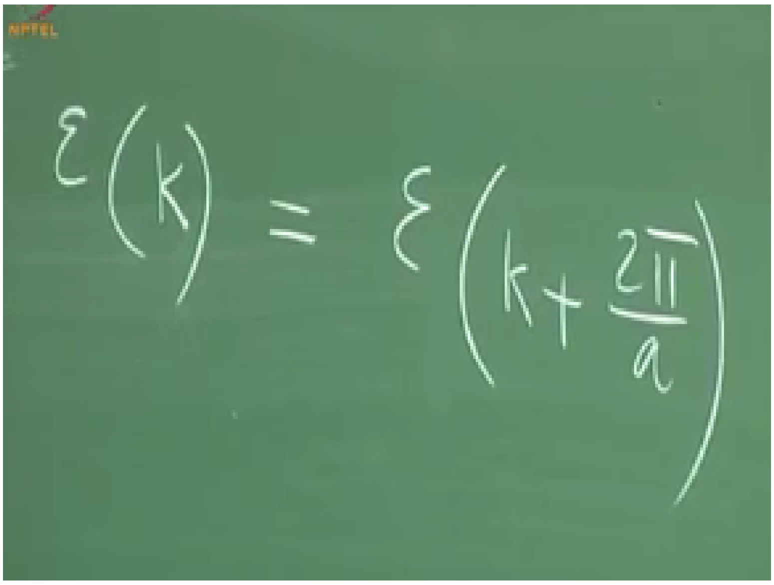

$$\varepsilon(k) = \varepsilon\left(k + \frac{2\pi}{a}\right)$$

Now, this new form of the function is also psi of x. This means that energy that is represented by this function and the energy that is represented by this way function. Both the energies must be same and therefore we can write the energy which is the function of k, should be the same if the k is replaced by k+ 2 pi /a, okay. So, this part is energy associated with this function, here you have k.

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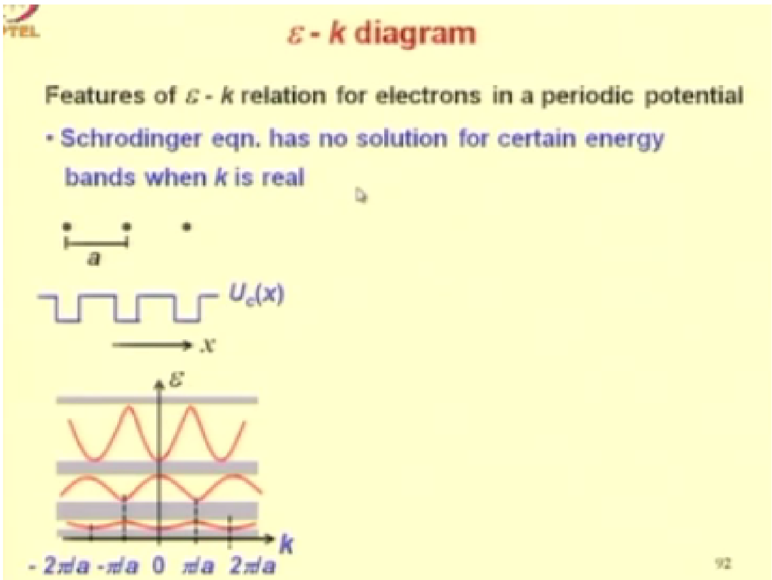

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- Schrodinger eqn. has no solution for certain energy bands when k is real

And this part is energy associated with this function where you have k+2 pi/ a here, okay. This is how we derive the condition that E is the periodic function of k with periodicity 2 pi/ a. Next, the Schrodinger equation has no solution for certain energy bands, when k is real. Now, let us see how we show this?

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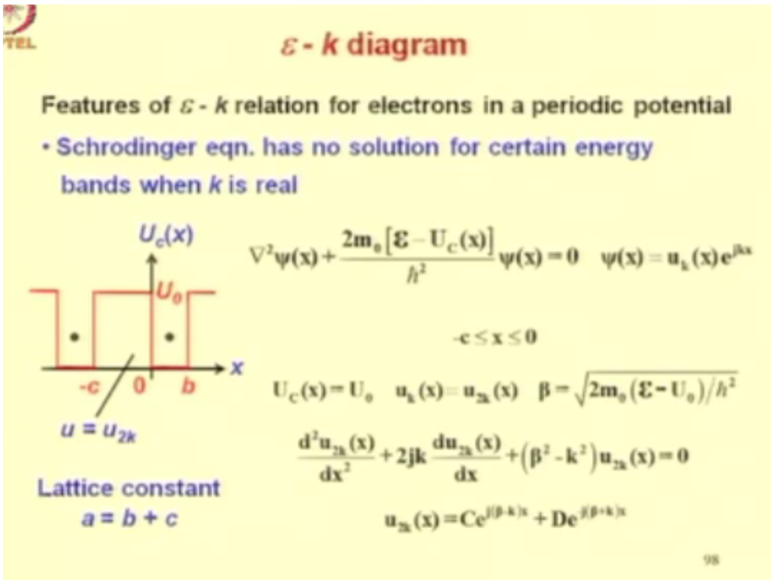

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- Schrodinger eqn. has no solution for certain energy bands when k is real

$$\nabla^2\psi(x)+\frac{2m_0\left[\mathcal{E}-U_C(x)\right]}{\hbar^2}\psi(x)=0 \quad \psi(x)=u_k(x)e^{jkx}$$

$$-c\le x\le 0$$

$$U_C(x)=U_0 \quad u_k(x)=u_{2k}(x) \quad \beta=\sqrt{2m_0(\mathcal{E}-U_0)/\hbar^2}$$

$$\frac{d^2u_{2k}(x)}{dx^2}+2jk\frac{du_{2k}(x)}{dx}+\left(\beta^2-k^2\right)u_{2k}(x)=0$$

$$u_{2k}(x)=Ce^{j(\beta-k)x}+De^{-j(\beta+k)x}$$

Lattice constant
$a = b + c$

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Now, this is our periodic potential approximate form, the points here indicate the location of atoms. The potential well here is having a length b, okay, the origin is set up here at the left end, the height of this potential barrier is U0 and the thickness of the barrier on the left hand side here is c. The distance between the 2 atoms which is a, is nothing but b+c, so this is the lattice concept.

Now, this your Schrodinger equation and this is your solution based on the Bloch theorem. Let us construct the interval 0 to bx; 0 to b that is this interval here. In this interval, the potential is 0, okay; the Ucx is 0 that is what is shown here. The envelope function or the Bloch function Ux, let us indicate that as U1x, the suffix k indicated that this Ux also contains k as a parameter, so this is the U1 function in this region.

The equation for U1 would be obtained by substituting this function writing here U1 instead of U of x, right here U1x, okay, substitute this here and this differential equation derived this particular differential equation, where we have used alpha to indicate this term, which is square root of 2m0 energy/ h cross square, so this term you obtained from this part of this equation.

So, in a simplified form, when you write this is the way the equation will turn up, this differential equation has a solution of this form a* e power j * alpha –kx+b * e power – j* alpha+kx; because the second order differential equation. Now, this solution can be easily seen by substitution, you are getting alpha – k because you have alpha square – k square here as a coefficient, okay.

So, you get alpha – k as well as alpha +k, the 2 things. If you do a similar solution for x line between 0 and –c, that is this region. Now, here your Uc of x = U0, so this U0 is the value of the crystal potential in this region. The Bloch function is U2x, now we define a parameter beta, which is different from alpha in this term that here instead of energy for alpha, you have energy – U0, which is the potential here.

