Relativistic Quantum Mechanics
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Lecture - 16
Arrow of time and particle-antiparticle asymmetry, Band theory for Graphene

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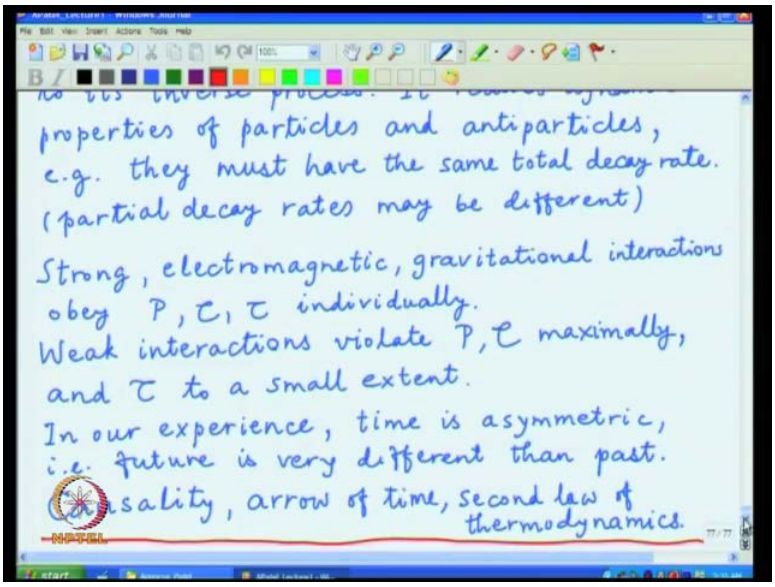

In the previous lecture, I discuss the time reversal symmetry. And showed that the Dirac equation does obey this symmetry; the symmetry extends too many other interactions as well and we have an only a tiny violation of a time reversal symmetry in the weak interactions. This observation in some sense is hard to grasp, because we have a very strong sense of arrow of time. And so there is enough confusion about how there could be a strong asymmetry in our observation as far as time is concerned while the dynamical equations show a only a tiny violation of time reversal. And I would like to clarify a few points regarding that the first point is that time itself is treated in quantum theory as a parameters.

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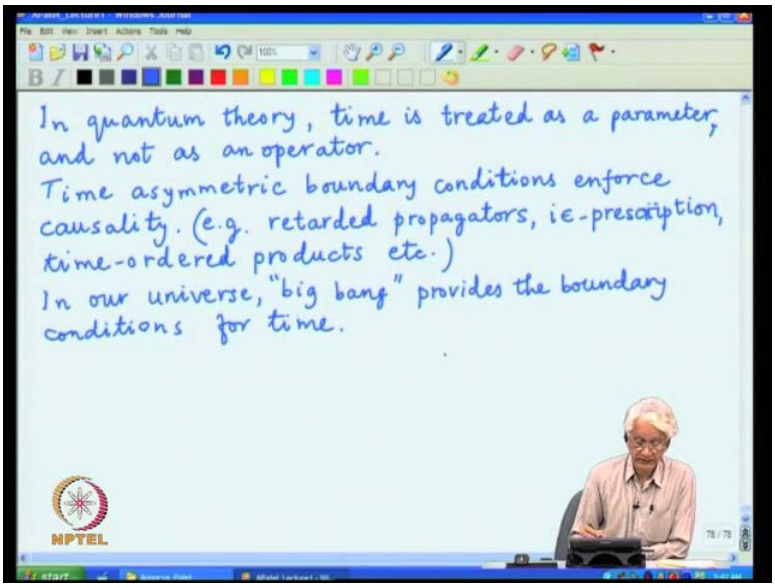

