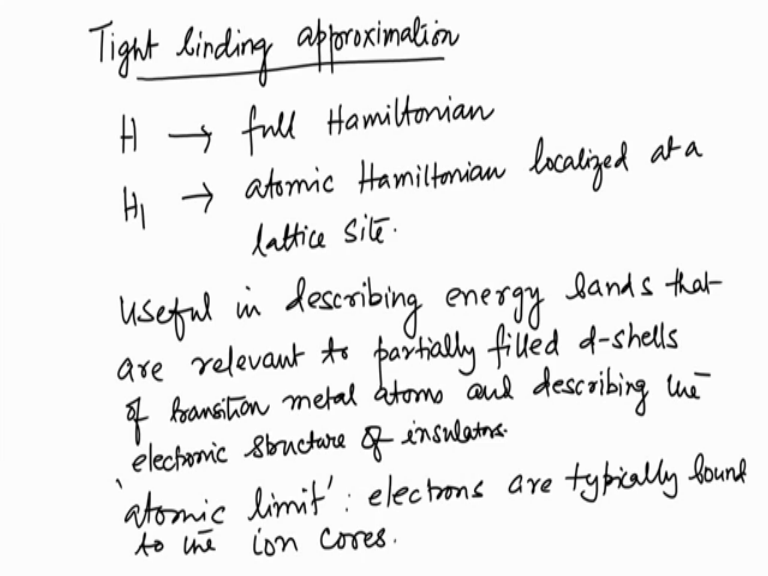
Advanced Condensed Matter Physics
Prof. Saurabh Basu
Department of Physics
Indian Institute of Technology, Guwahati

Lecture – 06
Tight Binding Hamiltonian, Hubbard model

So, we shall carry on with the applications of this second quantized formalism that we have learnt so far. And this time we are going to apply it to real materials or rather the models which actually mimicrial materials. So, in that context we will look at tight binding approximation today.

(Refer Slide Time: 00:49)



Tight binding approximation

$H \rightarrow$ full Hamiltonian

$H_1 \rightarrow$ atomic Hamiltonian localized at a lattice site.

Useful in describing energy bands that are relevant to partially filled d-shells of transition metal atoms and describing the electronic structure of insulators.

'atomic limit': electrons are typically bound to the ion cores.

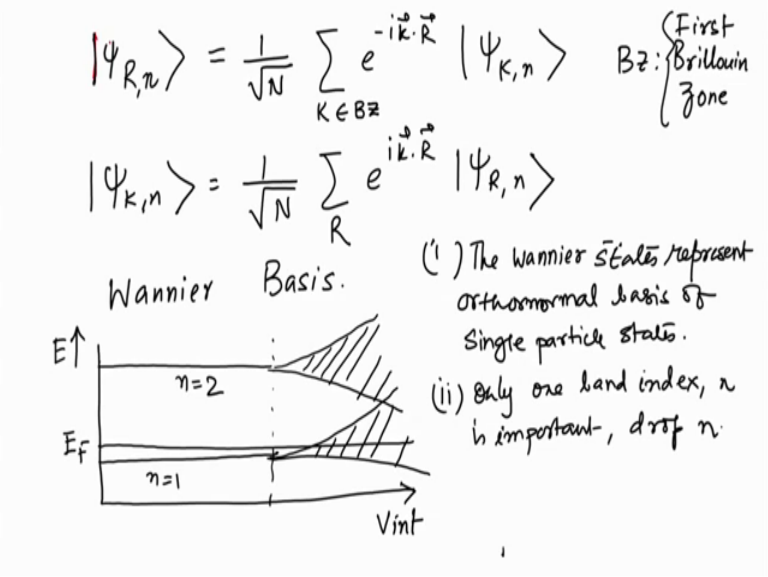
So, I am assuming that you have done tight binding approximation in your solid state physics course when you wanted to calculate the electronic structure or the electronic band structure of metals and in that context you have learned that we assume that in the vicinity of each lattice point, the full periodic crystal Hamiltonian, which is given by H. So, H is the full Hamiltonian is approximated by H 1 which is an atomic Hamiltonian and localized at a lattice site.

So, the approximation is about full periodic Hamiltonian, which we assume that it is now a localized atomic Hamiltonian which is localized or rather only confined to a lattice site. So, the overlap of the atomic wave functions is still enough for us to consider that there is we are talking about a real material and not talking about isolated atoms or ions, but it is not so much that the independent electron or rather the isolated atom information is not completely dumped.

So, it is just the balance between that we are saying that the wave function is just restricted to a site, and it is minimally overlapping with the wave function to a neighbouring site, but; however, we are still acknowledging there is some very minimal overlap so, that the isolated atomic description is not completely overthrown, but the presence of other atoms are being acknowledged at the same time. And this approximation is useful in describing energy bands that is that are relevant to two partially filled d-shells of transition metal atoms and describing the electronic structure of insulators.

So, this Hamiltonian within the tight binding approximation is what we are going to see now. So, we have tightly bound electrons to the iron cores and we are pretty much this is called as the atomic limit and this word is used to denote that the electrons are typically bound to the iron cores. To write down the Hamiltonian in a formal manner, let us introduce the wave function of the electrons in this atomic limit.

(Refer Slide Time: 05:45)



$$|\psi_{R,n}\rangle = \frac{1}{\sqrt{N}} \sum_{K \in BZ} e^{-i\vec{k}\cdot\vec{R}} |\psi_{K,n}\rangle \qquad BZ: \begin{cases} \text{First} \\ \text{Brillouin} \\ \text{Zone} \end{cases}$$

$$|\psi_{K,n}\rangle = \frac{1}{\sqrt{N}} \sum_{R} e^{i\vec{k}\cdot\vec{R}} |\psi_{R,n}\rangle$$

Wannier Basis.

(i) The wannier states represent orthonormal basis of single particle states.

(ii) Only one band index, n is important, drop n.

As a psi of R n will tell you what n is R is of course, a site or lattice site where an atom or an iron is located and n is actually an orbital which we are going to come to and this has a normalization factor like this, and then you have an exponential minus i k dot R and in the momentum space it is written as this.

So, let us put a comma in between and there is a K that is only restricted to the first Brillouin zone. I mean when I say B Z. So, B Z for me stands for Brillouin zone and we say the mostly we say the first Brillouin zone. So, we use this notation that the BZ actually talks about the first Brillouin zone.

So, this is the wave function of the electron which is localized at a given iron core or at a given lattice site and so, there is a free part which is given by exponential minus i k dot R and there is also this psi k n, where n is as I said is the orbital index, and R is a location of the lattice. And you can write also the psi k n and just by taking the Fourier transform and which will come with a simple.

So, psi k n is written as 1 by root over N and this sum over R exponential i k dot R and psi R n. So, thus for this system which comprises of vanishingly weak inter atomic overlap, this are called as the Wannier basis. And these are localized written the wave functions are written in the localized Wannier basis and now this for an interacting Hamiltonian the Wannier basis is certainly not the Eigen basis of the problem, but; however, we can still they are still helpful and let us give you a picture physical picture that what we are trying to talk about.

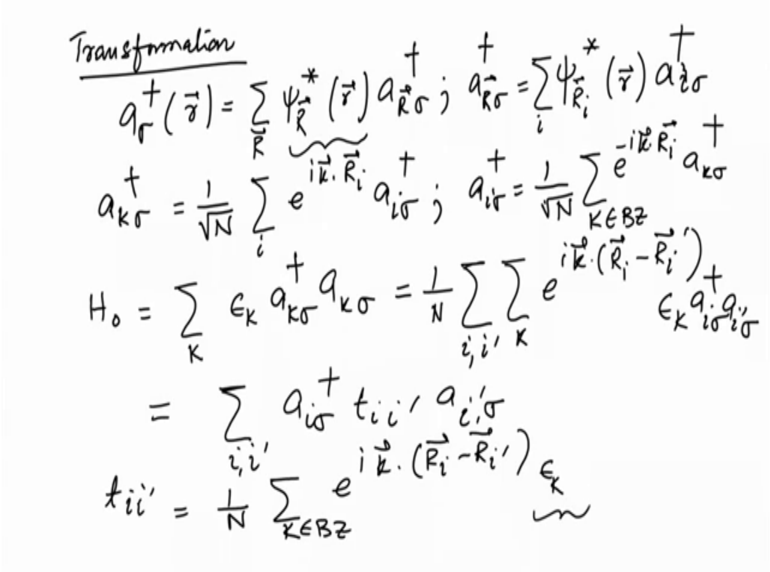
So, this is my energy axis and this is what I say that it is my interaction is in this along this axis. And when we have this each of these orbitals what happens is that, at 0 interaction these are discrete energy values. So, this one corresponds to say n equal to 1 and the other corresponds to say this n equal to 1 and these are n equal to 2 and so on, but; however, when the interaction becomes larger than some value these start you know branching out like this, and they spread out like this and these form the energy bands and again I assume that you have done the first course of solid state physics in which the formation of energy bands are taught.

So, beyond a certain interaction potential between the energy levels we would have these individual orbitals from transform from being single particle discrete single particle states, and to they will fan out or they will branch out like this and for being energy bands.

Now, they will be called as insulators or conductors depending on the position of the Fermi level and let us say. So, as I told this is the energy axis. So, let us say the Fermi level is somewhere here and let us call that as EF and then if the Fermi level falls in the spectrum of the available energy states within that spectrum, and then it is called as a metal and otherwise it is called as an insulator. So,.

