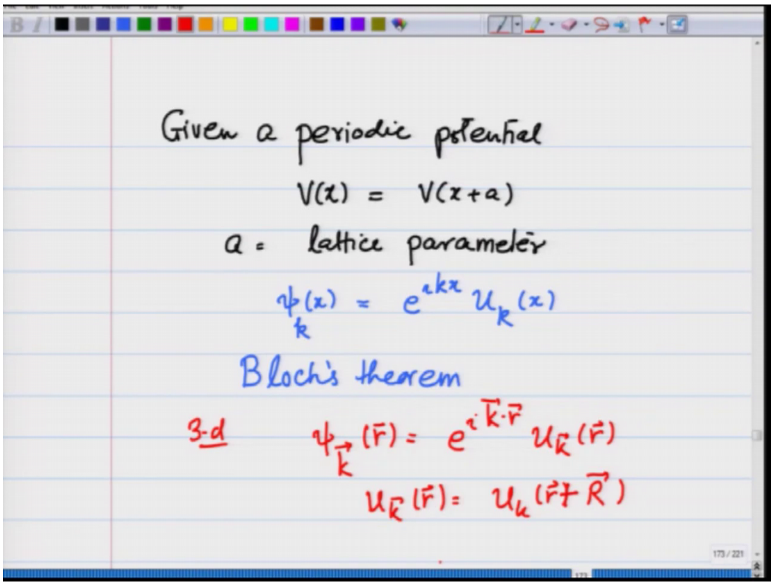
**Introduction to Solid State Physics**
**Prof. Manoj K. Harbola**
**Prof. Satyajit Banerjee**
**Department of Physics**
**Indian Institute of Technology, Kanpur**

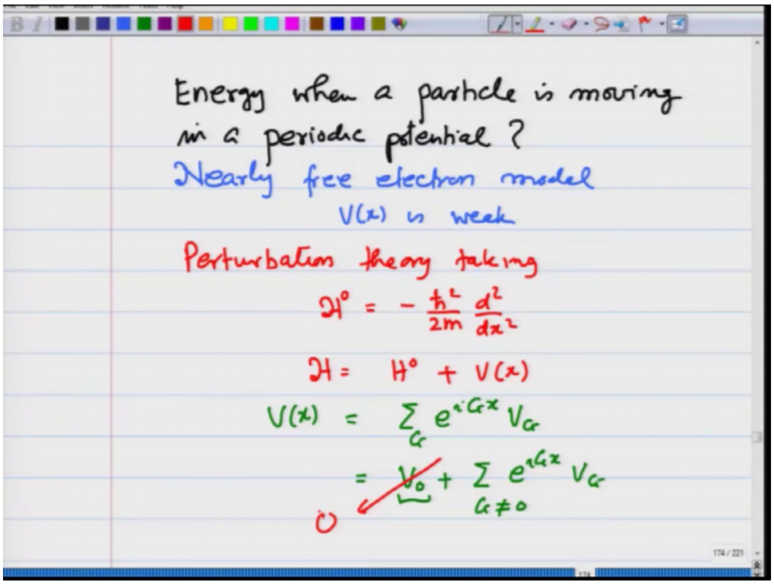
**Lecture – 58**
**Mixing of plane waves to get Bloch Wavefunction – I**

(Refer Slide Time: 00:19)




In the lecture so far what I have argued is that, given a periodic potential V x equals v x plus a where a is the lattice parameter. The wave function has the form psi x and we label it with k equals e raised to i k x a periodic function u k x and this is known as the Bloch's theorem. Then once we know this general form and let me also write this for three dimensions 3-d, the Blochs theorem says that there is a k vector r is going to be equal to e raised to i k dot r u k r where u k r is equal to u k r plus the lattice vector r. This periodic with lattice vector minimum being primitive lattice vector. So, it is periodic over that. This was the effect on the wave function how about the energy.