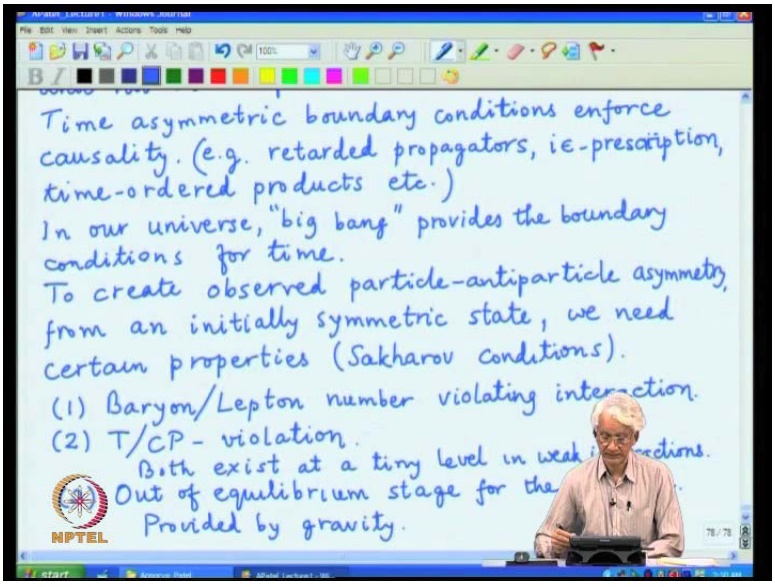

And, we often talk about the system evolving from some initial state under the influence of certain Hamiltonian to a final state. And so time is the descriptor of the change in the state from the initial point to the final point. And that description as a parameter is quite a different language then treating other objects in quantum theory as operators. And in particular time and space do get mixed because of relativity. But it is very easy to treat the space coordinates as operator, as you can talk about their measurements and their uncertainty and things of that sort. But time is literally not at the same level; we cannot define some operator whose exception value will give time. It is not really the part of the formulism, as we have developed; and this distinction of the treating the time as a

parameter. And not as an operator opens a new direction in which time can be labeled. And that is provided as boundary conditions on time.

So, we have; so called time asymmetric boundary conditions, which enforce the principle of causality. So, complete solution the problem requires always 2 parts; 1 is a set of dynamical equations. We have differential equations of various types. And then the boundary conditions, which will allow you to complete the solutions and the equations, may be time reversal symmetric, but the boundary conditions may not be. And if that is the case, then we do you have a sense of time through the boundary conditions. And this appears in quantum field theory under various labels; which go under the names of retarded propagators. There is a trick to ensure this thing which goes under the name I epsilon. Prescription many times the expectation values are evaluated as time order products etcetera. But all these consequences are arising from the particular boundary conditions that we choose. And that boundary condition is strongly connected with our sense of time and what we understand to be cause and what will be the effect.

So, this is one way of bringing in time asymmetry even when the equations of motions are completely time reversal symmetry. But as I said there is a little bit of violation of time reversal through the weak interaction. And we have to understand how that also contributes to the observed time asymmetry in the universe. And in particular what we need is a particle, antiparticle symmetry in the universe; which arises from this time reversal violating interactions. Even in the presence of these asymmetric boundary conditions.

So, in our universe this boundary conditions is provided by the; so, called the big bang at the beginning of time. And how the system will evolve after that particular instance and to create the observed particle, antiparticle, asymmetry from an initially symmetric state; we need certain extra conditions. And these conditions of properties go under the name of Sakharov; who clearly spelled them out. And we can now understand what these conditions are in a simple enough language; I will just list them 1 by 1; that we want to go from a symmetric state to asymmetric state. And that clearly requires a contribution to an interaction that it breaks this particular symmetry.

So, this in our universe the particle antiparticle symmetry is defined; in terms of baryon number or lepton number of the various states. So, to produce this symmetry; we

certainly need a interaction, which violates baryon and lepton number; this interaction does exist in the structure of it interactions, but it is a tiny effect. The second thing which is required is that 1 has to evolve and produce this effect; and that will not happen unless the violations rule itself asymmetric. So, we still made on top of that a property which makes violation time asymmetric. And that is the condition that the time reversal or equivalently C P symmetry should be violated; again this property exists in the weak interactions, but to a tiny extend; so, this 2 are there.

And, the third property which is needed is that; 1 will not evolve from a particular state unless the reserve driving force. And if you start in equilibrium state 1 will always remain in equilibrium state that is the way we define equilibrium. So, the third condition is that universe must be out of equilibrium. And that out of equilibrium dynamics will produce the driving force to take advantage of this asymmetry. And this out of equilibrium causes arises from a different interaction and that interaction is gravity. And it is simple enough to understand that the gravitational force, which is always attractive, cannot come to equilibrium by itself; we need both attractive and a repulsive forces to be able to achieve equilibrium. And pure attractive gravity always leads to a collapse state like a black hole.