So, how do we actually exploit this Wannier basis to write down the ore to form the Eigen states of the general Hamiltonian the full periodic Hamiltonian? So, two things that need to be kept in mind one is that that the Wannier states represent orthonormal basis of single particle states. The word orthonormal means it is both orthogonal and normalized and it is also we can see that one can actually drop the band index because only one band index or orbital index as we have said band index n is important is important as we have shown yet only n equal to one is important. So, we can drop the index n and drop n ok.

(Refer Slide Time: 12:19)



Transformation

$$a_\sigma^\dagger(\vec r) = \sum_{\vec R} \utilde{\psi_{\vec R}^*(\vec r)}\, a_{\vec R\sigma}^\dagger ; \quad a_{\vec R\sigma}^\dagger = \sum_i \psi_{\vec R_i}^*(\vec r)\, a_{i\sigma}^\dagger$$

$$a_{k\sigma}^\dagger = \frac{1}{\sqrt N}\sum_i e^{i\vec k\cdot\vec R_i}\, a_{i\sigma}^\dagger ; \quad a_{i\sigma}^\dagger = \frac{1}{\sqrt N}\sum_{k\in BZ} e^{-i\vec k\cdot\vec R_i}\, a_{k\sigma}^\dagger$$

$$H_0 = \sum_k \epsilon_k\, a_{k\sigma}^\dagger a_{k\sigma} = \frac{1}{N}\sum_{i,i'}\sum_k e^{i\vec k\cdot(\vec R_i - \vec R_{i'})}\, \epsilon_k\, a_{i\sigma}^\dagger a_{i'\sigma}$$

$$= \sum_{i,i'} a_{i\sigma}^\dagger\, t_{ii'}\, a_{i'\sigma}$$

$$t_{ii'} = \frac{1}{N}\sum_{k\in BZ} e^{i\vec k\cdot(\vec R_i - \vec R_{i'})}\, \utilde{\epsilon_k}$$

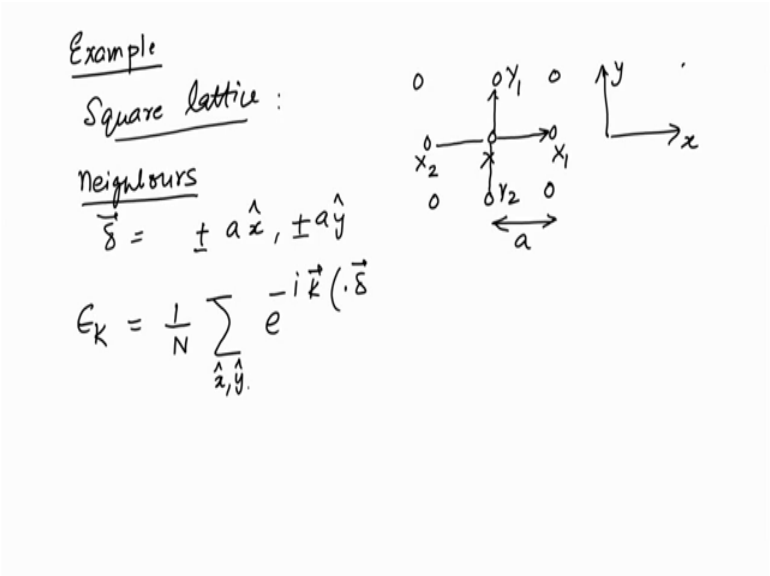
So, now allow us to introduce a transformation of the form a sigma r equal to sum over R and psi R star and it is r and a R sigma dagger or we can write the Fourier transform of this as a R equal to sum over i psi of R i and r and this is a i sigma dagger. So, this is how the operators are defined in terms of the Wannier functions look these size are the Wannier functions that we have just spoken and we have dropped the band index and as we introduce new operators the creation operators in terms of the Wannier basis.

And a momentum space representations is equally possible which is given by a k sigma equal to 1 by root over N an exponential i k dot R i and a i sigma and similarly the Fourier transform of that is a i sigma dagger equal to 1 by this is i 1 by root over N and this is equal to sum over k which belongs to the first Brillouin zone and then you have an exponential minus i k dot R i and a k sigma dagger.

So, this transformation can be used to write down the generic single particle Hamiltonian as H 0 is equal to sum over k epsilon k a k sigma dagger a k sigma which finally, gives me it is equal to 1 over N because from both the operators we get 1 over root N. So, that becomes 1 over N and there is a i and i prime and also there is a k. So, that gives me a exponential i k R i minus R i prime and then there is an epsilon k and there is a a i sigma dagger a i prime sigma and so, that can be written as sum over i and i prime and a i sigma dagger t i i prime and a i prime sigma.

So, this t i i prime is equal to 1 over n sum over k again k belonging to the first Brillouin zone and this is equal to an exponential i k R i minus R i prime and then there is an epsilon k and so, let us take a particular. So, this is the formula for the or rather the Hamiltonian and the t i i prime represents this, and let us see the example of a square lattice.

(Refer Slide Time: 16:44)



Example

Square lattice :

Neighbours

$\vec{\delta} = \pm a\hat{x}, \pm a\hat{y}$

$\epsilon_K = \frac{1}{N} \sum_{\hat{x},\hat{y}} e^{-i\vec{k}(\cdot\vec{\delta}}$

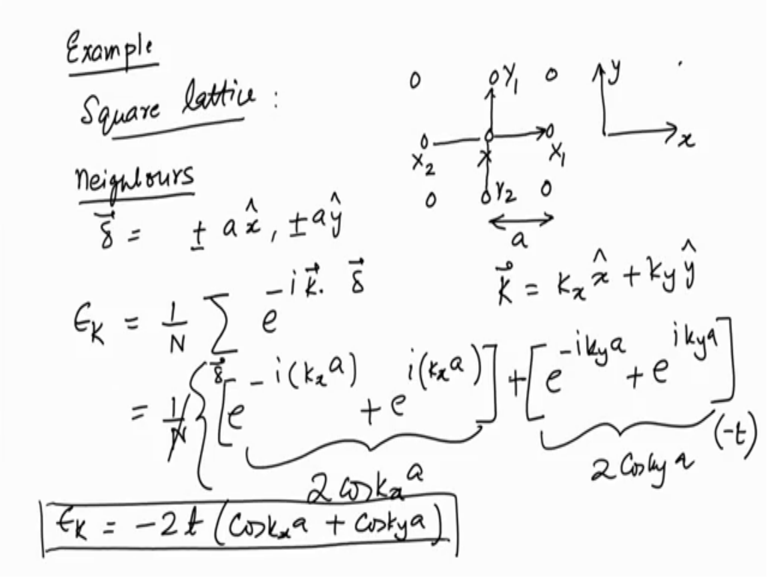
And what is the square lattice you have these are the positions of the lattice points where which is occupied by the atoms or the ion cores. So, this is my x direction and this is my y direction and let us say that this is called which is called as a lattice spacing which is of a and then this direction is called as the x cap direction and this is as the y cap direction. So, we have for a particular site we have four neighbours. So, an electron actually can hop in a lattice on a on a two dimensional square lattice from this point let us call this point as o or let us call this point as x or will be indistinguishable in this matrix of the lattice points that are shown here.

So, from this lattice point x, it can go to x 1 which is on the positive x axis towards the positive x axis it can go to x 2 which is in the negative x axis, and it can go to y 1 which is in the positive y direction and it can also go to y 2 which is in the negative y direction. So, the neighbours for in a square lattice is given by plus a x cap and a minus a x cap and a plus a y cap as I said a is called as a lattice constant and there is also a minus a y cap.

So, these are the four neighbours of a lattice site for a 2D square lattice two dimensional square lattice ok. So, we so, to write down the tight binding model we need an information about the neighbours, which are the most dominant contributor to the Hamiltonian. So, then I can write down this epsilon k which is the single particle energy spectrum as written in this slide here.

So, this epsilon k can be written as a 1 over n again taking a Fourier transform and there is. So, it is x cap and y cap and this will be like exponential minus i k and then it will be all the let us call these neighbours by a name let us call them as delta. So, it is dot delta and there is a sum over in you can write it x cap y cap, but let us write it as delta sum over delta and this delta are these all these neighbours and this is equal to.