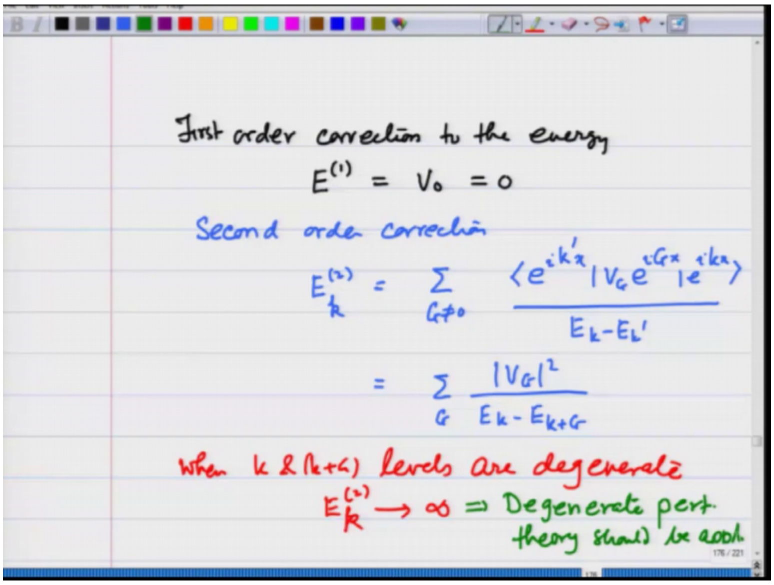
(Refer Slide Time: 01:44)




When a particle is moving in a periodic potential, we considered what I call the nearly free electron model in which V x is weak. And therefore, we could apply perturbation theory taking the unperturbed Hamiltonian H 0 to be only the kinetic energy operator and adding to it the weak periodic potential.

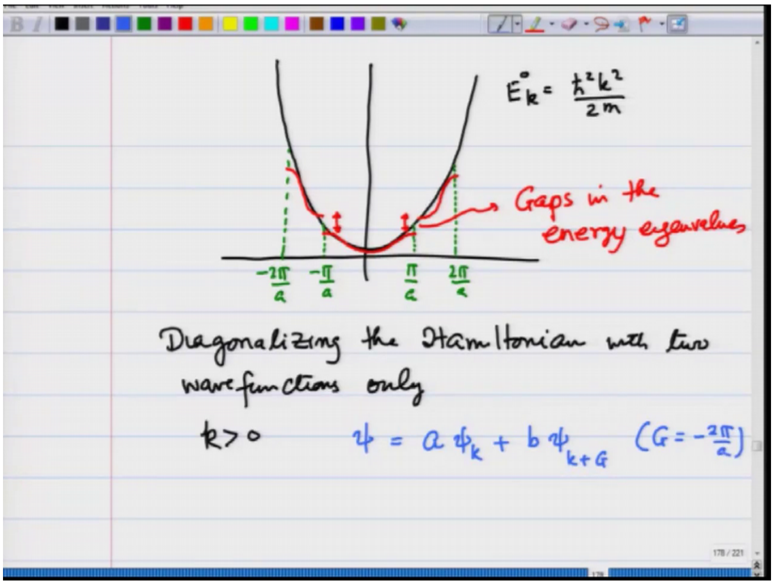
The potential has the form V x equals summation E raised to i G x V G summed over G from which I can separate the G equals 0 component which is V 0 plus summation E raised to i Gx V G; G naught equal to 0 and you see this G equals 0 component is a constant. So, it just refers to the reference point of the potential and we took this to be 0.

(Refer Slide Time: 03:32)




In that case when I applied the perturbation theory, we found that the first order correction to the energy E 1 was equal to V 0 which is 0 and the second order correction E 2 which is given as summation G naught equal to 0 E raised to i k prime x V G e raised to i G x e raised to i k x divided by E k minus E k prime; this is second order correction for the k'th level. This comes out to be equal to mod V G square over E k minus E k plus G summed over G. This is all fine as long as k and k plus G are not degenerate, when k and k plus G levels are degenerate, then E 2 k goes to infinity. Our perturbation result does not hold anymore and what we did then is we applied implies degenerate perturbation theory should be applied.