So, if you start from an extended object; it certainly going to collapse due to gravity. And that is non Perturbative evolution driven from the extended object to collapsed object monotonically. And given this dynamics this 3 Sakharov conditions; 1 can understand that you can develop particle, antiparticle and asymmetry in the universe even, if the original state was symmetric; to understand the actual observed value of this asymmetry is much difficult task. And even all these ingredients it is a problem which has to been fully solved. There are various models; which take advantages of features. And. then they gives certain some estimates, but we still not develop a model which is completely satisfactory in particular. There are lot of conjurors that there must be interactions beyond the usual set of 4, that we treat most often in higher energy physicals this 4 consist of a strong electromagnetic weak and the gravitational interactions.

So, I will leave this discussion of time reversal symmetry; how it is broken? How it can lead to particle antiparticle asymmetry at this particular stage? And further details can be obtained only in a detail calculations and extensions of the; so, called standard model of particle physics. Now, I want to go to a completely different topic, which illustrates

many features of relativistic quantum mechanics in a contest, which is very different than the normal subject of high energy physics. The relativistic quantum mechanics which we looked requires electrons protons and other particles moving at speed at very close that of light. And that occurs only at very high energy process is typically encountered; in accelerators and collision process like cosmic rays, but not in our routine life. And so many of them, kind of remain out of reach most common situations in physics.

But it turns out that, there is a new system which has been investigated in recent years; where this features appear in condors matter physics at energy level, which can be encountered in simple table top experiments. And that is why it has been useful as a laboratory tool, to understand many unusual properties which we have seen in the case of solutions to the Dirac equation. And I would discuss these things in a little bit detail to illustrate, how the unusual features seen in case of particular system can be associated with prediction coming from the Dirac equation. And this system happens to be a material called Graphene; this is a condensed matter system obeying Dirac equation in 2 plus 1 dimensions.

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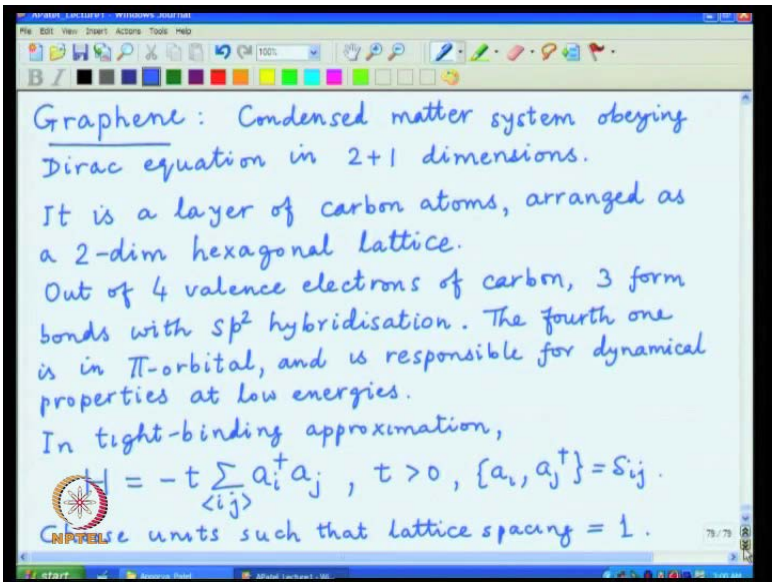

Now, in terms of its material content; Graphene is a layer a single layer of carbon atoms arranged as 2 dimensions in space hexagonal lattice. Now, carbon as 4 valence electrons and in a hexagonal lattice each carbon has 3neighbors to which it forms bonds. So, out of the 4 valance electrons 3 of them are occupied inside the bonds; while the fourth one

remains free. In the terminology of the chemistry this 3 bonds form. So, called S P 2 hybridization structure and connects to the neighbors. And the fourth one goes in to so, called phi orbital which just lies above and below the layer of carbon atoms. And that fourth electron is responsible for many of the dynamical properties of this Graphene by dynamical properties. I mean those important that low energy like transport or conduction of various types; essentially describe by how this fourth electron is going to move around; on this sheet of Graphene. And we want to study essentially the dynamics of this fourth electron by looking at a simple model.