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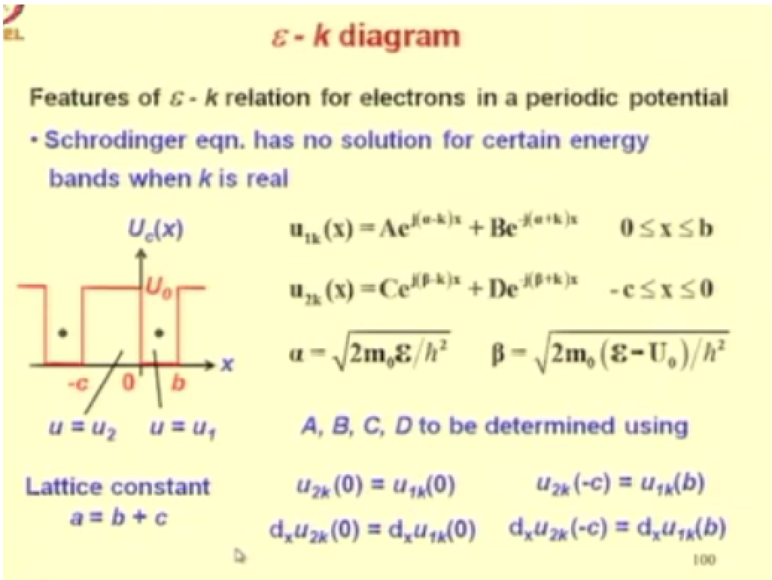

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- Schrodinger eqn. has no solution for certain energy bands when k is real

$$u_{1k}(x) = Ae^{j(\alpha-k)x} + Be^{-j(\alpha+k)x} \qquad 0 \le x \le b$$

$$u_{2k}(x) = Ce^{j(\beta-k)x} + De^{-j(\beta+k)x} \qquad -c \le x \le 0$$

$$\alpha = \sqrt{2m_0\mathcal{E}/\hbar^2} \qquad \beta = \sqrt{2m_0(\mathcal{E}-U_0)/\hbar^2}$$

A, B, C, D to be determined using

Lattice constant
$a = b + c$

$$u_{2k}(0) = u_{1k}(0) \qquad u_{2k}(-c) = u_{1k}(b)$$

$$d_x u_{2k}(0) = d_x u_{1k}(0) \qquad d_x u_{2k}(-c) = d_x u_{1k}(b)$$

Now, in terms of this beta, if you write the differential equation for U2 of x, obtained by substituting this function into this Schrodinger equation, then this is your differentia equation and this is your solution, this similar to the solution U1 x with alpha replaced by beta. So, this is the summary of the solution for U1 of x and U2 of x valid for the 2 ranges x between 0 and b and x between – c and 0.

Now, the coefficients A, B, C and D are to be determined by using the following boundary conditions. Now, look at this boundary conditions; the boundary condition U2 at x =0, should be = U1 at x =0, because the wave function should be continuous across the boundary here, that is the statement, which is being made by this equation. Similarly, the derivative of the wave function should also be continuous here, now that is what is reflected by this equation.

So, d/dx of U2 at x = 0 = d/dx of U1 at x = 0. Now, exactly similar condition should apply at the other end either here or here. Now, because the function is periodic, we can say that the value of the wave function at this end should be equal to the value of the wave function at this end, right. This is the same as saying the value of the wave function when you approach this point from right should be the same as the value of the wave function, you approach the same point from left, okay.

So, this region is identical to this region and this region is identical to this region, so that is why this condition formulated, U2 at –c that is here = U1 at x = b, so U1 at x = b at this end, so value at this end here should be the same as the value at this end. Similarly, for the derivatives, okay. The derivatives should also be the same as at these 2 points. So, we substitute these boundary conditions in this equation to get A, B, C and D.

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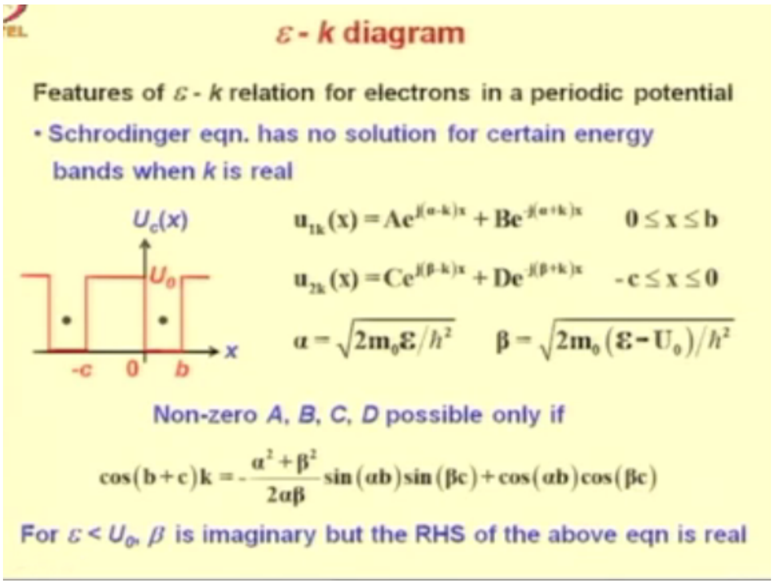

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- Schrodinger eqn. has no solution for certain energy bands when k is real

$$u_{1k}(x) = Ae^{j(\alpha-k)x} + Be^{-j(\alpha+k)x} \qquad 0 \le x \le b$$

$$u_{2k}(x) = Ce^{j(\beta-k)x} + De^{-j(\beta+k)x} \qquad -c \le x \le 0$$

$$\alpha = \sqrt{2m_0\mathcal{E}/h^2} \qquad \beta = \sqrt{2m_0(\mathcal{E}-U_0)/h^2}$$

Non-zero A, B, C, D possible only if

$$\cos(b+c)k = -\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\alpha b)\sin(\beta c) + \cos(\alpha b)\cos(\beta c)$$

For $\varepsilon < U_0$, β is imaginary but the RHS of the above eqn is real

Now, when you do that you will find that nonzero A, B, C, D is possible only, if this particular condition is satisfied, okay. So, this equation is obtained as follows, so you apply the boundary conditions that we have just talked about and write equations for A, B, C and D. Now, in these 4 equations, if you want nonzero A, B, C, D the only way it can be done is by getting this particular relation, so let me explain that.

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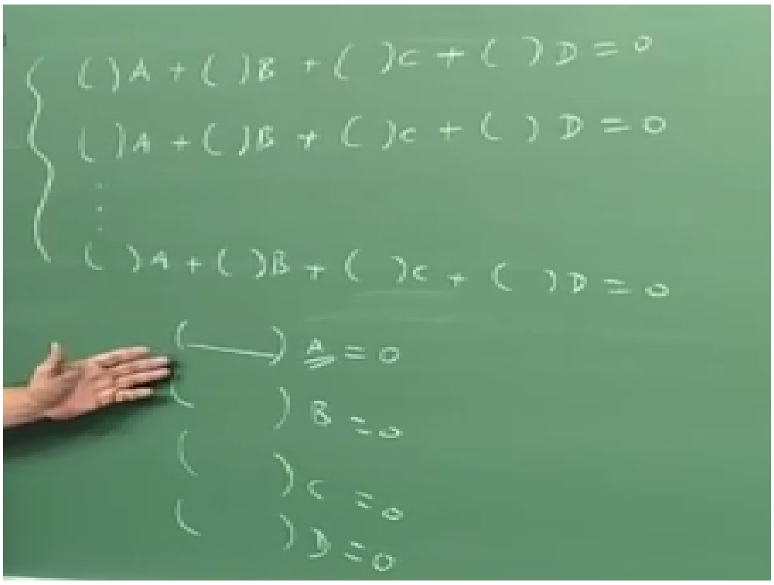

So, the equations will turn out to be of this form, something * A+something * B+something * C+something * D = 0. Now, all the 4 equations will have the same form with different coefficients coming here, so you have 4 such equations, okay you have 4 such equations. Now, evidently A = 0, B = 0, C = 0, D = 0 is the solution but it is the trivial solution, that solution would not work for you, okay.