(Refer Slide Time: 20:28)



Example

Square lattice :

neighbours

$\vec{\delta} = \pm a\hat{x}, \pm a\hat{y}$

$\vec{k} = k_x\hat{x} + k_y\hat{y}$

$$\epsilon_K = \frac{1}{N}\sum_{\vec{\delta}} e^{-i\vec{k}\cdot\vec{\delta}}$$

$$= \frac{1}{\cancel{N}}\left\{\underbrace{\left[e^{-i(k_x a)} + e^{i(k_x a)}\right]}_{2\cos k_x a} + \underbrace{\left[e^{-ik_y a} + e^{ik_y a}\right]}_{2\cos k_y a}\right. (-t)$$

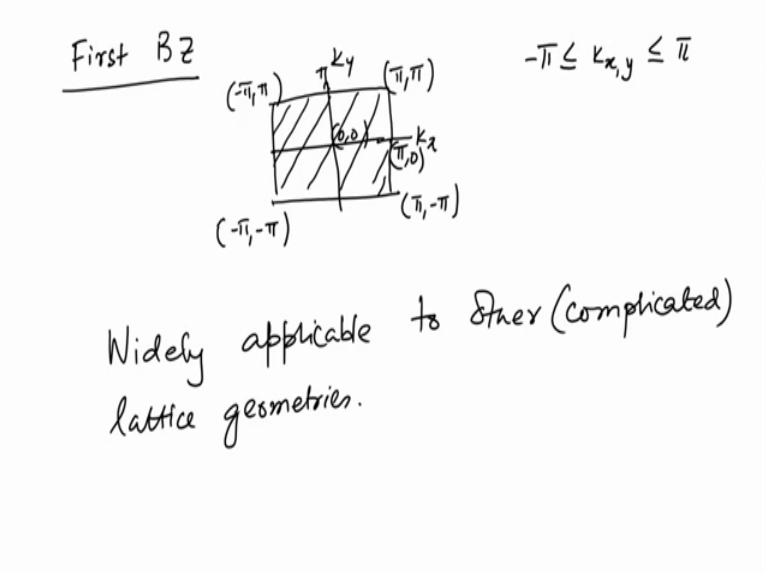
$$\boxed{\epsilon_K = -2t\left(\cos k_x a + \cos k_y a\right)}$$

So, this is simply I need to find the neighbours and then just take a k dot delta, where k is just a generic vector in two dimension which is k x x cap plus a k y y cap. So, this will give me a 1 over n and I have an exponential minus i k x a a and I have also a exponential minus exponential i k x a. So, this is for the term that is for delta to be plus a x cap and delta to be minus a x cap and for the plus a y cap and minus a y cap are similarly given by. So, this is will be simply equal to.

So, I should have ok. So, these are simple to see you should verify them. So, k y a and exponential i k y a. So, this is nothing, but twice of cos k x a and this is nothing, but twice of cosine k y a and hence my epsilon k becomes equal to with an amplitude that is given by that as minus p and then there is a sum. So, because this will take care of this 1 over n and I will have.

So, this 1 over n will not be there if I do the sum and I have a minus 2 t cosine k x a and a cosine k y a as the dispersion or the energy momentum relation for an electron a tight binding electron in a square lattice. Now this formalism is very important because this as I said that in a variety of real materials this tight binding approximation is very helpful in finding the e versus k relation and this can be plotted on a two dimensional k x k y plane and one can find that that how the dispersion looks like over the first Brillouin zone what I mean by first Brillouin zone is that for k x to be.

(Refer Slide Time: 23:19)



First BZ

$-\pi \le k_{x,y} \le \pi$

Widely applicable to other (complicated) lattice geometries.

So, the first Brillouin zone of a square lattice is also a square lattice and it looks like this which is a. So, this is my k y and this is my k x. So, these are points which are pi and pi here. So, that we have a this point to b like pi pi and this point is like pi minus pi and this point is like minus pi minus pi and this point is minus pi pi and this is 0 0 and this point is called as pi 0. They have specific names we are not going into that you can look at any book on electronic structures and they have names such as m k gamma etcetera points and. So, this is my first Brillouin zone which I need to do all these sums that we have talked about. So, k x is between minus pi to pi and same for y.

So, now we can we know a lot of information about this square lattice or the energy dispersion tight binding dispersion in square lattice, we can calculate the electron velocity by taking a derivative with respect to k either k x or k y and then we can calculate the velocity of the electrons at one of those given points pi pi pi 0 0 0 etcetera this is called as a zone centres 0 0 is called as a zone centre and pi pi is called as a zone corner.

So, we can calculate at thus these special points we can calculate the velocity and we can also find out the effective mass of electrons by which is which comes out from the inverse of the second derivative of this of this energy dispersion or with respect to k x or k y. Now so, this is also widely applicable to other and let me write in bracket as complicated lattice geometries and by complicated we mean other kinds of lattice geometries such as the triangular lattice, the Honeycomb lattice, Kagome lattice and so on and one of the famous examples is given by Graphene.

(Refer Slide Time: 26:39)

Graphene

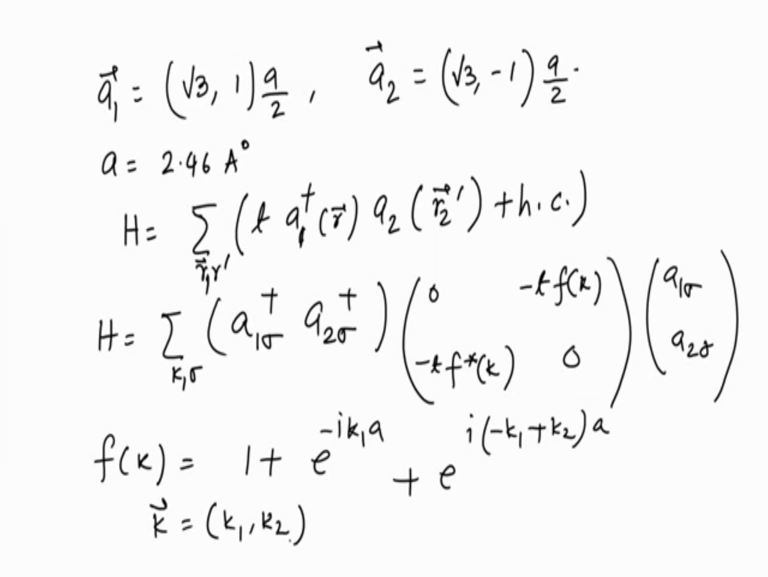
And this Graphene was discovered in 2004 by two scientists called Novoselov and Gaim and this was their from Manchester united kingdom and they were awarded Nobel Prize in 2010.

So, this is the citation for the Nobel Prize that they have got this was in 2010 from the from Sweden and then this is the structure of grapheme, it is one atom thick honeycomb structure. So, it is the best 2 D material that you can find in nature and it is just like a thin sheet absolutely one atomic layer thin sheet of carbon atoms, which are which are there arranged in the hexagonal form or the honeycomb form and to find out the tight binding dispersion of electrons in graphene we note this figures and this gives the unit vectors of graphene. So, graphene is a it has two atoms per unit cell. So, one atom is by the filled circle and the other is the filled and the open circle with the filled circle inside, these are the two atoms per unit cell and these are the basis vectors that one can see.

So, they are basically the carbon atoms are arranged in the hexagonal lattice as we have shown, and they are connected by very strong covalent bonds of the sigma orbitals and they derive from the s p 2 hybridization of these atomic orbitals and the remaining p z orbital has a weak overlap and forms a narrow band of the pi orbital states. One should look up the structure of graphene more carefully and understand that to the first approximation these pi electrons they can be represented or denoted by a tight binding Hamiltonian with a hopping energy minus t between the neighbouring atoms.

And to describe the the spectrum energy spectrum of the system and one actually can think of a unit cell consisting of two atoms as I told earlier, enclosed in a in this forming this honeycomb structure they are given by say a 1 and a 2 and from the figure one can write down that a 1 is equal to root 3, 1 and a by 2 and the a 2 equal to root 3 minus 1 a by 2 and this a is called as a lattice constant.

(Refer Slide Time: 29:41)



$$\vec{a}_1 = (\sqrt{3}, 1)\frac{a}{2}, \quad \vec{a}_2 = (\sqrt{3}, -1)\frac{a}{2}.$$

$$a = 2.46\ A^{\circ}$$

$$H = \sum_{\vec{r},r'} \left(t\, a_1^{\dagger}(\vec{r})\, a_2(\vec{r}_2{}') + h.c.\right)$$

$$H = \sum_{k,\sigma} \left(a_{1\sigma}^{\dagger}\ a_{2\sigma}^{\dagger}\right) \begin{pmatrix} 0 & -tf(k) \\ -tf^{*}(k) & 0 \end{pmatrix} \begin{pmatrix} a_{1\sigma} \\ a_{2\sigma} \end{pmatrix}$$

$$f(k) = 1 + e^{-ik_1 a} + e^{i(-k_1+k_2)a}$$

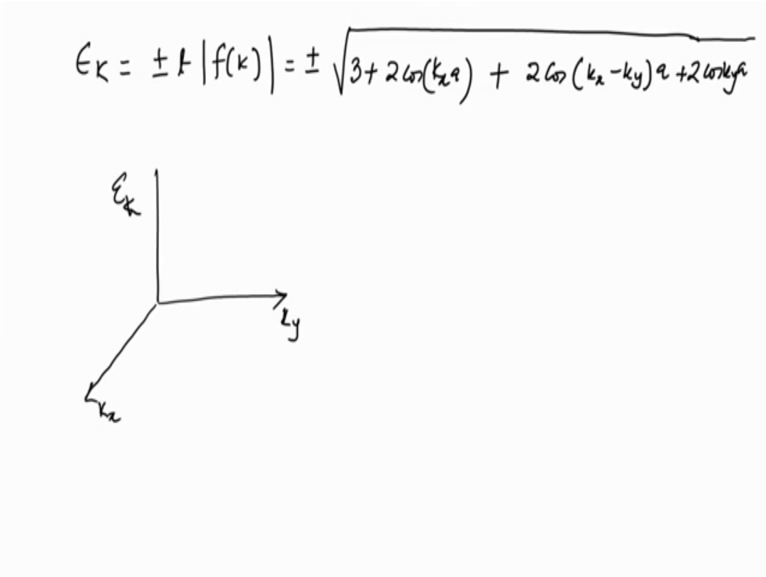
$$\vec{k} = (k_1, k_2)$$

It has a value that is known which is equal to 2.46 angstrom and so, the tight binding model for this though slightly more complicated than the square lattice which is what we have written earlier because of the presence of two kinds of atoms per unit cell, we can still write down in simple enough fashion as there is a r and r prime. So, and this is equal to some t a a 1 dagger r, a 2 dagger a 2 r prime plus Hermitian conjugate you will often find that in the tight binding Hamiltonian written in literature it is written with a Hermitian conjugate to make the Hamiltonian real or rather to give the Hamiltonian is still is.