So, simple model is provided by the so, called tight banding approximations. We have the Hamiltonian of the system which means essentially this fourth electron, whatever it does. And it only has kinetic energy which is described by some hoping parameter labeled here; as t connecting neighboring sides. And the creation and annihilation of operators described by a dagger and a. So, this particular term means that an electron at site j is taken out from that particular location. And deposited at site i which is a neighbor of that particular site. And this nearest neighbor coupling is essential all that remain in tied bonding approximation. Because of the translation of the invariance of the system, there is no potential energy appearing at all this is only the kinetic energy part. And in real life the objects which appear over here the quotient t which describes the strength of this hopping is positive.

And, the operators which appear in this expression are farm ionic. So, they have the anti commutation rule, given by a dagger anti commutator equal to delta i j. So, this is a simple enough model to describe Graphene. And we want to see what this produces when explicitly evaluated on this geometry of this hexagonal lattice formed by carbon atoms. And we will see that description produces Dirac equation for electron with sufficiently low energy. And in this calculation I have already made certain choose of units. And that will help to keep the algebra simple enough. So, lattice spacing of carbon atoms is just chosen to be 1. And when necessary this can be reduced back by dimensional counting. So, now let us work out the details of the lattice structure. I will draw the simple minded diagram for a hexagonal lattice; where, this is hexagonal and pattern repeats and so on.

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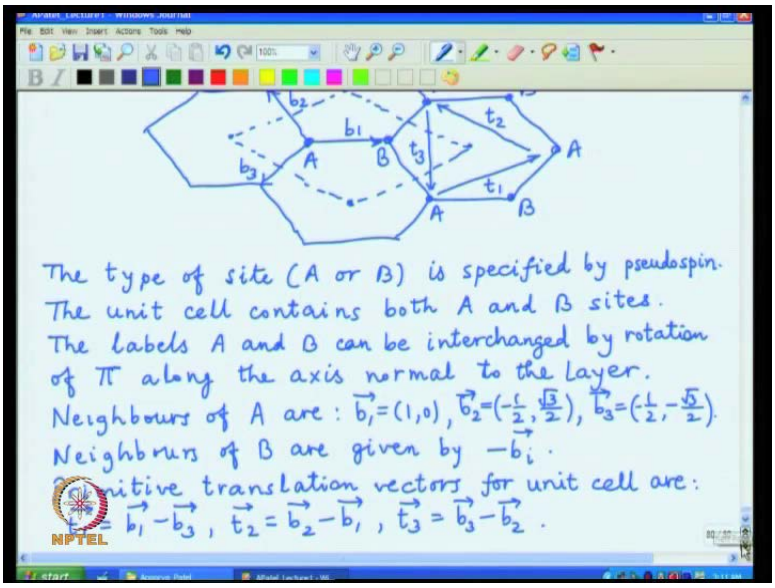

And, so forth it is clear that there are 2 types of sites. And I will generically label them A and B where a have bonds porting. And 3 direction separated by 140 degrees. And B has again 3 bonds are separated by 120 degrees. But the directions of these bonds between A and B are different; there related with respect to rotation by 60 degrees. And this makes this site A and B in equivalent. And we will explicitly keep track of this site by introducing a new label; which physically specified; whether, the site is of type A or B.

And, so we will have new label which can will takes 2 values. And those values are A or B will treat it the same way as we treats 2 values of spins. So, this object is commonly referred to as pseudo spin. It has nothing to do with angular momentum, it gives the position label. And 1 can now see this hexagonal structure can be described in terms of unit cell; which periodically repeats over the whole space. And this periodically repeating unit cell can be obtained by connecting the centers of the hexagonal, it has the rhombus shape. And this unit cell contains these 2 degrees of freedom A and B.

So, this label our pseudo spin. Now, refers to 2 degrees of freedom inside a unit cell. So, there are 2 degrees of freedom per unit cell, will some over the unit cells is in translation symmetry as usual. And 1 can also observe that, 1 can interchange these 2 labels by rotation of pi along axis normal to the sheet of Graphene. So, this is an important index and we need to know its meaning as well as how it can be manipulated given this label. Now, it is a straight forward algebra to work out the properties of the unit cell. The

Fourier transform version which, defines the brillouin zone. And then do the calculation of the Hamiltonian in terms of the vectors describing the unit cell as well as those corresponding to the brillouin zone; for that we have a need the various vectors connecting 1 site to it is neighbors, because the Hamiltonian has these nearest neighbor interactions.