So, only other solution that you can get, how do you find that? Well you take you express A in terms of B, C and D and substitute here, then you express B in terms of C and D, substitute in the next equation, then you express C in terms of D and that is how you can convert this entire equation to an equation of the form something * A = 0 or something * B =0, so all these 4 equations can be converted into this form, right.

Something * C = 0, or same thing = 0, so if you do not want to a solution A = 0, the only other nonzero solution for A is possible, if you set this term in the bracket to 0, now this is the term that we are talking about here, okay. So, when you set that term to 0, you get this equation, okay. So, the coefficient of A or you can take coefficient of B, right, you can take coefficient of any of these.

Now, this is the key result, based on which we can show the existence of forbidden bands, let us see how? Now, first point to note is that for E less than U0, so U0 is the height for energy less than U0, beta is imaginary you can see here, if E is less than U0 this negative and therefore beta is imaginary but the right hand side of the above equation is real. So, here even if beta is imaginary, this will be real; this is an important point to note.

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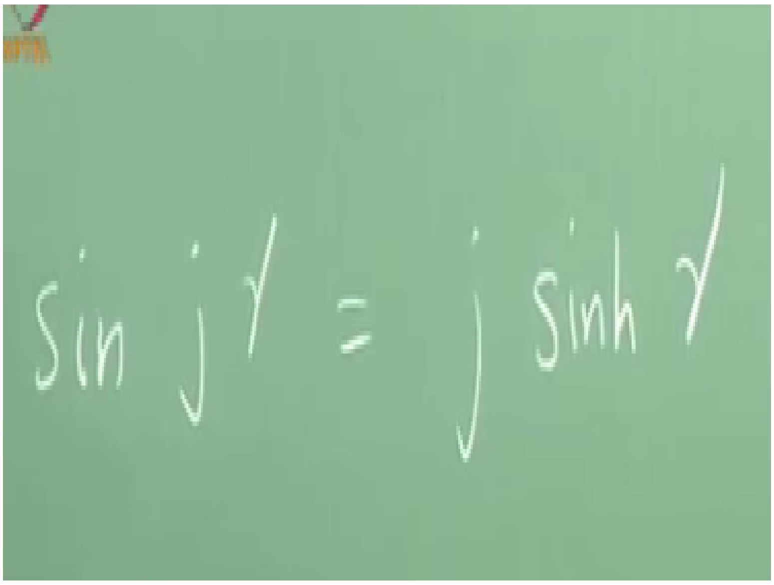

$$\sin j\gamma = j \sinh \gamma$$

Now, how do you get this? Because beta square is real even though beta is imaginary, now here this beta you can write it as some j times some constant, now sin of j times some constant is nothing but j times sin hyperbolic of the same constant, sin of j * some gamma let us say is = j * sin hyperbolic gamma, you can show this very easily, right using exponentials.

So, what will happen is that, similar condition can be shown for cos of imaginary constant here, so a well, we actually do not need that part, we need only this part here, so here you will get a j out; out of the sin and this beta will also contain a j and this j and the j coming out here, when you write this in terms of sin hyperbolic function of a real quantity, so that j will cancel and that is how this part will be real, okay.

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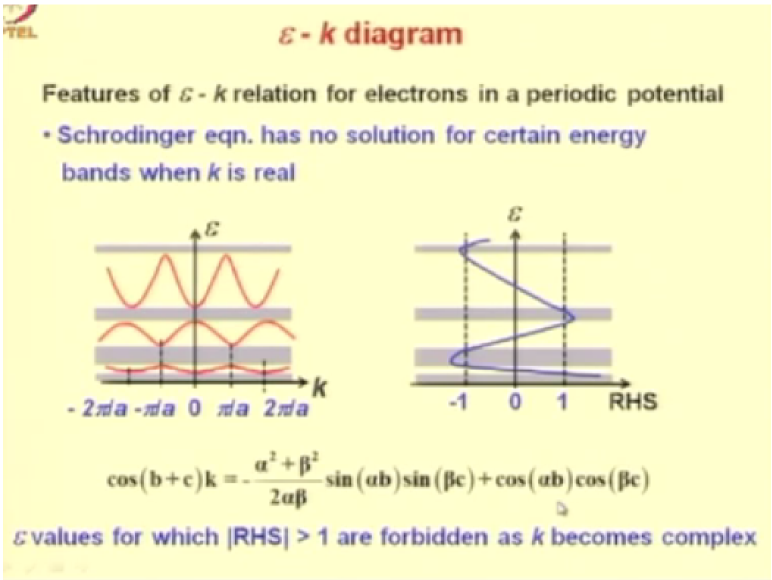

ε - *k* diagram

Features of ε - *k* relation for electrons in a periodic potential

- Schrodinger eqn. has no solution for certain energy bands when *k* is real

$$\cos(b+c)k = -\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\alpha b)\sin(\beta c)+\cos(\alpha b)\cos(\beta c)$$

ε values for which |RHS| > 1 are forbidden as *k* becomes complex

In fact, this part is real even when this j is imaginary. Now, let us look at this function on a plot, so the right hand side of the function that is this part has been plotted as a function of energy because alpha and beta, alpha and beta here, alpha beta, these are functions of energy, which we have defined in the previous slide. So, therefore this whole thing is the function of energy.

So, when you plot, you get a periodic function of energy, the right hand side is a periodic function of energy. Evidently, because sin, cosine and so on these are all periodic functions. Now, what is important here to note; is that the amplitude of this variation goes beyond 1, okay, so it go below -1 and above +1. Now, this is the important result that tells you why certain energies are not possible, okay for electrons in a crystal.

Because if the right hand side here goes either less than -1 or more than 1, then that is not allowed because the cos function has a maximum value of 1, if I take the amplitude, magnitude of this function it cannot exceed 1. Therefore, for those values of E for which the magnitude of this function exceeds 1, that is indicated by this boundary, okay; -1 and +1 here. So, when this function goes beyond process these boundaries, in that region the solution of the Schrodinger equation does not exist, okay.

Because, k is no more real for this regions. So, these regions are therefore shaded to show the forbidden bands, so these bands of energies, here. Similarly these where the right hand side is going the magnitude of the right hand side is going beyond 1, these energies are not allowed because for these energies the k is not real, so the E values for which the modulus of right hand side is more than one forbidden as, k becomes complex.

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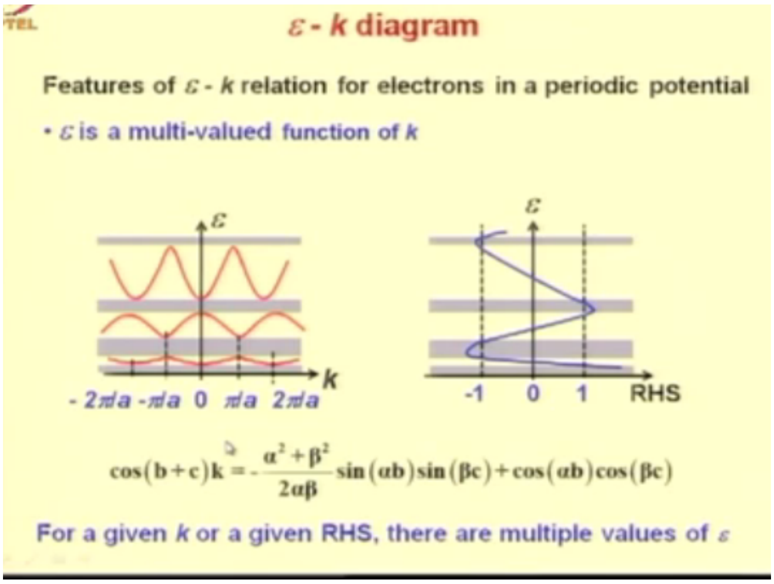

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- ε is a multi-valued function of k

$$\cos(b+c)k = -\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\alpha b)\sin(\beta c)+\cos(\alpha b)\cos(\beta c)$$

For a given k or a given RHS, there are multiple values of ε

Now, these are the bands that are shown on the Ek diagram here, okay so each of this bands shown here actually correspond to these bands, which arise from this particular equation. Now, let us look at the final feature of the Ek diagram, this is that E is the multivalued function of k, how do you get this? Well that is also obtained very easily from this graph, which clearly shows that for a given k or a given right hand side; for a given k or a given value of the right hand side there are multiple values of E.