So, the energy spectrum is real. So, that is why this Hermitian conjugate is added and this sum is overall the nearest neighbour basis vectors of the unit cell that is shown there this is a problem that is given to you to solve I am only outlining the solution of this problem and this Hamiltonian can now be written in the momentum space as rather.

So, this is equal to a a 1 sigma dagger a 2 sigma dagger and then it is 0 and the t f of k I will tell you f of k is a function of k and minus t f star k and a 0 and this is equal to a 1 sigma and a 2 sigma. This is the form of the Hamiltonian and it has simply has to be diagonalized in order to find the energy Eigenvalues it is just a 2 by 2 matrix that one has to diagonalize where f of k is simply equal to 1 plus exponential minus k 1 a and plus exponential i minus k 1 plus k 2 a, where k vector is written as k 1 having two components k 1 and k 2 because we are talking about a two dimensional system and finally, you should be able to write.

(Refer Slide Time: 32:48)



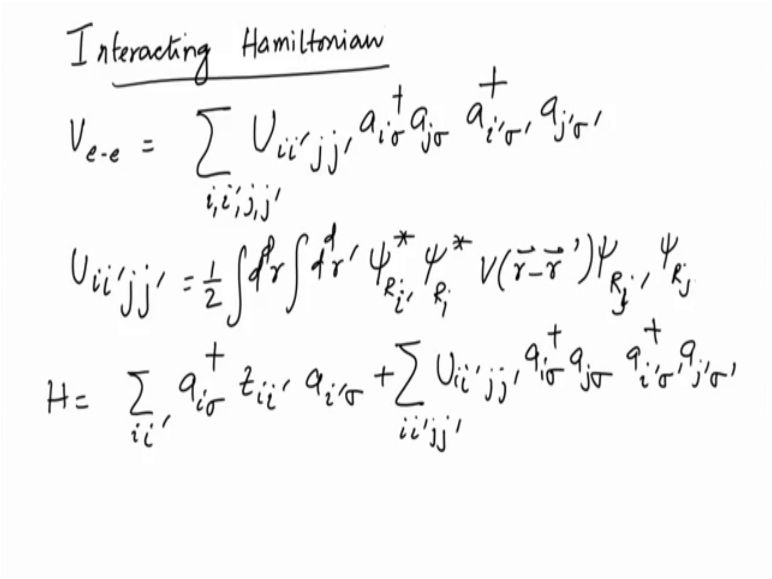
$$\epsilon_k = \pm t\,|f(k)| = \pm\sqrt{3 + 2\cos(k_x a) + 2\cos(k_x - k_y)a + 2\cos k_y a}$$

The dispersion as a plus minus t f of k, and this is equal to a plus minus and then we have 3 plus 2 cosine k 1 a if you like you can call the k 1 to be. So, we can simply call this as k x, k y and maybe it is better to write with the k x and k y instead of k 1 and k 2 because which is what you are more familiar with it is k x a and a plus 2 cosine k x minus k y a and up to cosine k y a.

So, that is the dispersion and this of course, because of the plus minus sign it has two bands and let me write down this together there. So, this is the dispersion and there is an upper band and there is a lower band upper band is given by the positive sign and then there is a lower band that is given by the negative sign and in fact, you should try to plot it on a do a three dimensional plot of epsilon k being in the z axis, and a k x and a k y say in the. So, let this be k x and the k y and if you plot epsilon k, you will see some nice structures which I leave it as an example or rather a problem that needs to be solved. And you will find that these two bands actually touch at 6 points in the Brillouin zone and near those 6 points the energy dispersion is not parabolic it is rather it is linear.

So, these linear dispersions are called as the Dirac cones and because linear dispersion is found in relativistic particles such as a photon, and the energy dispersion close to those points where they touch they represent or rather resemble that of massless electrons and that is why they are called Massless Dirac fermions. So, most of it we leave it as an exercise for you to solve let us go to the an interaction term and write that interaction term in some simple form for the two particle interaction.

(Refer Slide Time: 35:51)



Interacting Hamiltonian

$$V_{e-e} = \sum_{i,i',j,j'} U_{ii'jj'}\, a^{+}_{i\sigma} a_{j\sigma}\, a^{+}_{i'\sigma'} a_{j'\sigma'}$$

$$U_{ii'jj'} = \frac{1}{2}\int d\vec{r} \int d\vec{r}\,'\, \psi^{*}_{R_{i'}} \psi^{*}_{R_i}\, V(\vec{r}-\vec{r}\,')\, \psi_{R_{j'}} \psi_{R_j}$$

$$H = \sum_{ii'} a^{+}_{i\sigma} t_{ii'} a_{i'\sigma} + \sum_{ii'jj'} U_{ii'jj'}\, a^{+}_{i\sigma} a_{j\sigma}\, a^{+}_{i'\sigma'} a_{j'\sigma'}$$

So, interacting Hamiltonian; a bit of a summary if you like that we have done the second quantized formalism, we have introduced the creation and the annihilation operators and we have written down generic Hamiltonian which includes single particle Hamiltonian and a Hamiltonian which consists of two particle interactions. As we have said earlier that there could be higher body interactions but usually they are too weak and most of the time they are unsolvable and the two particle interactions are good enough for describing most of the systems that we come across, and from there on we have done the single particle Hamiltonian and that Hamiltonian has only a single particle term which can be solved it is a kinetic energy mostly it is a kinetic energy part of the Hamiltonian, there could be also an onsite potential which it may include.

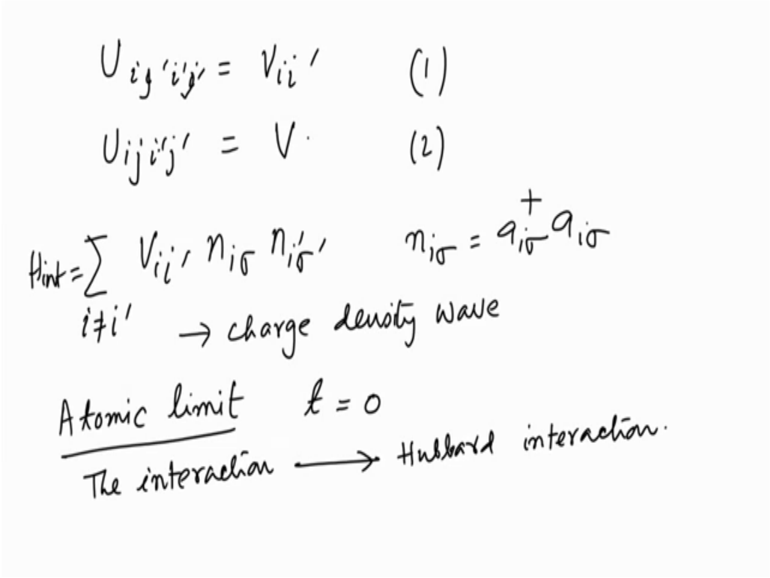
And we have also now seen today it is about the tight binding Hamiltonian, let us now talk about the interaction Hamiltonian, again we will write it in a generic fashion. So, it is an electron electron interaction and we have i, i prime j, j prime and this is like U i, i prime j j prime and there is a a i sigma dagger, a j sigma and a i prime sigma prime dagger and a j prime sigma prime. So, once again just to make the notation clear that there are two particles interacting via some interaction strength U i i i prime j j prime and these two particles are at i and i prime and they have spin sigma and sigma prime and after the scatter.

So, interaction is a type of scattering which we are going to see elaborately later and then they go on to sites which are j and j prime, and maybe the sigma becomes sigma prime and sigma prime becomes sigma or sigma retains as sigma and sigma prime become retains is retained as sigma prime. This is a generic Hamiltonian and if you like the the amplitude of the term is written as this thing is like half and a d d r and d d r prime and there is a psi R j star and psi R i star and there is a V r minus r prime and these are of course, the psi's are of course, functions of r and r prime and we have then we have a psi R i prime and psi R j prime here we have dropped the. So, maybe we have not kept that same notation let us just make it a little more careful.

So, we have and let us not keep this and so, we write this as R i and R i prime and this is r j and r j prime ok. So, that and then the full Hamiltonian looks like i i prime a i sigma dagger t i i prime, a i prime sigma now we have gotten back the spin and this we have neglected the spin, because most of the time the interaction between two particles is spinning independent it may not be, but occasionally it is. So, it is i i prime j j prime and we have U i i prime j j prime and now I have a i sigma dagger, a j sigma a I prime sigma prime and a j prime sigma prime.