So, the neighbors of sites A there are given by 3 unit vectors. And we can easily see their components as b 1 b 2 and b 3 in terms of 3 unit vectors rotated by 120 degrees. And neighbors of B are just given by the vectors directed in the opposite sites. So, for example, on this diagram this label b 1 is here b 2 is here and b 3 is here. Now, the periodicity vectors of the unit cell are given by; the translation vectors connecting an identical set of sites. For example, A to A or equivalently B to B and those can be again defined on the same diagram by this. So, called primitive translation vectors and they in the convention which I will use are; t 1, t 2, t 3 as shown here. They connect site A to another site of type A. So, this are all B and we can easily work out, what this expressions for this primitive translation vectors are; it is just a combinations of 2 nearest neighbor unit vectors added with a appropriate Vectorial rule.

So, these primitive translations vectors for the unit cell are; t 1 is equal to b 1 minus b 3, t 2 is equal to b 2 minus b 1and, t 3 is equal to b 3 minus b 2. We are working in a 2 dimensional space. So, only 2 of the 3 vector linearly independent and we can take any 2 of these 3 to form that particular basis. And I will work essentially with t 1 and t 2. The third one is just a combination of 2 or rather you can easily see that t 1 plus t 2 plus t 3 is equal to zero. But somehow it is convenient to use all 3 in simplifying the algebra.

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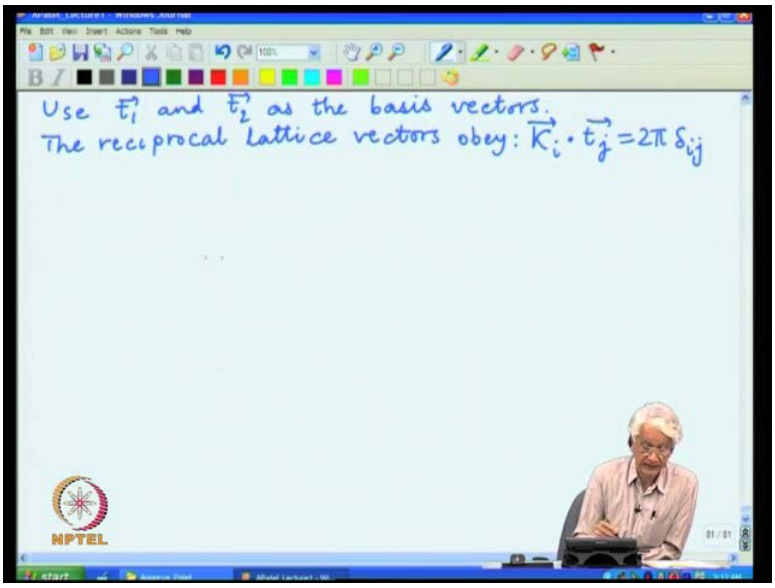