We can see that here for any given k, there are many values of E, that is again because of the periodic nature of the right hand side, okay and that is why here E is the multivalued function of k, so for any k, you have multiple values of E. So, that is how one can show the 3 important features of the Ek diagram of an electron in a periodic potential.

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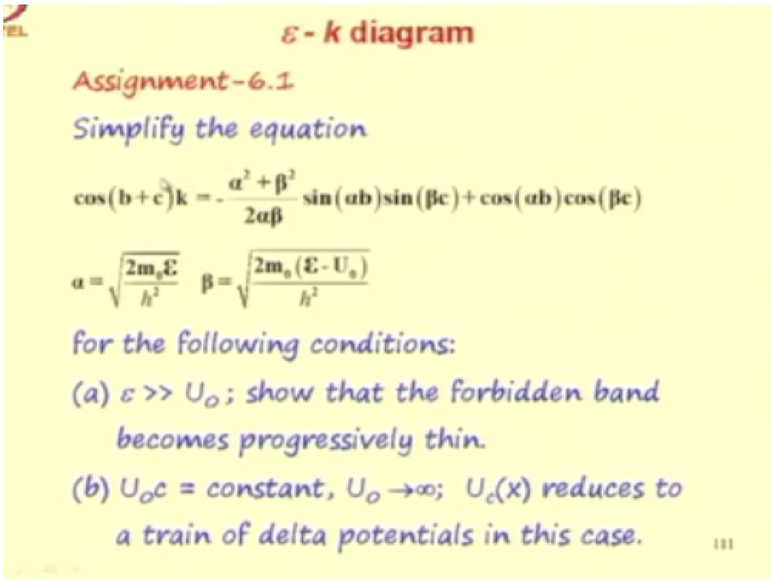

ε - k diagram

Assignment-6.1

Simplify the equation

$$\cos(b+c)k = -\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\alpha b)\sin(\beta c)+\cos(\alpha b)\cos(\beta c)$$

$$\alpha = \sqrt{\frac{2m_0\mathcal{E}}{\hbar^2}} \quad \beta = \sqrt{\frac{2m_0(\mathcal{E}-U_0)}{\hbar^2}}$$

for the following conditions:

(a) $\varepsilon >> U_O$; show that the forbidden band becomes progressively thin.

(b) U_Oc = constant, $U_O \rightarrow \infty$; $U_c(x)$ reduces to a train of delta potentials in this case.

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Now, here is an assignment for you, simplify the equation cosine of b+c * k = - of alpha square+beta square / 2 alpha beta * sin of alpha b * sin of beta c+cos of alpha b * cos of beta c, where alpha and beta are given by these quantities for the following conditions. A; the energy of the electron is much greater than U0, which is the height of the rectangular periodic rectangular potential distribution, okay.

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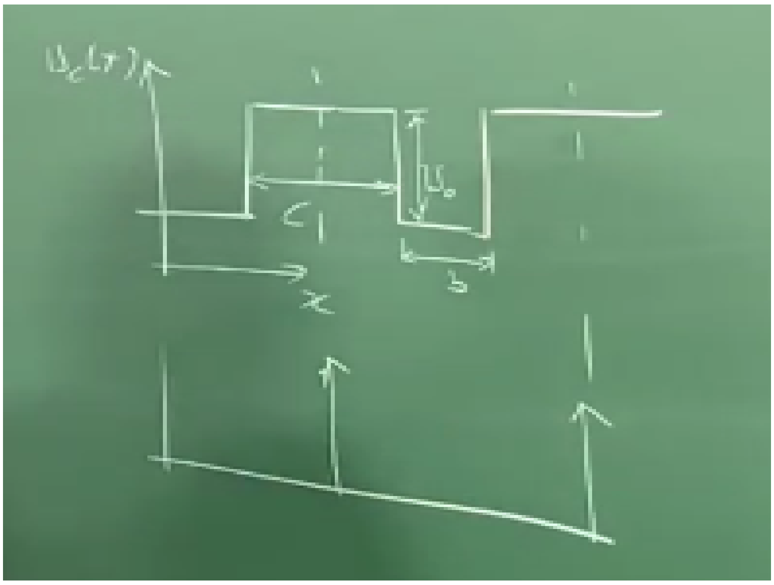

And therefore from your result show that the forbidden band becomes progressively thin as energy becomes more and more; as energy becomes higher and higher. Part B; assume U0 * c is a constant, so U0 * c, let me draw that potential distribution for you here, now this distance is c and this height is U0, okay and this distance is b, so this your rectangular potential. This is x and this is Uc of x.

So, we are saying; assume U0*c that is the area under this as a constant and let U0 go to infinity, okay. So, U0 is going to infinity that means this region will become a delta function, so for this limit, when you maintain the area constant but make U0 infinite here, this will be replaced by delta function. Similarly, we will have another delta function here, somewhere here, so you are replacing this rectangular potential periodic potential distribution by a train of delta functions.

So, for this case, Ucx reduces to a train of delta potentials, okay. So, find out if you use this approximation, what is the simplification that results for this particular equation? It will turn out be much simpler and easier to interpret.

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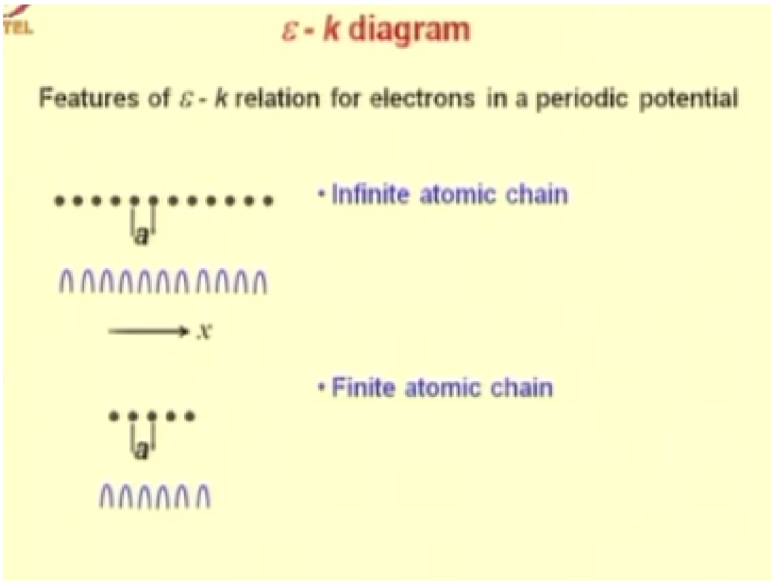

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- Infinite atomic chain
- Finite atomic chain

Now, let us point out what happens if instead of an infinite atomic chain you have a finite atomic chain, so you have a periodic crystal potential but you have a finite number of periods in the potential as against the infinite number of periods for which we have just now derived the Ek relation and energy band picture, so what differences will arises if the atomic chain is made finite?