(Refer Slide Time: 05:25)

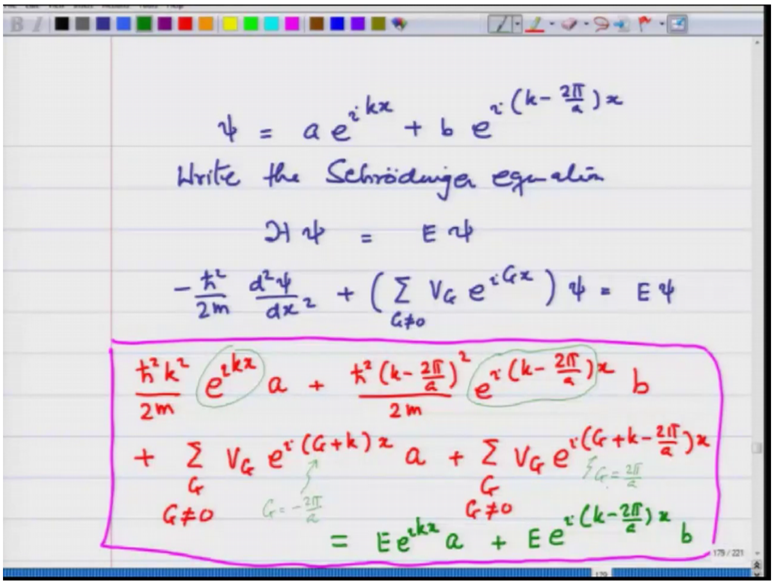



When we apply degenerate perturbation theory what we found is, that if I have this unperturbed energy curve like this E 0 k equals h cross square k square over 2 m. At the points, the Brillouin zone let me make two of them. This is pi over a 2 pi over a, minus pi over a, minus 2 pi over a. This is where E k and E k plus j become degenerate.

For example for k equals pi by a E k minus 2 pi by a will become degenerate for k equals two pi by a 2 pi by a minus 4 pi by a will become degenerate and then what happens is that a gap opens up near the Brillouin zone boundary. And therefore, energy does not remain continuous anymore rather it will become something like this and there is this gap which opens up. So, you have gaps in the energy. So, these are called the gaps in the energy eigenvalues. These energies are not there anymore and we got this by applying degenerate perturbation theory.

Let us now look at this result from the point of view of diagonalizing the Hamiltonian with two wave functions only. I will consider case where k is greater than 0. So, I am considering the case where I am on the right side of k equals 0 and I will consider the wave function side to be some constant a psi k plus where psi k is understood by E raised to i k x b psi k plus G. We are now in this case because I am taking k equals 0 k greater than 0 G should be equal to minus 2 pi by a because the degeneracy opens up at k equals pi by a. So, I am mixing these two levels and seeing what the energy would look like.

(Refer Slide Time: 08:11)

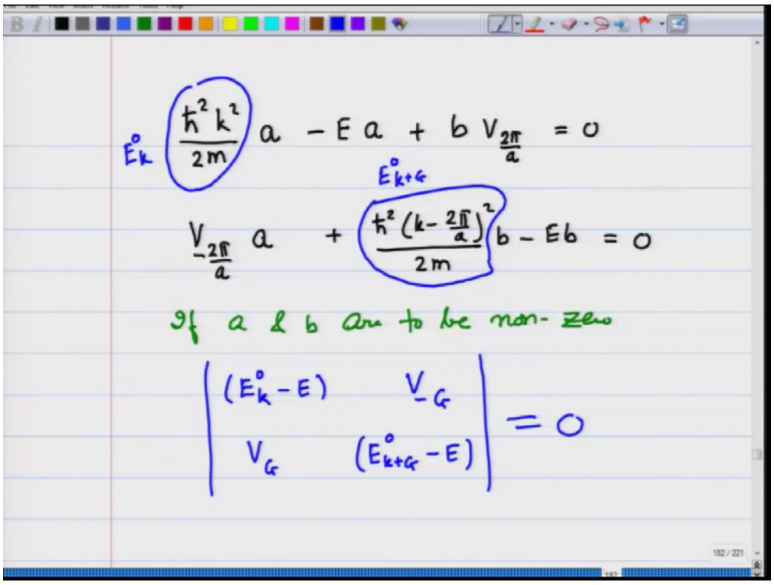



So, let me write it explicitly I am looking at psi equals a e raised to i k x plus b E raised to i k minus 2 pi by a x. If I now write the Schrodinger equation, then I have H psi equals E psi and I have h s minus h cross square over 2 m d 2 psi over d x square plus summation V G G naught equal to 0 E raised to i G x times psi equals E psi.