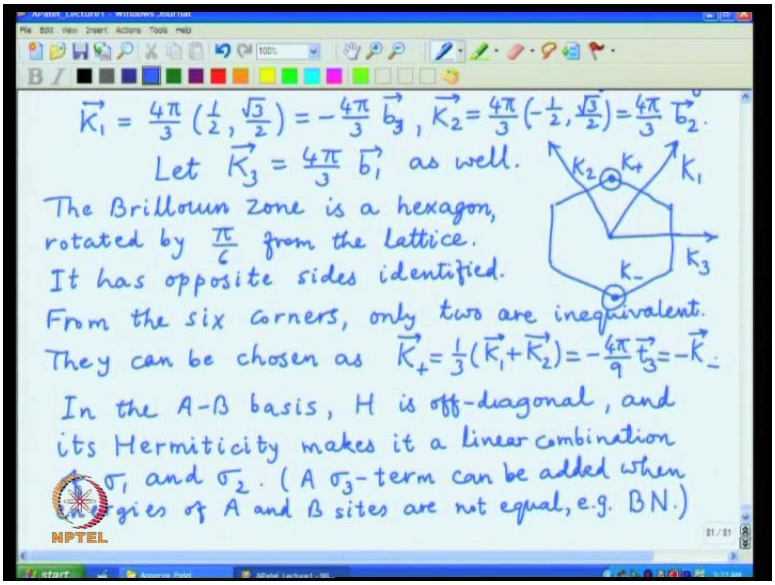

So, use t 1 and t 2 as the basis vectors. So, given this primitive vectors the brillouin zone is now specified by the so, called reciprocal lattice vectors. And that relation is just a orthogonality relation between this reciprocal lattice vectors K and this primitive vector t producing 2 pi times a chronicle delta. And given this values of unit vectors t; we can easily solve what this K would be and the solutions are K 1 is proportional to b 3while K 2 is proportional to b 2. And we can just by analogy extend a these 2 basis vectors to a third one. And I will call it K 3which will be proportional to b 1. So, now these vectors K 1 K 2 K 3 form a brillouin zone. And that brillouin zone is also has a hexagon.

But it is rotated by and an angle of pi by 6 from the original lattice. So, we can draw it in the same kind of structure which I drew on the previous page as a hexagon oriented as shown. And vectors which we have will again connect the centers of these hexagons. So, K 1 points along that direction shown, K 2 has another direction rotated by 60 degrees. And K 3 as I have defined points along the third direction again rotated by 60 degrees. So, now we have to work out the geometry of this brillouin zone; in particular the band structure of the electrons describing low energy. Excitation is given the Fermi levels embedded inside this brillouin zone.

The brillouin zone is again periodic structures. It has the opposite site identified with each other. And because of that periodicity out of the 6 corners only 2 are in equivalent. And we will choose them as the points marked on the diagram 1 of them will call K plus. And the diametrically opposite 1 we will call K minus in terms of the reciprocal lattice vector K plus is one third of K 1plus K 2 and by doing the algebra its easierly seen that this is proportional to at translation vector t 3. And we will define the K minus to be just the opposite of K plus. So, this is essentially all the lattice algebra required. Now, to re-express the Hamiltonian in a form; where 1 can see the excitation spectrum in particular transforming from the position space to the momentum space, through a Fourier transform.

It will allow us to construct the Hamiltonians in terms of the momentum vectors and immediately giving the energy momentum desperation relation. So, now what we have is a simple structure. Since the Hamiltonian has only terms connecting A sites with B's sites. And it is hermitian so, in the A B basis the H is off diagonal. And its hermitian character makes it a linear combination of the 2 Pauli matrices sigma 1 and sigma 2. We only have a 2 dimension situation. And only 2 sigma matrices appear in the Hamiltonian, which I started with. But it is possible to get third term in the Hamiltonian, which corresponds to the third Pauli metric sigma 3. And in this A and B basis it correspond to situation where, the energy at site A is somehow different then energy at site B, it is a diagonal term in the Hamiltonian.

And, then the atom sitting A and B cannot be exactly the same. But we can have a same hexagonal structure based on not just a single type of atom, but 1 type of atom at site A. And another type of atom its site B then their energies will be different and Hamiltonian will have a third term. So, sigma 3 terms can be added, when energies of A and B sites

are not equal. And a simple example of such situation is the chemical compound boron nitride; both boron and nitrogen are neighbors of carbon in the periodic table. Boron has 1 less electron nitrogen has 1 more and they can form the same kind of bond as carbon forms with its 3 s p to hybridize electrons. But the pi electron structure is different for boron and nitrogen. And that is making the energy at site A and B slightly unequal and that difference produces a sigma 3 terms in the Hamiltonian.