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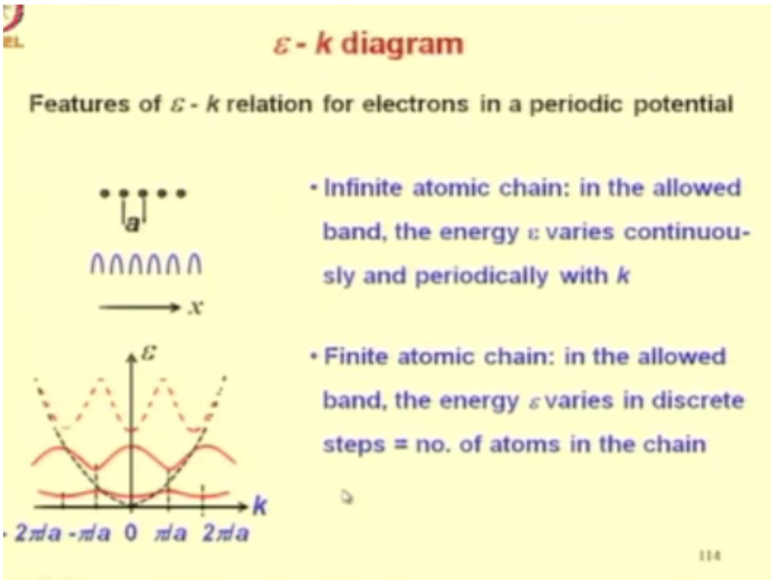

ε - k diagram

Features of ε - k relation for electrons in a periodic potential

- Infinite atomic chain: in the allowed band, the energy ε varies continuously and periodically with k
- Finite atomic chain: in the allowed band, the energy ε varies in discrete steps = no. of atoms in the chain

For an infinite atomic chain in the allowed band the energy E varies continuously and periodically with k, this what you can see, so this is the allowed band of energy, is the another allowed band of energy, this another allowed band and in the allowed bands, the E varies continuously and periodically with k. Now, what will happen if you have a finite atomic chain?

In this case, in the allowed band the energy E varies in discrete steps and the number of discrete steps is equal to the number of atoms in the chain. So, here is an example shown for this band. Now similar discretisation will happen for each of the other bands which have not been shown in this figure. So, you can see here that this allowed band there are 5 discrete energy levels; 1, 2, 3, 4, and 5, why?

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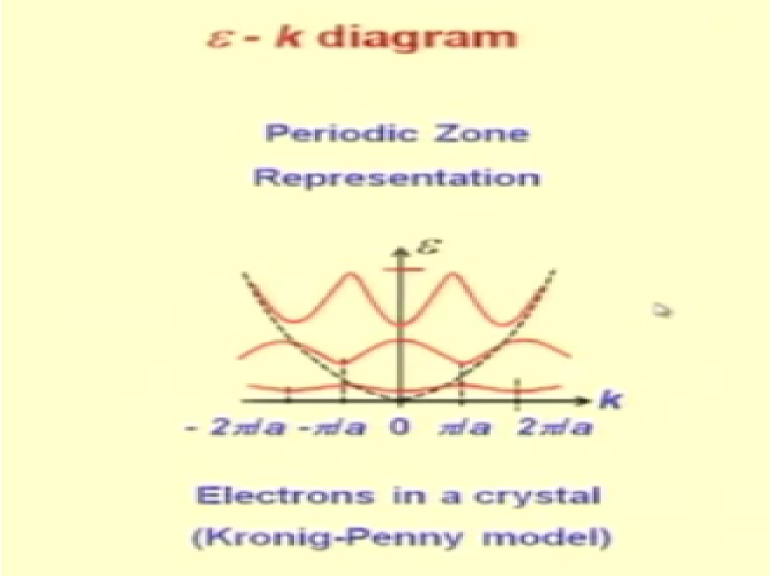

ε - k diagram

Periodic Zone Representation

Electrons in a crystal (Kronig-Penny model)

Because there are 5 atoms here, 1, 2, 3, 4, 5, so 5 atoms in the chain and therefore this allowed bands get discretised into 5 energies. Now, let us come to some aspects of the representation of the Ek diagram. Because the Ek diagram is periodic, it is not necessarily to show many periods of the diagram because information is contained in one period and in fact because the Ek relation is E1, you can even take one half of the period, okay.

And that will give you all the information that is required to construct the entire periodic Ek diagram. So, let us look at this. Now the way we have shown the Ek diagrams so far, it is called the periodic zone representation, okay. Let us look at this various features once again, so here the periodicity = 2pi/ a, so you have marked here 0 pi/ a 2 pi/a and so on. Now, this is the kind of Ek variation which results from the Kronig Penny model, which assumes the rectangular potential distribution; periodic rectangular potential distribution.

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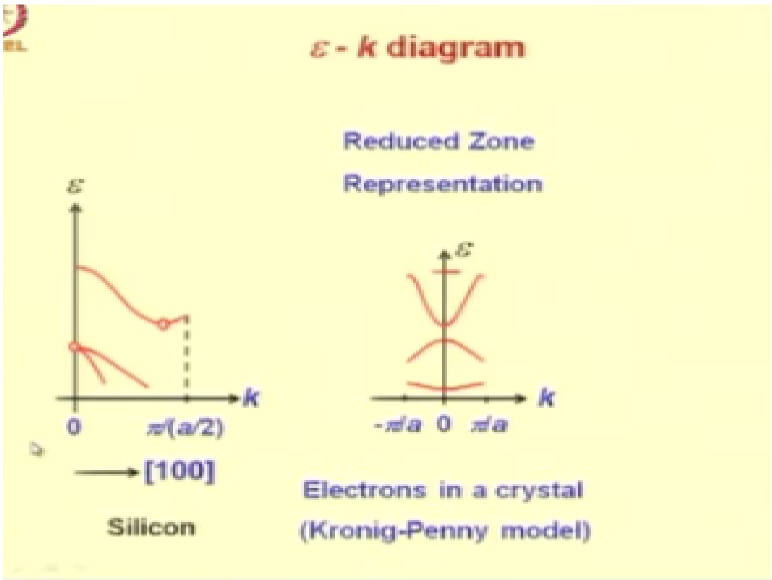

ε - k diagram

Reduced Zone Representation

Silicon

Electrons in a crystal (Kronig-Penny model)

Now, something that I have not mention earlier what is this curve here? Now this curve is a parabola that you would get for the free electron, right. So, for free electron, the Ek relation is a parabola. So, that is what is shown here superpose just for you to be able to compare, the picture for a free electron and the picture for electron in a periodic potential. Now, the reduced zone representation represents the Ek behaviour in just one period okay, 0 to pi/ a and 0 to – pi/a, this is called the first Brillouin zone, okay.

This is called the Brillouin zone because this Ek diagram the way we have determine it the procedure that we have just outlined the Kronig Penny model happens to be the procedure suggested by Brillouin, where you derive the forbidden bands starting from the continuous energy band for free electrons. Now, let us consider the Ek picture for a real crystal, this was an ideal picture.

The Kronig Penny model is the ideal picture where you are assuming the potential; crystal potential to be periodic and rectangular of the shape, actual crystal potential is much more complex. Now, people have done calculations, okay for various real crystals. Let us look at the calculations for silicon, how do they look like? Now, this is the Ek diagram that you will come across in books shown for silicon.

First, let us explain the various aspects of this diagram, now this 100 within brackets, this actually shows a certain orientation of the crystal, you know silicon is a 3 dimensional crystal, so there can be many directions, which you can consider and you can consider the Ek diagram in various directions, right. It is not a one dimensional situation like what we have analysed so far.

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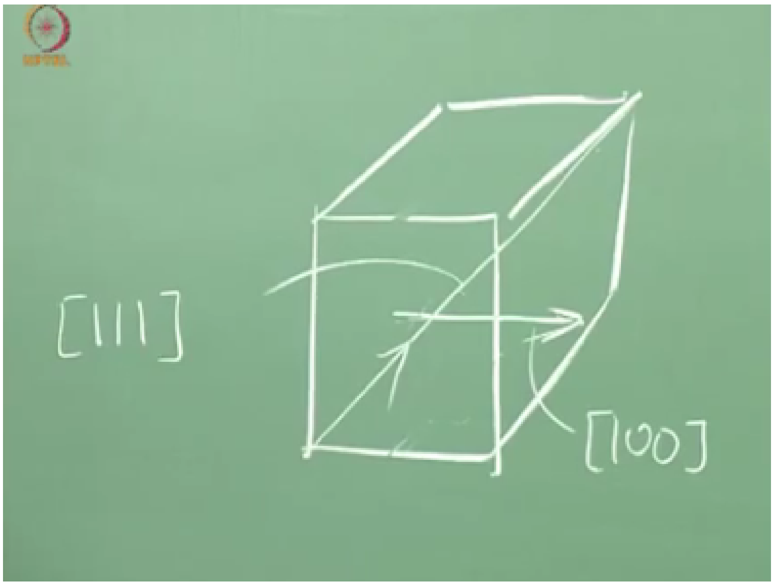

So, for example this is the crystal, now you can move in these direction or you could move in the diagonal directions, so let us say from something like this, right and you will get some Ek diagram because you will get some periodicity of the potential and you will get a different periodicity, if you are moving in this direction, right. Now, this is the direction that is called 100, it is perpendicular to the phases of the cubic of the unit cube of silicon.