So, that is the interaction term we have put in and this is the full Hamiltonian that one usually has to solve and most of the time this Hamiltonian has no solution that we have, and there are there could be many approximations in which we can write this and we have U we can have U i i prime and i prime i this could be a v i i prime and or it could be simply you know all these.

(Refer Slide Time: 41:20)



$U_{ij'i'j'} = V_{ii'}$ (1)

$U_{iji'j'} = V$. (2)

$H_{int} = \sum_{i \neq i'} V_{ii'} n_{i\sigma} n_{i'\sigma'}$ $\quad n_{i\sigma} = a^{+}_{i\sigma} a_{i\sigma}$

$\rightarrow$ charge density wave

<u>Atomic limit</u> $t = 0$

The interaction $\longrightarrow$ Hubbard interaction.

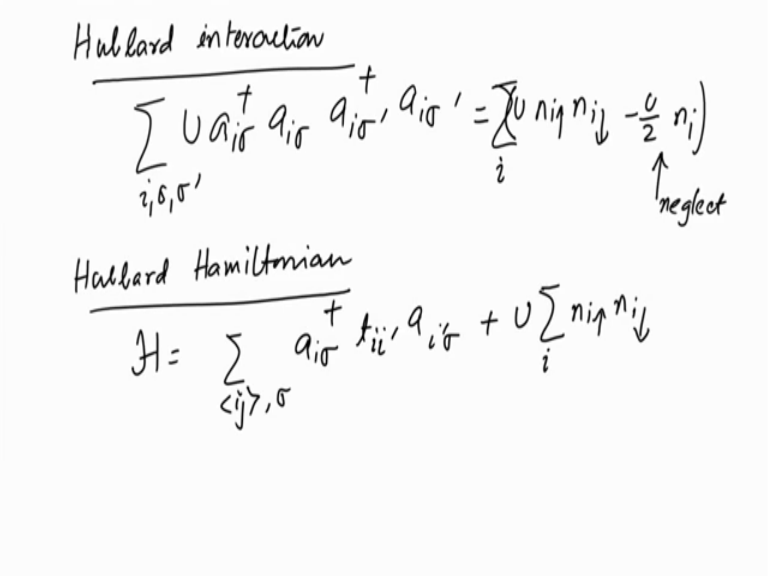
So, U so, this is equal to maybe i j i prime j prime as we have written could be simply it depends on two indices or it may actually depend on one index. So, it is i j and i prime j prime this is equal to simply equal to V and these are some of these things that we want to discuss now.

So, let us now discuss specific types of interactions and call these as maybe 1 and maybe this is 2, let us see specifically what one does. So, when we have U i j i prime and j prime equal to depends only on two indices that is V i i prime as it is shown in the above equation, then I have i not equal to i prime the V i i prime n i sigma n i prime sigma prime is the interaction term and this is the interaction term that we have for. So, n i sigma equal to a i sigma dagger a i sigma, and this is let us call it as H interaction and this is the form. So, this is going to give me a charge density wave type of modulation.

So, because you have a density which is n i sigma at a given site and in another site it is going to be probably in the neighbouring site it is going to be n i prime sigma prime. So, one is going to have a charge density wave, and this may lead to charge density wave instabilities which those physics we will discuss later. Now in the atomic limit what can happen. So, let us define what is the atomic limit and atomic limits means the hopping which is denoted by t that is set equal to 0 or it tends to 0 becomes vanishingly small and the atoms are well separated with the overland between the neighbouring orbitals to be minimal if in this limit.

So, the atomic limit just to repeat it again it talks about the overlap of the atomic orbitals being minimum and the resultant interaction is called as the in that case the interaction is known as Hubbard interaction and this was by john Hubbard, who first wrote down this Hamiltonian way back in the 60s 1960s and in which case we have for this as we have written it for the second one that is or the interaction is completely independent of the indices i j and i prime j prime and it is equal to a constant and then we can write down this interaction.

(Refer Slide Time: 45:11)



Hubbard interaction

$$\sum_{i,\sigma,\sigma'} U a^{\dagger}_{i\sigma} a_{i\sigma} a^{\dagger}_{i\sigma'} a_{i\sigma'} = \sum_{i} \left(U n_{i\uparrow} n_{i\downarrow} - \underset{\overset{\uparrow}{\text{neglect}}}{\frac{U}{2} n_i} \right)$$

Hubbard Hamiltonian

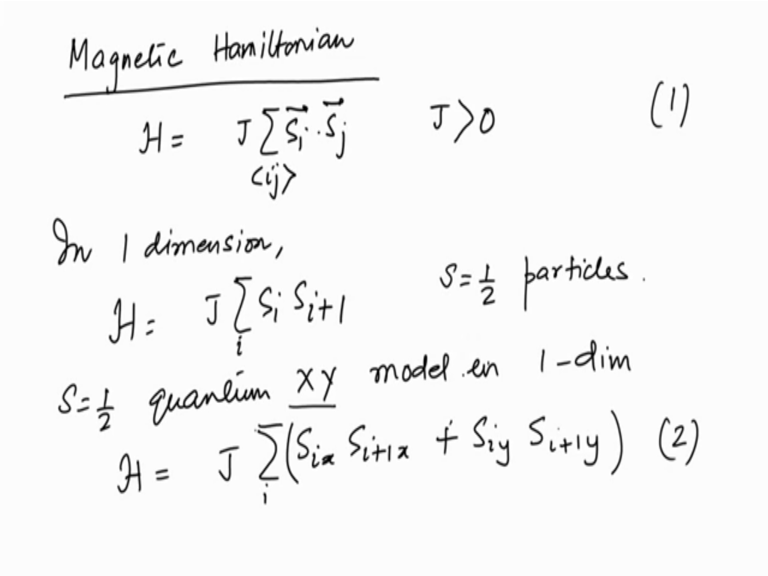
$$\mathcal{H} = \sum_{\langle ij \rangle, \sigma} a^{\dagger}_{i\sigma} t_{ii'} a_{i'\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

So, let us write it fresh to be U a i sigma dagger a i sigma a i sigma prime dagger a i sigma prime and there is a sum over i sigma and sigma prime and this can be written with a little bit of effort as n i up n i down sum over i and also a u by 2 n i. Now this last term is just a constant because it acts like a chemical potential which acts on a single site or rather it is a single particle operator, which will just shift the energy up or down and hence we can neglect that term.

So, the neglecting this term which we understand is going to shift the energy by a constant amount and as if it is just acts like a chemical potential. So, we will drop that and we will write the Hubbard Hamiltonian as H which is equal to i j and a sigma and a i sigma dagger t i i prime a i prime sigma, and a plus U n i up n i down. So, this is known as the Hubbard Hamiltonian and in fact, even though it is as I said that it is discovered in the sixties of the last century, there is still physics which are not understood and is often thought as the you know the research focus for many groups and it is still under active you know research. And especially it was under focus immediately after the discovery of the high temperature superconductors, in which it thought to away from half filling it thought to give rise to the correct physics and it is been debated since then in a number of variety of occasions.

So, well stop this discussion at this moment and let us go to another discussion in which we will talk about maybe let us talk about a magnetic Hamiltonian.

(Refer Slide Time: 48:00)



Magnetic Hamiltonian

$$\mathcal{H} = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j \qquad J>0 \qquad (1)$$

In 1 dimension,

$$\mathcal{H} = J\sum_{i} S_i S_{i+1} \qquad S=\frac{1}{2} \text{ particles.}$$

$S=\frac{1}{2}$ quantum $\underline{XY}$ model in 1-dim

$$\mathcal{H} = J\sum_{i}\left(S_{ix} S_{i+1x} + S_{iy} S_{i+1y}\right) \qquad (2)$$

And see that how this magnetic Hamiltonian gives rise to magnetic properties of materials, and by a magnetic Hamiltonian what I mean is that it is written as J and S i dot S j and where maybe it is just for the moment I assume that, j is greater than 0 and the sum is over nearest neighbour sites and this is why it is called a magnetic Hamiltonian because there is no Fermion or there is no kinetic energy of the Fermion it is basically two frozen spins are interacting via a strength J and so, the ground state properties of this model at low temperature has a long range anti ferromagnetic order and this long range anti ferromagnetic order is called as an nil state.

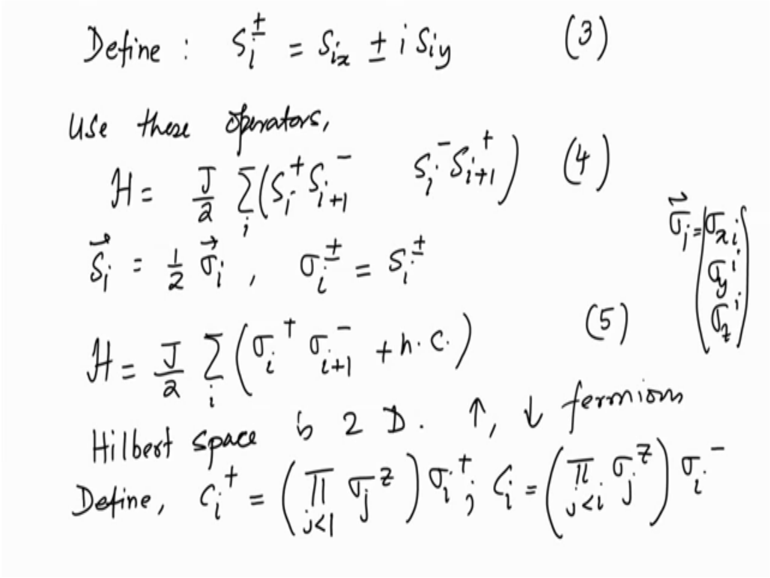
So, what I mean by long range anti ferromagnetic order is that, the spins are alternately pointing up and pointing down and there is a long range order in the system which means that the spins at i and spins at some distant j are linked or related and so, this the long range order is technically defined by a correlation function of S i and S j when i i and j are large. And the signature of a long range order is given by this correlation to decay in some exponential fashion as a function of the distance.