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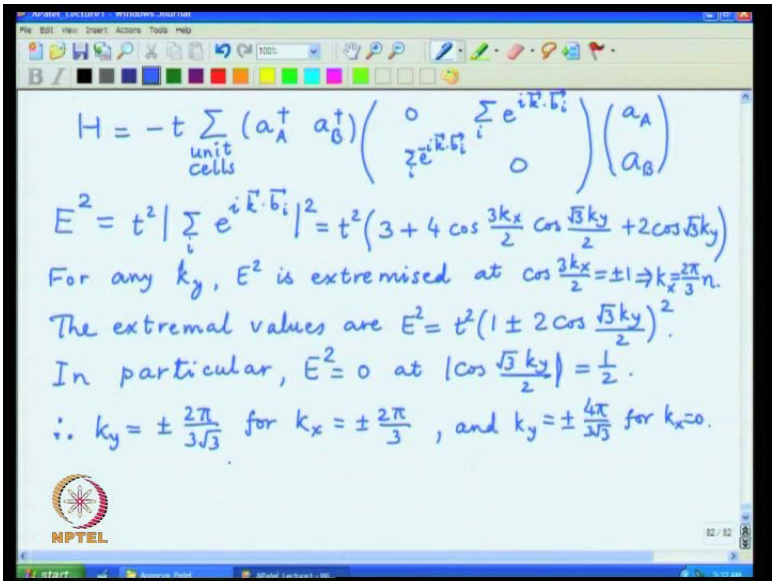

We can now easily write down the Hamiltonian in terms of a 2 by 2 metric structure. And that is now; so, summed over unit cells we separate out the A and B terms. The sum over the neighbor produce this factors e rest to i k dot b i corresponding to the Fourier transform, that unit vector pointed along that direction b i. And the term on the other side of the diagonal is complex conjugate corresponding to unit vectors pointed in the opposite directions. Neighbors of A are given b i, neighbors B are given by minus b i. And so we have this Hamiltonian now written in the 2 by 2 matrix form or equivalently written in the pseudo spin basis. Its hermitian and I have written only the examples in case of Graphene. If we are looking at boron nitrate then the 2 zeros; and the diagonal can be replaced by 2 different constants or if you subtract out a common energy it can be converted into plus some constant and minus some constant.

On the diagonal giving a matrix sigma 3, but I will not discuss this sigma 3 contribution any further. And only deal with Graphene given by this particular Hamiltonian. Now, we

are done the Fourier transform the operators have been simplified. And we can easily extract the energy in terms of the momentum k. And that is very easy to see Hamiltonian is trace less which means there will be paring of the Eigen values with every plus e, there always be a minus e; the sum of 2 has to be 0. And the product of these 2 Eigen values will be given by the determinant which can also be easily worked out. Sorry, I made a mistake here in the notion. Let me correct, it is a summation over i but the minus i in the exponent, the determinant is very easily given by the Eigen value.

So, we have the relation that product of plus e and minus e, which is the determinant or E square is equivalently the negative of the determinant can be written easily as p square. And these 2 factors are complex conjugate of each other. So, we have E square is equal to t square times this whole summation modulus square. And that can be explicitly evaluated as 3 plus 4 times cos 3 k x by 2 times cos root 3 k y by 2 and plus 2 times cos of root 3 k y. So, that is essentially the structure which we are interested in. It gives for a particular point in the brillouin zone specified by this momentum vectors k x k y. What is the corresponding energy? And that is the description of the band of Graphene. Now, to calculate it 1 can easily take this functions and plot them as the function of k x y.

And, it produces is a certain surface. And a graphics program can easily show that, I am only interested in particular extreme situations in particular small energy excitations. And those correspond to not the full length or width of the band. But rather it can be specified by giving the extreme values. The energy can take rather just the top of the band and the bottom of the band and everything in between is allowed. So, it can be worked out rather easily from these situations. So, any k y we have to find out E square is extremised at cos 3 x k by 2 is equal to plus or minus 1. And that implies k x is equal to 2 pi by 3 times some integer. And the extreme values are given by this particular value of k x plugged in. And 1 can see that there is a particular choice; the extreme value turns out to be 0 at cos root 3 k y by 2 equal to half in magnitude.

And, that means that when 1 plugs in both these k x and k y there will be certain points where there are 0 energy excitation available. And this points are given by k y equal to plus or minus 2 pi 3 root 3 for k x equal to plus or minus 2 pi by 3 and k y is equal to plus or minus 4 pi by 3 root 3 for k x equal to 0. And these are 6.2 here and 4 here and this point. Now, 1 can go back and look at the geometry are the 6 corners of the brillouin

zone. So, at the corners we have 0 energy excitations. And we will study now, the properties of excitations in the neighborhood of these corners in the next lecture.