Now, we will not discuss the orientation further, this is just to help you understand that Ek diagram is different in different orientations, so you can show the Ek diagram for k vector in this direction, you can show Ek diagram for k vector let us in this direction, these direction would be called 111, okay, why this is called 111 and why this is called 100? This is beyond this course, okay this you can if you are more interested in this, you can read up the books.

So, now for this 100 direction, from 0 to pi/a/2, now why is it a/2 here? Well, as we have said since the Ek diagram is E1, instead of showing from – pi/ a2+pi/ a in the entire first Brillouin zone, you can show even for half of this zone that is from 0 to pi/a, because this part and this part, they are symmetric, so that is what is done here, the diagram is shown only for this half of the Brillouin zone.

Now, the reason here you are using a/2, instead of a, is that, this is the one dimensional crystal, okay. Whereas, here the results are shown for a 3 dimensional crystal, where A is the lattice constant, it turns out that in when you are moving 100 direction that is the direction shown here, the periodicity is related to the location of the various planes atomic planes and 2 successive atomic planes, the distance is a/2; this is a and the successive 100 atomic planes it is a/2, so that is why the a/2 is coming here.

So, as against this kind of variation of Ek relation, here the Ek relation in silicon is something like this, this for the conduction band. In the valence band, this variation looks similar to this variation, right. So, this is conduction band and this; a valence band that is what is shown here. These are lower bands, so you have as you know you have many allowed bands, so normally we are interested in the outer most bands, which is the conduction band.

Because the electron, which have those energies, they contribute to the properties of the semiconductor, they participate in conduction and so on. Now, here there are 2 lines, so there are 2 overlapping Ek relations. Now, this is the complexity that arises because of the nature of ten crystal potential, which is much more complex than what we have considered here. We will not discuss this point further.

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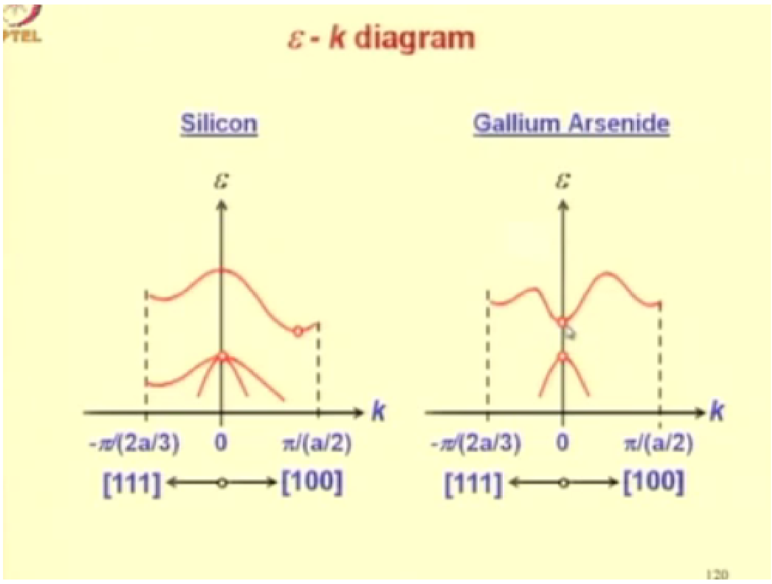

ε - k diagram

Now, normally what one does is, one uses the left hand side, to also provide information of the Ek diagram, if you were to move in the 111 direction. Now, please note the way it is shown here does not mean that 100 direction is exact opposite of 111 direction, right that is not what is meant here, so I have said this diagonal is a 111 direction, right and perpendicular to the phase is 100.

So, those are the directions, so the diagrams in those directions. Now, here instead of a/2, you have 2a/3 because in the 111 direction, the successive atomic planes the distance between them is 2a/3, you just accept this result without going into why it is 2a/3, now that you will study, if you study the crystal structure of silicon in detail. So, you can see when you move in 111 directions, the conduction band Ek relation is somewhat different, okay, both for conduction and valence bands.

The so called energy gap is actually the distance between the bottom of this Ek realtion for conduction band and the top of Ek relation for valence band. So, you see that this vertical distance between these 2 points in the 100 direction is different from the vertical distance between the points in 111 directions. Here, the gap is more, okay, here the gap is less, the vertical distance between these 2points is less.

Now, compare the Ek diagram of silicon with that of Gallium arsenide, where your crystal potential is different, right. So, if you do a numerical calculation for the crystal potential associated with Gallium arsenide, the band diagram which results look something like this. The key difference between the Ek diagram of gallium arsenide and Ek diagram of silicon is that the bottom of the Ek variation in the conduction band is shifted away from the Ek variation, bottom of the Ek variation of the valence band here.

So, there is a difference in k locations of this minimum and this maximum, whereas the minimum of the Ek relation of the conduction band in gallium arsenide is right above the maximum of the relation of the valence band. Now, this difference in the Ek diagrams is the reason why the gallium arsenide is called a direct band gap semiconductor and silicon is called the indirect band gap semiconductor, okay.

So, more about this later, the reason it is called direct is the vertical transition can be made from an electron can make a vertical transition down from conduction to valence band without changing its momentum right. Now, unfortunately this result is all right for free electrons, but not electrons in crystal and you have to restore to the Ek diagram to actually get these relations, okay and they will not be exactly identical to what we have discussed.

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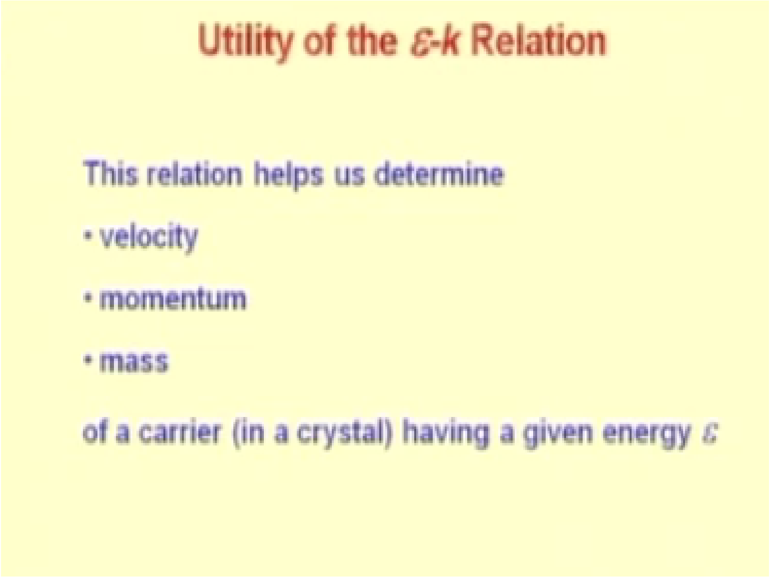