So, let me now apply this two psi and then I am going to have h cross square k square over 2 m w raised to i kx will come with a coefficient a plus h cross square k minus 2 pi by a square over 2 m e raised to i k minus 1 pi by a x come with the coefficient b plus summation G V G E raised to i G plus k x. This will come with a coefficient a G is not equal to 0 plus summation G V G e raised to i G plus k minus 2 pi by a x, this is also G naught equal to 0 equals E e raised to i kx with a coefficient a plus E e raised to i k minus 2 pi by a x b. This is the equation that we get for a and b. In this I will equate the coefficients of e raised to i kx on both sides e raised to i k minus 2 pi by a on both sides

So, you can see since G is not equal to 0, I will get G equals minus 2 pi by a here and that will give me the coefficient for k minus 2 pi by a x and I will have G equals 2 pi by a here and that will give me the coefficient for E raised to i kx.

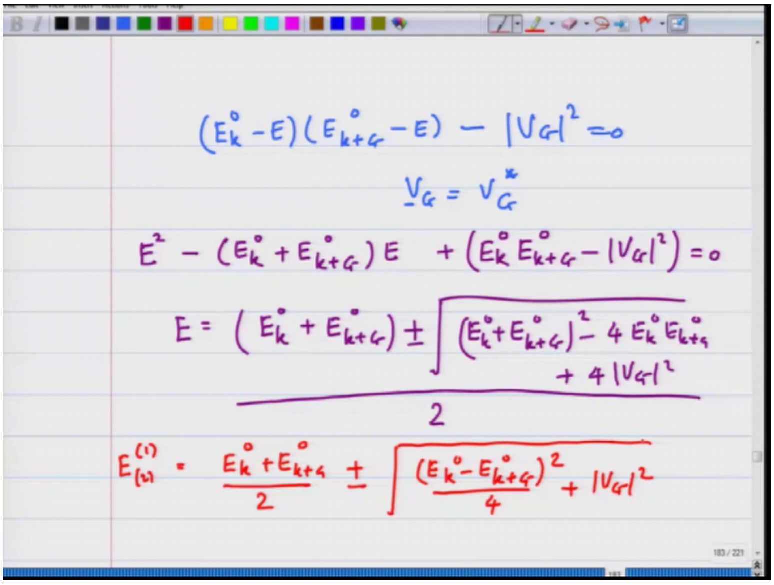
(Refer Slide Time: 11:31)




So, equating the coefficients of e raised to i kx and e raised to i k minus 2 pi by a x, I get h cross square k square over 2 m a minus E a plus b V 2 pi by a equals 0 and for the other equation, I get I will write the a part first.

So, I am going to get V minus 2 pi by a, a plus h cross square k minus 2 pi by a whole square over 2 m b minus E b equals 0. If a and b are to be non-zero, then I should have the determinant of let me write this term as E 0 k and this term as E 0 k plus G. So, that I get E k 0 minus E. Here I am going to get V G is minus 2 pi by a. So, minus G V G E k plus G 0 minus E determinant should be 0 and that will give me the eigenvalue E.

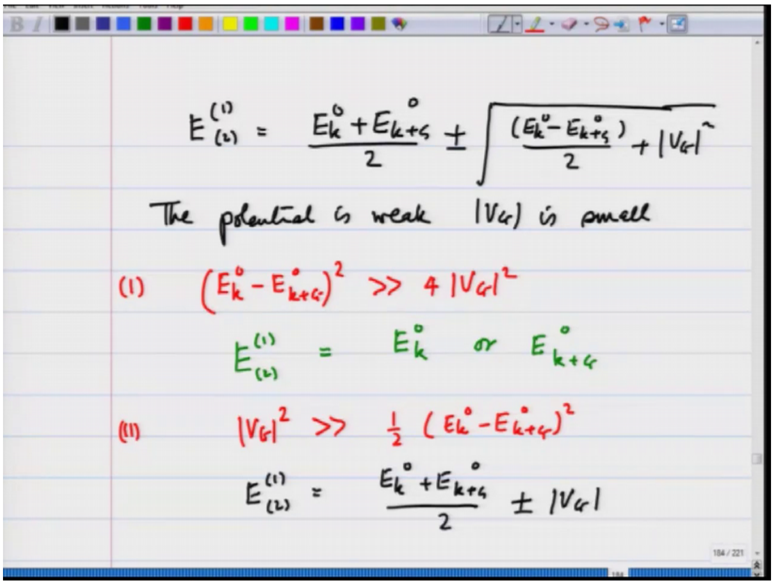
(Refer Slide Time: 13:30)




Let us solve this. When I solve this, I am going to get E k 0 minus E times E k plus G 0 minus E minus mod V G square is equal to 0. This comes out to be mod V G square because V minus G is equal to V G star and this equation then becomes E square minus E k 0 plus E k plus G 0 E plus E k 0, E k plus G 0 minus mod V G square equals 0. This is a quadratic equation in E.