So, this long range order is achieved below a certain temperature, which is a characteristic temperature for antiferromagnets and is called as an nil temperature and an effective theory can be written down in terms of the partition function and hence calculating the susceptibility and so on. It is difficult to solve this Hamiltonian in higher dimensions. In one dimension we can hope to solve this Hamiltonian with certain approximations and this is what I am going to show you now that how this Hamiltonian can be solved in one dimension and that to a restricted version of the Hamiltonian and how it can be solved using some transformations. So, let us write down the Hamiltonian in one dimension and that is equal to J and S i, S i plus 1 and there is a sum over i.

So, every spin at site i is interacting with it is neighbour at i plus 1 and these are assumed to be all spin half particles; that means, these values of s is are either up or down which we can represent by plus 1 or minus 1. And this model was exactly solved by bethe and then onwards by many others and it is known that there is no anti ferromagnetic long range order for this model, and the spin correlations have a power law that is the spins at site a and spins at site j where i and j are distant sites in the lattice, it does not have exponentially decaying correlations rather it has a power law of correlations and at the wave vector given by k equal to pi and. So, there are these physics which has already been known since the exact solution by bethe, we are not attempting that solution rather we would take a simpler model which is called as the quantum x y model.

So, we will do a S equal to half quantum x y model in 1-dimension. And let us write down this Hamiltonian which is the starting point of our discussion now and this is equal to S i x S i plus 1 x and plus S i y and S i plus 1 y. So, the interaction for the spin components are only taken to be in the x and the y directions; however, the system is a one dimensional chain of spins there is no s z component or the interaction between the s z components are neglected and that is why this name is x y model. So, this is the Hamiltonian that we want to solve and see that what it gives us.

(Refer Slide Time: 53:44)



Define : $S_i^{\pm} = S_{ix} \pm i S_{iy}$ (3)

Use these operators,

$\mathcal{H} = \frac{J}{2} \sum_i \left(S_i^+ S_{i+1}^- \quad S_i^- S_{i+1}^+ \right)$ (4)

$\vec{S}_i = \frac{1}{2} \vec{\sigma}_i$, $\sigma_i^{\pm} = S_i^{\pm}$

$\vec{\sigma}_i = \begin{pmatrix} \sigma_{xi} \\ \sigma_y^i \\ \sigma_z^i \end{pmatrix}$

$\mathcal{H} = \frac{J}{2} \sum_i \left(\sigma_i^+ \sigma_{i+1}^- + h.c. \right)$ (5)

Hilbert space is 2 D. ↑, ↓ fermions

Define, $c_i^+ = \left(\prod_{j<l} \sigma_j^z \right) \sigma_i^+$; $c_i = \left(\prod_{j<i} \sigma_j^z \right) \sigma_i^-$

So, if you define operators which are S i plus minus this is equal to S i x plus minus i S i y. So, I these are called raising and lowering operators.

So, I am making this or rather constructing this raising and lowering operators from the x and y components of the spin at a given site, and there is a plus and a minus sign are related to the plus and the minus which means S i plus equal to S i x plus i S y and similarly for the minus sign. So, if I use these operators to write down the Hamiltonian, this you should do it and convince yourself. So, the Hamiltonian is J over 2 and S i plus S i plus 1 minus and a plus S i minus and S i plus 1 plus. As I said you should check that that how this Hamiltonian written in let us call it as equation 1, let us call this as equation 2 and let us call this transformation as equation 3 and equation 4. So, you should see that how equation 2 becomes equation 4 via this transformation.

Now, if you write further that these a size are simply equal to half sigma is where sigma is are the Pauli matrices sigma i vector is a matrix or rather it is a it is equal to sigma x i, sigma y i and sigma z i. So, this is the definition of sigma i there is a H cross which has been taken as 1 here, otherwise you could have written it as H cross over 2 it really does not matter in this case even if we take H process 1 it is and it is a normal practice to take H cross equal to 1 for this particular cases. And in which case your sigma i plus minus becomes equal to your S i plus minus ok. So, you have a size now the spin vectors are defined in terms of the Pauli spin matrices and the raising and the lowering of the Pauli spin matrices are nothing, but the raising and the lowering of these spin operators s operators.

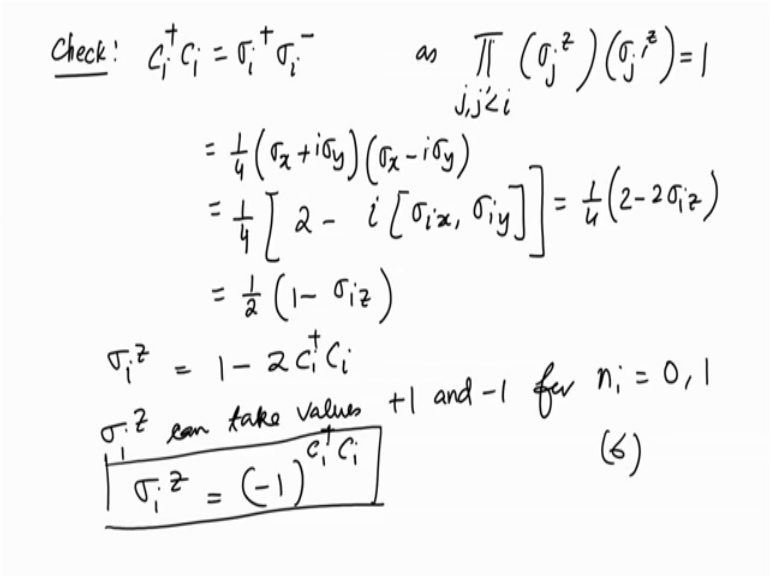
So, now what we can using this we want to write down the same Hamiltonian in 4 in terms of the Pauli matrices and that is written as sum over i and a sigma i plus and a sigma i plus minus 1 plus the Hermitian conjugate. So, the Hermitian conjugate will be sigma i minus and a sigma i plus 1 plus. So, the Hilbert space is two dimensional, Hilbert space is two dimensional and it is consists of spin up and spin down fermions.

Now it is important to realize there are no fermions so far in the Hamiltonian 5 however, these spin matrices they correspond to fermions and these are the spin half objects correspond to fermionic particles and that is why these up and down spins they correspond to fermionic operators or rather fermions and so, the only thing that you should keep in mind is that the sigma is are not fermion operators at the sigma i actually at different sides they commute and not anti commute as the fermion operators would have done.

So, if there is any hope to transform this Hamiltonian into a Fermionic Hamiltonian we have to do a careful transformation and which is what we are going to do. So, this Hamiltonian is written in terms of Pauli speed matrices and we shall transform this Hamiltonian to a Fermionic Hamiltonian and how do we do that let us define C i dagger equal to this you should do it carefully because this algebra slightly involved algebra that is going to follow, and sigma i plus an similarly C i is defined as j i and sigma j z sigma i minus.

So, these are the transformations that we do for from the pauli spin matrices to the fermionic operators. And now writing down a transformation does not guarantee that these are fermionic operators unless they satisfy the anti commutation relations that we have spoken about. So, we have to check that whether they correspond to the or rather they satisfy the anti commutation relations the c operators. So, one can check.

(Refer Slide Time: 59:46)



<u>Check:</u> $c_i^\dagger c_i = \sigma_i^+ \sigma_i^-$ as $\prod_{j,j'<i} (\sigma_j^z)(\sigma_{j'}^z) = 1$

$$= \frac{1}{4}(\sigma_x + i\sigma_y)(\sigma_x - i\sigma_y)$$

$$= \frac{1}{4}\left[2 - i[\sigma_{ix}, \sigma_{iy}]\right] = \frac{1}{4}(2 - 2\sigma_{iz})$$

$$= \frac{1}{2}(1 - \sigma_{iz})$$

$$\sigma_i^z = 1 - 2c_i^\dagger c_i$$

σ_i^z can take values $+1$ and -1 for $n_i = 0, 1$

$$\boxed{\sigma_i^z = (-1)^{c_i^\dagger c_i}} \qquad (6)$$

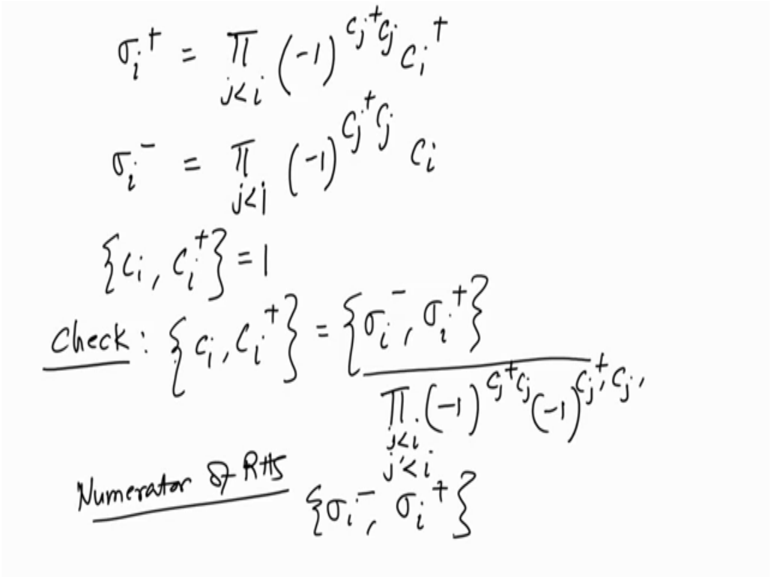
So, please check this that C i dagger C i equal to sigma i plus sigma i minus and this is true because you are the product of sigma j z and sigma j prime z it is equal to 1 for all sorry for all j j prime less than some i ok.