Utility of the ε-k Relation

This relation helps us determine

- velocity
- momentum
- mass

of a carrier (in a crystal) having a given energy ε

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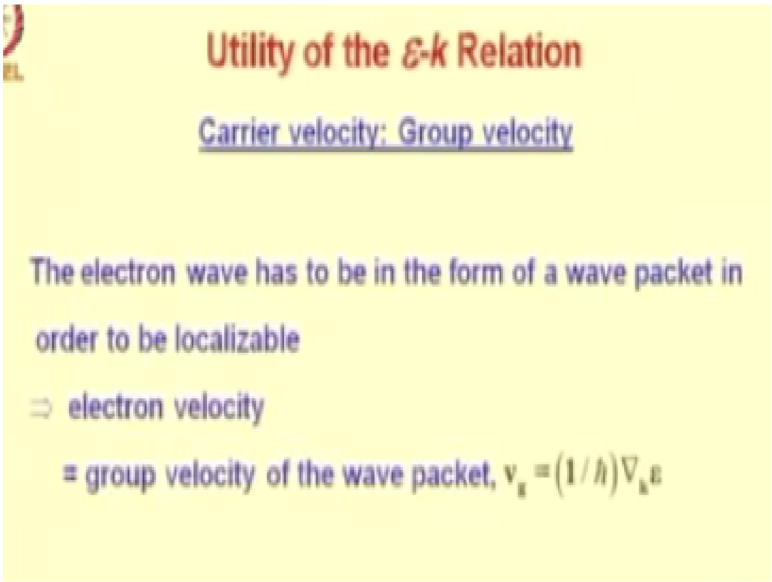

Utility of the ε-k Relation

Carrier velocity: Group velocity

The electron wave has to be in the form of a wave packet in order to be localizable

$\Rightarrow$ electron velocity

$\equiv$ group velocity of the wave packet, $v_g = (1/\hbar)\nabla_k \varepsilon$

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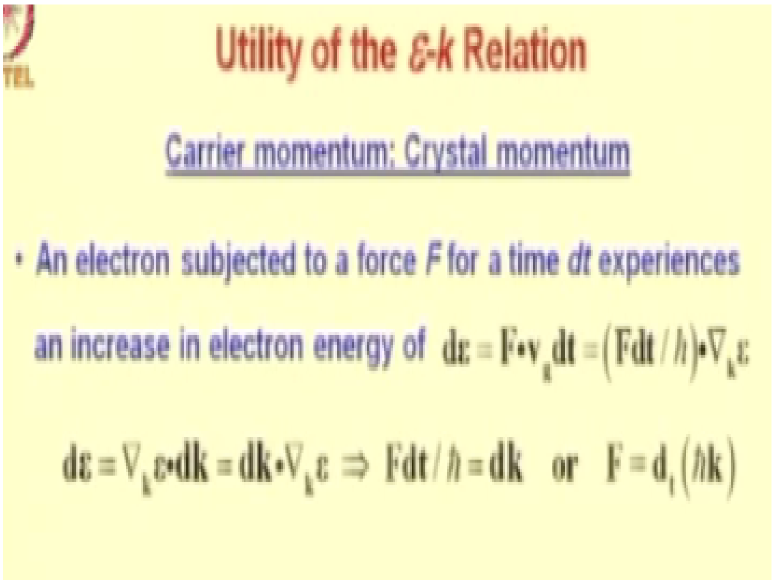

Utility of the ε-k Relation

Carrier momentum: Crystal momentum

- An electron subjected to a force *F* for a time *dt* experiences an increase in electron energy of $d\varepsilon = \mathbf{F}\cdot\mathbf{v}_g dt = (\mathbf{F}dt/\hbar)\cdot\nabla_k\varepsilon$

$$d\varepsilon = \nabla_k\varepsilon\cdot d\mathbf{k} = d\mathbf{k}\cdot\nabla_k\varepsilon \Rightarrow \mathbf{F}dt/\hbar = d\mathbf{k} \quad \text{or} \quad \mathbf{F} = d_t(\hbar\mathbf{k})$$

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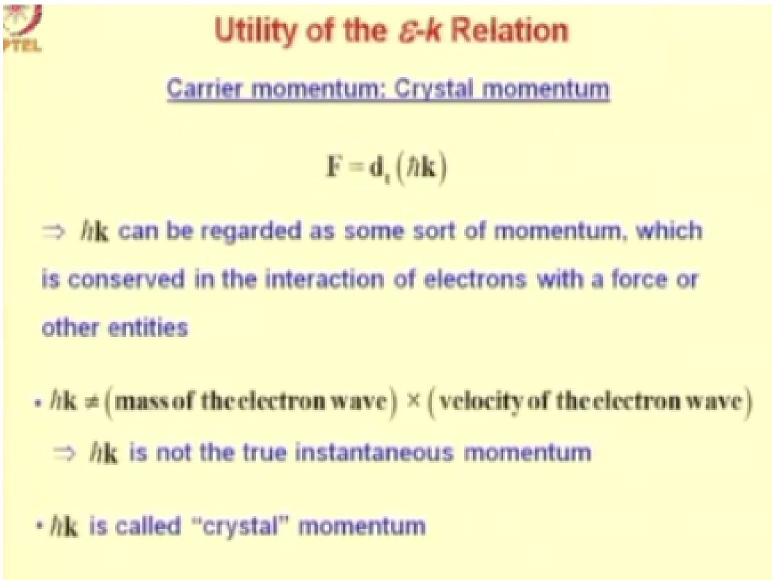

Utility of the ε-k Relation

Carrier momentum: Crystal momentum

$$\mathbf{F} = d_t(\hbar\mathbf{k})$$

$\Rightarrow$ $\hbar\mathbf{k}$ can be regarded as some sort of momentum, which is conserved in the interaction of electrons with a force or other entities

- $\hbar\mathbf{k} \neq (\text{mass of the electron wave}) \times (\text{velocity of the electron wave})$

  $\Rightarrow$ $\hbar\mathbf{k}$ is not the true instantaneous momentum

- $\hbar\mathbf{k}$ is called “crystal” momentum

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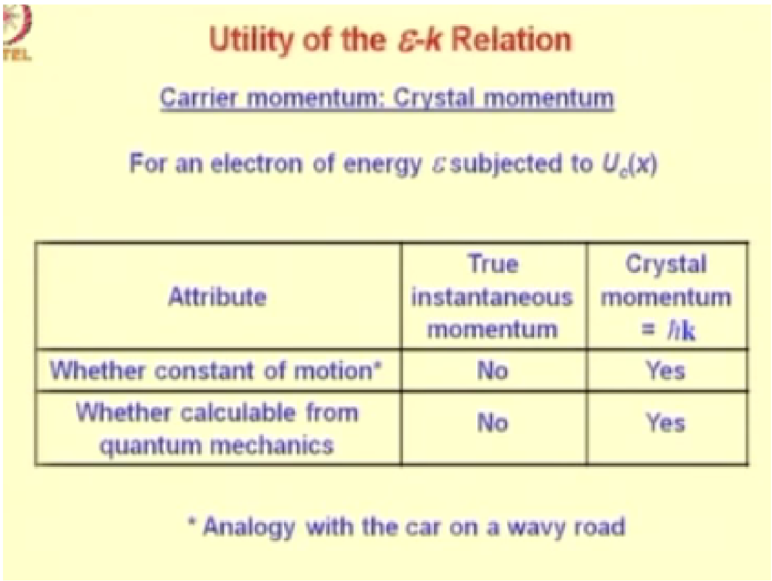

Utility of the ε-k Relation

Carrier momentum: Crystal momentum

For an electron of energy ε subjected to $U_c(x)$

Attribute	True instantaneous momentum	Crystal momentum = $\hbar\mathbf{k}$
Whether constant of motion*	No	Yes
Whether calculable from quantum mechanics	No	Yes