So, the solutions for E r E k 0 plus E k plus G 0 plus or minus square root of E k 0 plus E k plus G 0 square minus 4 E k 0 E k plus G 0 plus 4 mod V G square divided by 2. And therefore, I get two solutions E 1 is equal to E k 0 plus E k plus G 0 divided by 2 plus I can write 2 here for the lower side plus or minus square root of E k 0 minus E k plus G 0 square divided by 4 plus mod V G square. And deriving this, I have taken this 2 inside the square root sign and therefore, it goes as 1 over 4 and this is what we get.

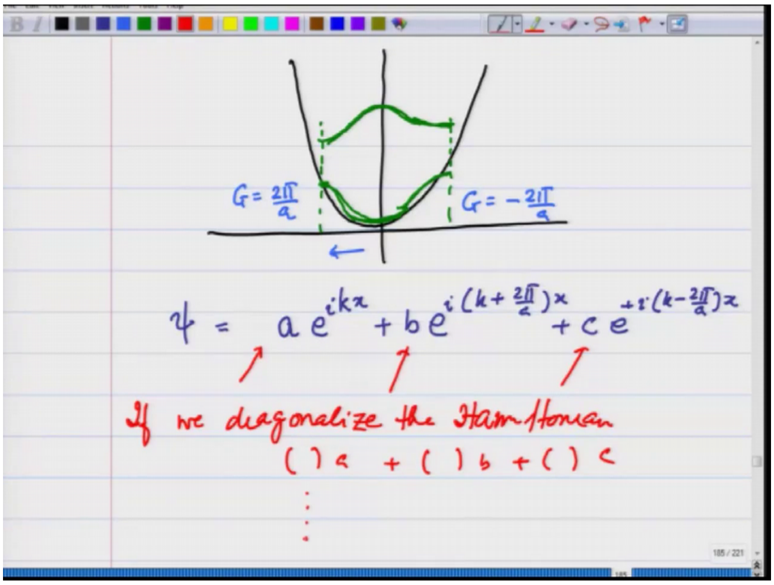
(Refer Slide Time: 15:39)




So, what we have is that E 1 or 2 is equal to E k 0 plus E k plus G 0 divided by 2 plus or minus square root of E k 0 minus E k plus G 0 divided by 2 plus mod V G square. Now since V the potential is weak, V G can be very small is small. Now take two cases; 1, E k 0 minus E k plus G 0 square is much much much greater than 4 V G square.

In that case I am going to get E 1 or 2 is equal to E k 0 or E k plus G 0 not much different. It is like first order perturbation theory where the first order correction was 0, second order correction is small. On the other hand, if I take V G square to be much much much greater than 1 half E k 0 minus E k plus G 0 square; that means, I am reaching the regime of the points where E k 0 and E k plus G 0 are very close. I am reaching near the Brillouin zone, then I get E 1 or 2 is equal to E k 0 plus E k plus G 0 divided by 2 plus or minus mod V G. Precisely is the result that we got through degenerate perturbation theory.

(Refer Slide Time: 17:52)