So, if that is the case then we can write this down as a one fourth of sigma x plus sigma i sigma y and sigma x minus i sigma y. So, sigma i will be half of sigma x plus I sigma y and sigma i minus will be half of sigma x minus i sigma y, and this if you expand it becomes equal to one-fourth of 2 minus i and a sigma i x and a sigma i y and this is equal to a one fourth of 2 minus 2 sigma i z which is nothing, but equal to half one minus sigma i z so, C i plus C i minus which is a number operator for the fermions is written as half into 1 minus sigma i z.

So, if I do the reverse transformation. So, my sigma i z is equal to 1 minus twice of C i dagger C i. Now it is known that C i dagger C i is equal to either 0 or 1 for fermions at a given site that is a restriction on the number of occupancy of the number of fermions at a given site going to the Pauli’s exclusion principle.

Now, you see that if C i dagger C i is equal to 0, then my sigma i z equal to 1. So, and if C i dagger C i equal to 1 then this is equal to sigma i z equal to minus 1. So, sigma i z can take value sigma i z can take values plus 1 and minus 1 for n i to be 0 or 1. So, we can write sigma i z equal to minus 1 whole to the power C i daggers C i. Now this is a clever way of writing if C i dagger C i equal to 1 then sigma i z is equal to equal to minus 1 if C i dagger C i equal to 1, then it is equal ton minus 1 and if it is equal to 0 then it is equal to plus 1. So, that is the that is the thing that we have decided or rather we have gotten from this earlier step. So, my sigma i z can be written in terms of the fermionic operators as this all right.

(Refer Slide Time: 63:43)



$$\sigma_i^+ = \prod_{j<i} (-1)^{c_j^\dagger c_j} c_i^\dagger$$

$$\sigma_i^- = \prod_{j<i} (-1)^{c_j^\dagger c_j} c_i$$

$$\{c_i, c_i^\dagger\} = 1$$

Check: $\{c_i, c_i^\dagger\} = \dfrac{\{\sigma_i^-, \sigma_i^+\}}{\prod_{j<i,\, j'<i} (-1)^{c_j^\dagger c_j} (-1)^{c_{j'}^\dagger c_{j'}}}$

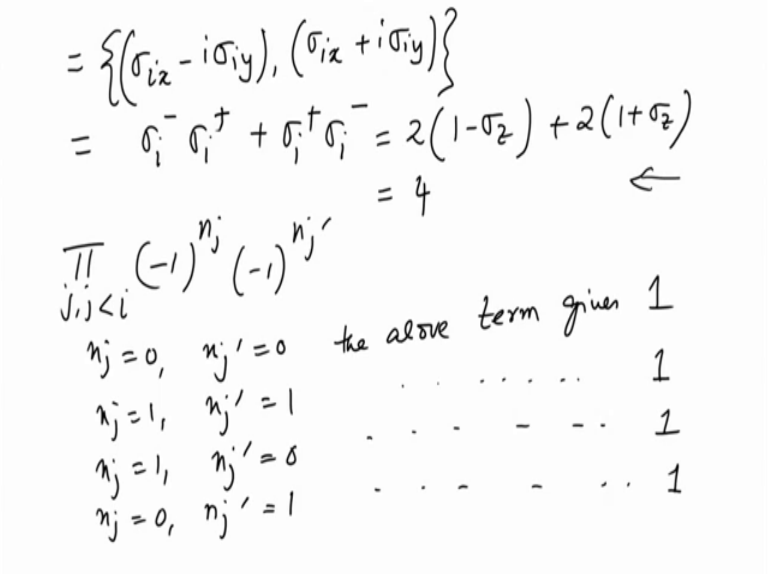
Numerator of RHS $\{\sigma_i^-, \sigma_i^+\}$

So, if we have this for the sigma i z then we have sigma i plus can be written as a product for all j less than i and the minus 1 c j dagger c j and a C i dagger. So, this is in the exponent. So, let me write it little neatly here ok.

So, that is my that is my sigma i raising or the plus 1 and for the sigma i lowering or the minus 1 this is equal to j less than i and a minus 1 C j dagger C j and a C i. So, you have to convince yourself that this is the right transformations between the raising and the lowering spin matrices Pauli spin matrices with the fermionic operators and it has to be also checked that C i C i dagger is equal to 1.

So, the fermionic anti commutation relations should give you 1 at a given site and this means that C i C i dagger plus a C i dagger C i which should give you 1 and that can be checked from the fact that. So, check this I am almost doing it for you, but you should also do it yourself to check that so, C i. So, C i and a C i dagger which is equal to a sigma i minus and the sigma i plus and this divided by this product. So, it is which is j less than i and j prime less than i as well and we have a minus 1 whole to the power c j dagger c j and minus 1 whole to the power c j prime dagger c j prime and this is the definition of the anti commutation relations in terms of this Pauli matrices and let us only take this the numerator. So, the numerator is of the right hand side, which is sigma i plus minus with a sigma i plus and that can be written as.

(Refer Slide Time: 66:39)



$$= \{(\sigma_{ix} - i\sigma_{iy}), (\sigma_{ix} + i\sigma_{iy})\}$$

$$= \sigma_i^- \sigma_i^+ + \sigma_i^+ \sigma_i^- = 2(1-\sigma_z) + 2(1+\sigma_z)$$

$$= 4 \leftarrow$$

$\prod_{j,j'<i} (-1)^{n_j} (-1)^{n_j'}$ the above term gives 1

$n_j = 0, \quad n_j' = 0$ 1

$n_j = 1, \quad n_j' = 1$ . . . - - . 1

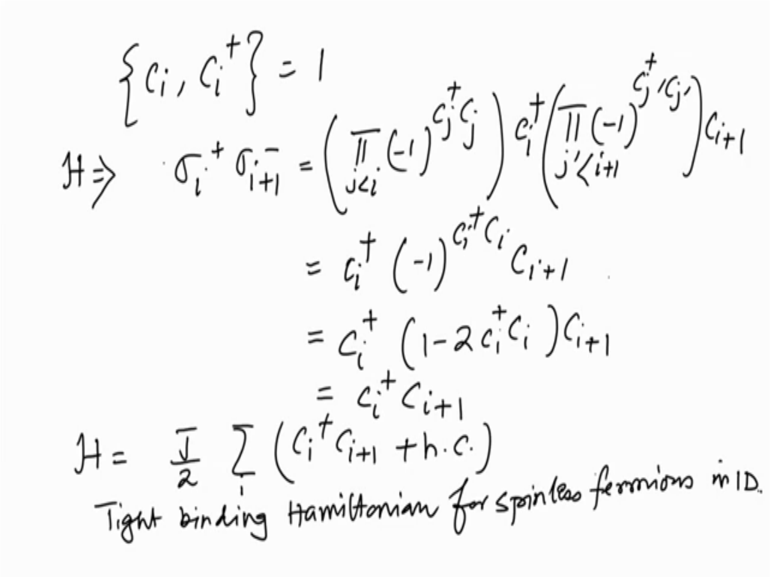
$n_j = 1, \quad n_j' = 0$ . . - - . . 1

$n_j = 0, \quad n_j' = 1$

Sigma i x minus i sigma i y and that has to be taken the anti commutation has to be taken with this. And this can be written down as minus sigma i plus plus sigma i plus sigma i minus which is equal to twice of 1 minus sigma z plus twice of 1 plus sigma z.

So, this is equal to 4 and interestingly this denominator which contains this term the product of j and j prime both less than i and a minus 1 whole to the power n j and a minus 1 whole to the power n j prime. So, it gives rise to four possibilities for n j to be 0 and 1 and n j prime to be 0 and 1. So, if you look at this then n j equal to 0 and n j prime equal to 0, then this term that the above term gives 1 and similarly for n j equal to 1 n j prime equal to 1 again the above term gives 1 and for n j equal to 1 and n j prime equal to 0 again the above term gives 1, and n j equal to 0 and n j prime equal to 1 the above term again gives 1. So, these four ones will actually cancel with the four that you are seeing here and I will finally, get the commutation relations that.