* Analogy with the car on a wavy road

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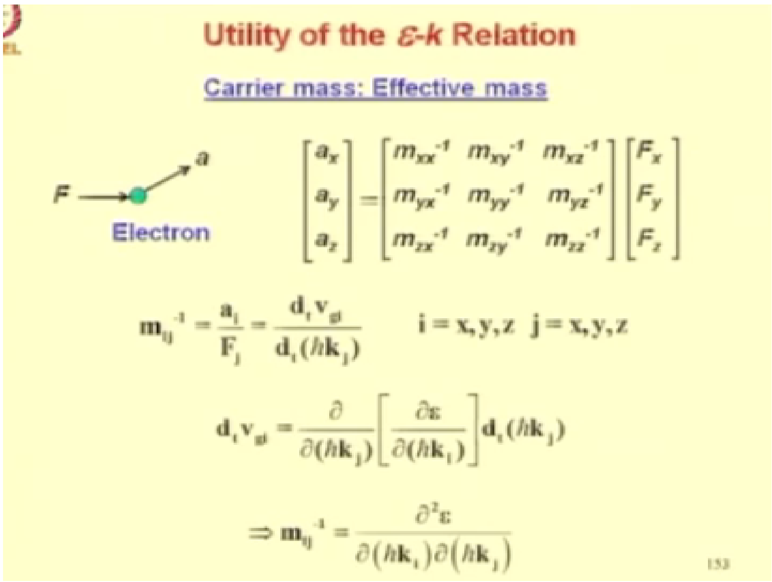

Utility of the ε-k Relation

Carrier mass: Effective mass

$$\begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix} = \begin{bmatrix} m_{xx}^{-1} & m_{xy}^{-1} & m_{xz}^{-1} \\ m_{yx}^{-1} & m_{yy}^{-1} & m_{yz}^{-1} \\ m_{zx}^{-1} & m_{zy}^{-1} & m_{zz}^{-1} \end{bmatrix} \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix}$$

$$\mathbf{m}_{ij}^{-1} = \frac{\mathbf{a}_i}{\mathbf{F}_j} = \frac{\mathbf{d}_t \mathbf{v}_{gi}}{\mathbf{d}_t(\hbar\mathbf{k}_j)} \qquad \mathbf{i} = \mathbf{x},\mathbf{y},\mathbf{z} \quad \mathbf{j} = \mathbf{x},\mathbf{y},\mathbf{z}$$

$$\mathbf{d}_t \mathbf{v}_{gi} = \frac{\partial}{\partial(\hbar\mathbf{k}_j)}\left[\frac{\partial\varepsilon}{\partial(\hbar\mathbf{k}_i)}\right]\mathbf{d}_t(\hbar\mathbf{k}_j)$$

$$\Rightarrow \mathbf{m}_{ij}^{-1} = \frac{\partial^2\varepsilon}{\partial(\hbar\mathbf{k}_i)\partial(\hbar\mathbf{k}_j)}$$

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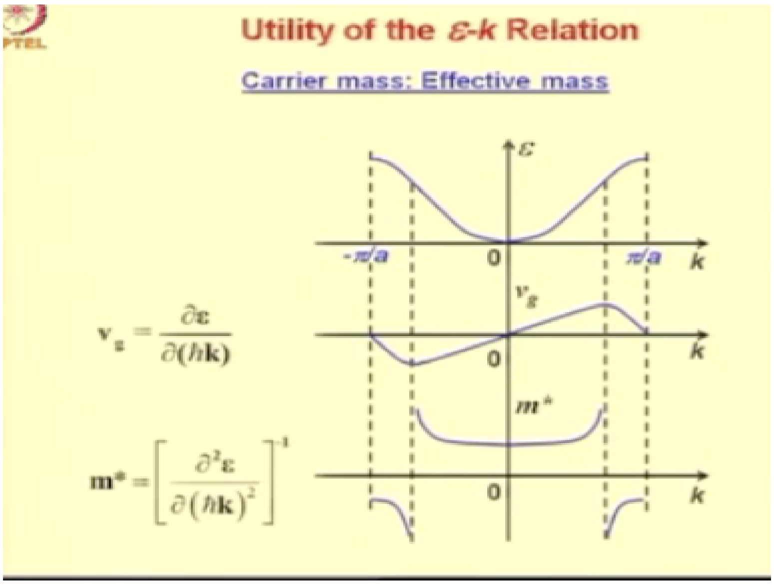

Utility of the $\mathcal{E}$-k Relation

Carrier mass: Effective mass

$$v_g = \frac{\partial \varepsilon}{\partial(\hbar \mathbf{k})}$$

$$m^* = \left[\frac{\partial^2 \varepsilon}{\partial(\hbar \mathbf{k})^2}\right]^{-1}$$

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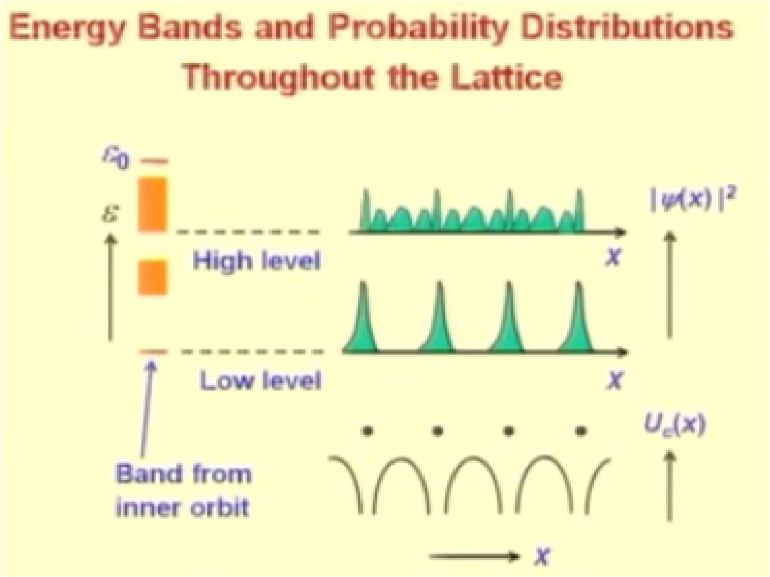

Energy Bands and Probability Distributions Throughout the Lattice

Now, this is the point that we will start within the next class, since we have come to the end of the lecture, let us make summary of the important points. So, in this lecture, we have discussed determination of the Ek diagram in a quantitative fashion in detail. This determination was discussed for a periodic crystal potential, we assume an idealised crystal potential, which has a rectangular periodic shape.

And then we showed how you can solve the Schrodinger equation for this potential and derive 3 important features of the Ek diagram of electrons in a crystal. These 3 features are 1; is that the Ek relation is periodic with periodicity = 2 pi/ distance between the atoms, so we have assumed an idealised one dimensional situation. The next feature is that for certain energies the Schrodinger equation does not have a solution and therefore these energies are not allowed for the electrons.

And the third important feature is that the energy as a function of the momentum or the wave vector k, a is a multivalued function that is for any given value of k, there are multiple value of E as against this, for example for a free electron for any given value of k, there is only one value of E, even for an electron in a rectangular potential well for any given value of k, there is only one value of E, okay.

So, the differences between the Ek relations of free electron the electron in a rectangular potential well and the electron in a periodic potential were clearly brought out by discussing how the Schrodinger equations is solved. Now, we have outlined the various steps of the solution for what is called a Kronig Penny model, okay idealised periodic rectangular potential distribution.

Now, the features from here can also be the qualitative features of this solution can be applied even to real crystals. So, we have discussed, so the shape of the Ek relation for real crystal such as silicon and gallium arsenide. Now, we want to make a point, that while the various steps of the Schrodinger; solution to the Schrodinger equation for a periodic crystal potential outline, we have not really gone through the various steps in detail.

Because such a derivation can go on to 2 or 3 classes and one can always read it up because it is available in various books. So, we have focussed ourselves on the outline of the key steps in the procedure. In the next class, we are going to see the utility of the Ek relation, how it can be used to find out the effective mass, the velocity and the crystal momentum of the electron in a crystal and we will also begin a discussion of how one can calculate the Ex diagram of devices.