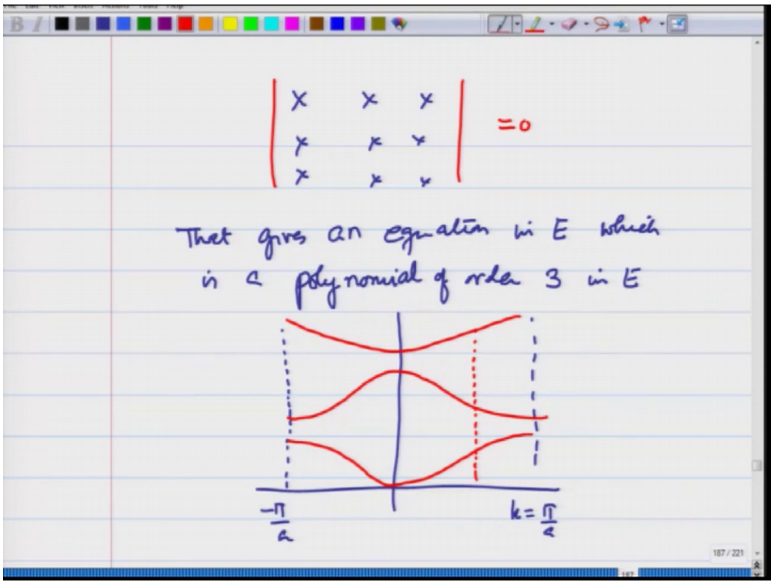

So, this again tells you that if I have this energy curve near k equals 0 or so, the energy remains roughly either E k 0 or E k. I will show you how this curve comes later E k plus G 0 and as you approach the Brillouin zone, there is a gap that opens up as you approach the brillouin zone, there is a gap that opens up.

So, energy curves look like this. Besides the result we got earlier, this we did through two plane waves mixing. Now for this, I had to take G equals minus 2 pi by a when I was going towards the right and I will have to take G equals 2 pi by a. This part I did not do, but you can easily see since everything is symmetric; you can repeat this calculation. So, I had to take G equals 2 pi by a when I was considering k on this side.

Suppose I do not want to do that I do not want to consider which G to take which not to take. I will take an expansion where I will take psi to be a mixture of three plane waves e raised to i kx plus b e erased to i k plus 2 pi by a x plus c e raised to i k minus 2 pi by a x. I do not have to now worry whether I am taking G equals plus 2 pi by a minus 2 pi by a and so on and again repeat the same calculation.

Now, I have three coefficients. So, I will have an equation for these three coefficients and if we diagonalize the Hamiltonian, I will have three equations; some coefficient a plus, some coefficient b plus some coefficient c three equations like these and for a b c to be nonzero, the determinant of these coefficients will have to be 0.

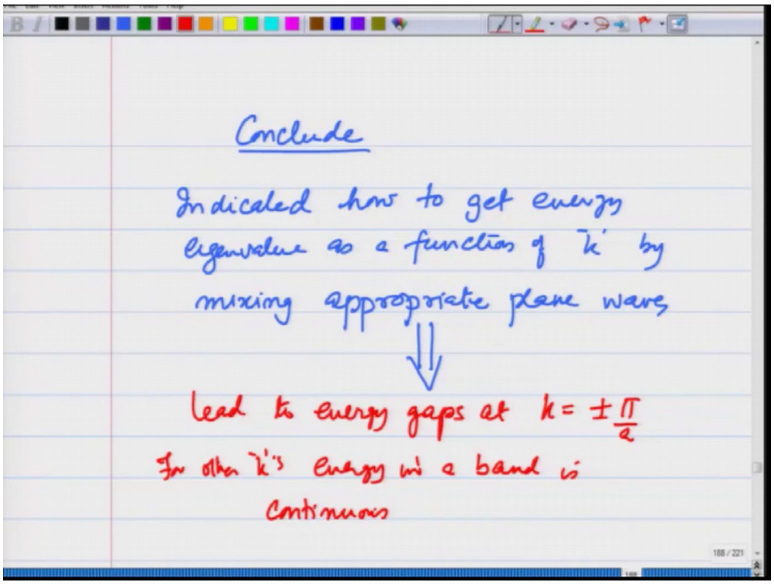
(Refer Slide Time: 20:10)




And that will give. So, these are the coefficients and that gives an equation in E or for E which is a polynomial of order 3 in E. And then you will have to calculate the eigenvalues of E through a computer and what you will find and this I will give as an assignment. Again if I can find myself between k equals pi by a and I will give you reason why I can confine myself between k equals pi by a and minus pi by a, you will find that you will get energy for different case like this and there will be a band like this. So, you will get 3 eigenvalues for each k because I mix three plane waves and you will find a band structure like this.

More plane waves I add, more the bands you will get and I will do that in the next lecture and you will also see why I am confining myself to minus pi by a 2 pi by a.

(Refer Slide Time: 21:31)




So, we conclude in this lecture, what I have done is indicated how to get energy eigenvalue as a function of k by mixing appropriate plane waves. And these also lead to energy gaps at k equals plus minus pi by a, for other case energy in a band is continuous. I will build upon this argument in the next lecture and give a proof based on this plane wave expansion give a proof for the Blochs theorem again.