(Refer Slide Time: 68:47)



$$\{c_i, c_i^{\dagger}\} = 1$$

$$\mathcal{H} \Rightarrow \quad \sigma_i^{+} \sigma_{i+1}^{-} = \left(\prod_{j<i} (-1)^{c_j^{\dagger} c_j}\right) c_i^{\dagger} \left(\prod_{j'<i+1} (-1)^{c_{j'}^{\dagger} c_{j'}}\right) c_{i+1}$$

$$= c_i^{\dagger} (-1)^{c_i^{\dagger} c_i} c_{i+1}$$

$$= c_i^{\dagger} (1 - 2 c_i^{\dagger} c_i) c_{i+1}$$

$$= c_i^{\dagger} c_{i+1}$$

$$\mathcal{H} = \frac{J}{2} \sum_i \left(c_i^{\dagger} c_{i+1} + h.c.\right)$$

Tight binding Hamiltonian for spinless fermions in 1D.

We want that is C i C i dagger should be equal to 1. So, the Hamiltonian takes a form which is equal to which is as we have written it down earlier. So, we will simply write down one of the terms which is sigma i plus and the sigma i 1 and now this thing would be written in terms of the fermionic operators and the fermionic operators are a product for j less than i minus 1 whole to the power c j dagger c j, I want to write down the fermionic operators explicitly we could have written it n j as well.

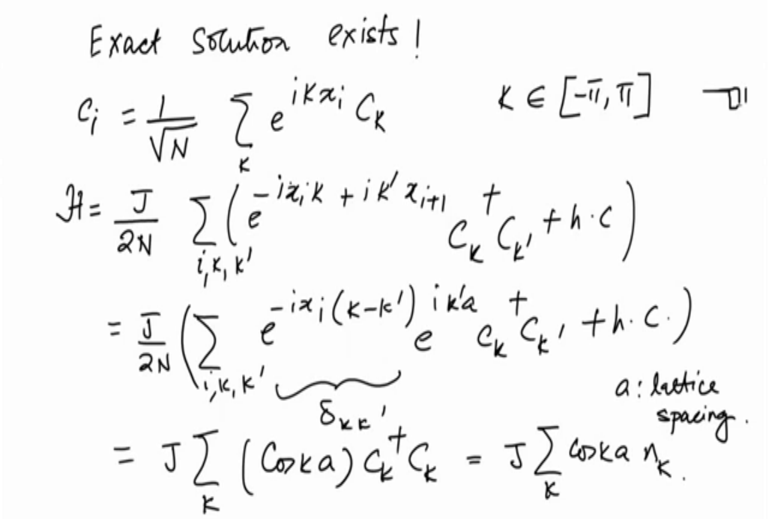
So, there is a C i dagger and then there is another bracket of this thing and which is a j prime is equal to i plus 1 and a minus 1 whole to the power c j dagger c j prime and c j, c j dagger prime daggers c j and this is with C i plus 1. So, this is the term if you recognize that this term is there in the Hamiltonian as written in equation let us call this as equation. So, this is an equation 5. So, so let us call this equation as equation 6 and we have checked. So, this is one term in the Hamiltonian that is written there.

And this if you simplify it becomes equal to C i dagger minus 1 whole to the power C i dagger C i and C i plus 1. So, this is what comes and this can be rewritten as C i dagger 1 minus 2 C i dagger C i and a C i plus 1 as you know that this is equal to either plus 1 or minus 1 which is written by these 1 minus 2 C i dagger C i because C i dagger C i can be either 0 or 1 and this can be hence written as C i dagger C i plus 1.

So, now it becomes a fully Fermionic Hamiltonian and the Hermitian conjugate as we have seen in equation 5 will come out as C i and C i plus 1 dagger. So, we will write down the full Hamiltonian completely now in fermionic terms with a J by 2 and a sum over i and a C i dagger C i plus 1 plus a hermitian conjugate and so, this is the called as the tight binding Hamiltonian which we have already seen earlier. So, tight binding Hamiltonian now we do not have any spin index so, these are for spinless fermions in one dimension so, spinless fermions in 1 D. So, this is up the problem that it boils down to starting from the Hamiltonian one as we have seen it here or rather to which is a simplified version of one and written in one dimension.

So, this is the spineless fermions and there is a it can be exactly solvable. So, exact solution exists.

(Refer Slide Time: 72:40)



Exact Solution exists!

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{ikx_i} c_k \qquad k \in [-\pi, \pi] \quad \text{BZ}$$

$$\mathcal{H} = \frac{J}{2N} \sum_{i,k,k'} \left(e^{-ix_i k + ik' x_{i+1}} c_k^\dagger c_{k'} + h.c \right)$$

$$= \frac{J}{2N} \Big(\sum_{i,k,k'} \underbrace{e^{-ix_i(k-k')}}_{\delta_{kk'}} e^{ik'a} c_k^\dagger c_{k'} + h.c. \Big)$$

a: lattice spacing.

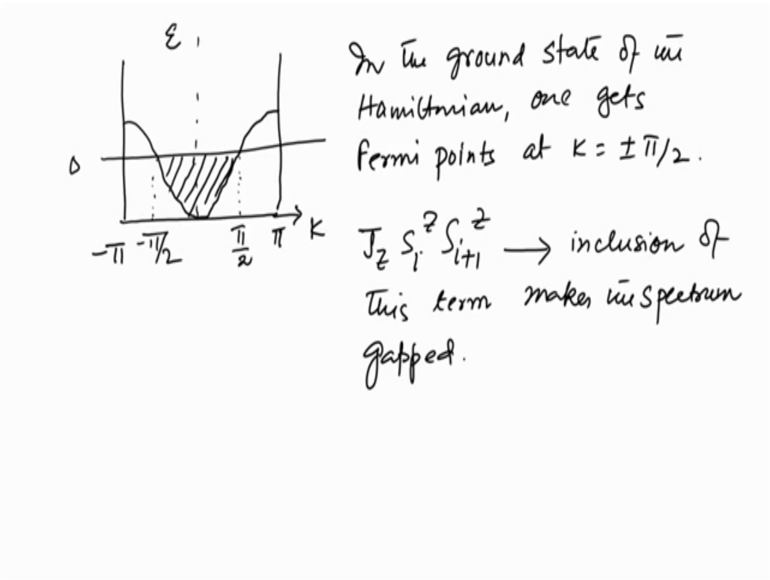
$$= J \sum_k (\cos ka) c_k^\dagger c_k = J \sum_k \cos ka \, n_k.$$

And why I write is that, it is quite unusual for an interacting problem or of many body Hamiltonian to have an exact solution, even if it is the case in one dimension. So, we will solve it using those. So, you rerun the whole thing in momentum space. So, that we can write down a C i equal to 1 by root over N and this is in one dimension. So, we can write it as exponential i k x i and a C k. So, k belongs to you know mind I mean in this range rather.

So, minus pi to pi which is the first Brillouin zone and if you do this momentum space transformation one gets that J by 2 N and i, k and k prime to be equal to exponential minus i x i k plus i k prime x i plus 1 and a C k dagger and the C k prime and plus the Hermitian conjugate that is going to be there and this is equal to j over 2 N and i, k, k prime exponential minus i x i k minus k prime and exponential i k prime and the C k, C k prime and plus a Hermitian conjugate as will be there and this is is basically the lattice spacing and this is.

So, this is equal to you are the definition along with this 1 over n is the definition of delta k k prime. So, this is becoming it becomes equal to J and there is a. So, this will give me a J and the sum over k cosine k a and this is equal to a C k dagger C k. So, this is simply J sum over k cosine k a n k. If you like take a equal to 1 the lattice spacing equal to 1 that does not cause any problem, but this is the exact solution of the Hamiltonian that we have started with equation 2 and what does this Hamiltonian tell you? That this tells me that the spectrum is like this and these are these points.

(Refer Slide Time: 75:57)



In the ground state of the Hamiltonian, one gets fermi points at $K = \pm\pi/2$.

$J_z S_i^z S_{i+1}^z \longrightarrow$ inclusion of this term makes the spectrum gapped.

So, this is the Fermi energy so, 0. So, this is my E versus K let me write it neatly this is equal to your epsilon and this is K and these are the points. So, this is that corner of the Brillouin zone. So, minus pi to plus pi and this is it cuts the Fermi energy at this is at pi over 2.

So, we have the Fermi points are at minus pi over 2 and plus pi over 2 so, the ground state. So, in the ground state of the Hamiltonian one gets Fermi it should be in three dimension, it should be Fermi surfaces; however, in one dimension these surfaces actually boil down to point. So, we will write as Fermi points at k equal to plus minus pi by 2. So, what it tells you is that there are gap less excitations so, which means that another fermion or one extra fermion can be added without any cost of energy at the Fermi level.

So, when you want to add a particle at in a system in a system of fermions because all the states all the way up to 0 to k by 2 are filled which are inside this parabola they are completely filled all the way up to k by 2 plus k by 2 and minus k by 2. So, if you want to introduce one Hamiltonian then sorry if you want to introduce one fermion that fermion has to be added at the Fermi level, and it costs no energy because the excitations are gapless; however,. So, it is known that the quantum x y model gives gapless excitations that is one can what I mean is that one can add one more fermion without any extra cost of energy.

However this situation will change if we add the z term. So, if we have a term which is z and z plus 1, this inclusion of this term of this term makes the spectrum gaped ok. So, we are really talking about a Magnetic Hamiltonian in one dimension which has an exact solution and this solution seemed to give us a magnetic metal or a kind of gapless excitations and in the event that you want to add a z component of the spin interaction along with the already the terms that appear in equation 2, this gapless situation will vanish and you will have a gapped situation which would be corresponding to an insulating scenario.