Module 24 – Lecture 11
t-J model, discrete symmetry groups, example square lattice

So, having discussed, this unconventional, d- wave pairing, we let us now look at, a model which can give rise to this D wave pairing, mathematical model, which is also relevant for these superconductors, which show, d-wave pairing. So, we have to write down a model almost with the kind of knowledge that we have about electron correlations and so on.

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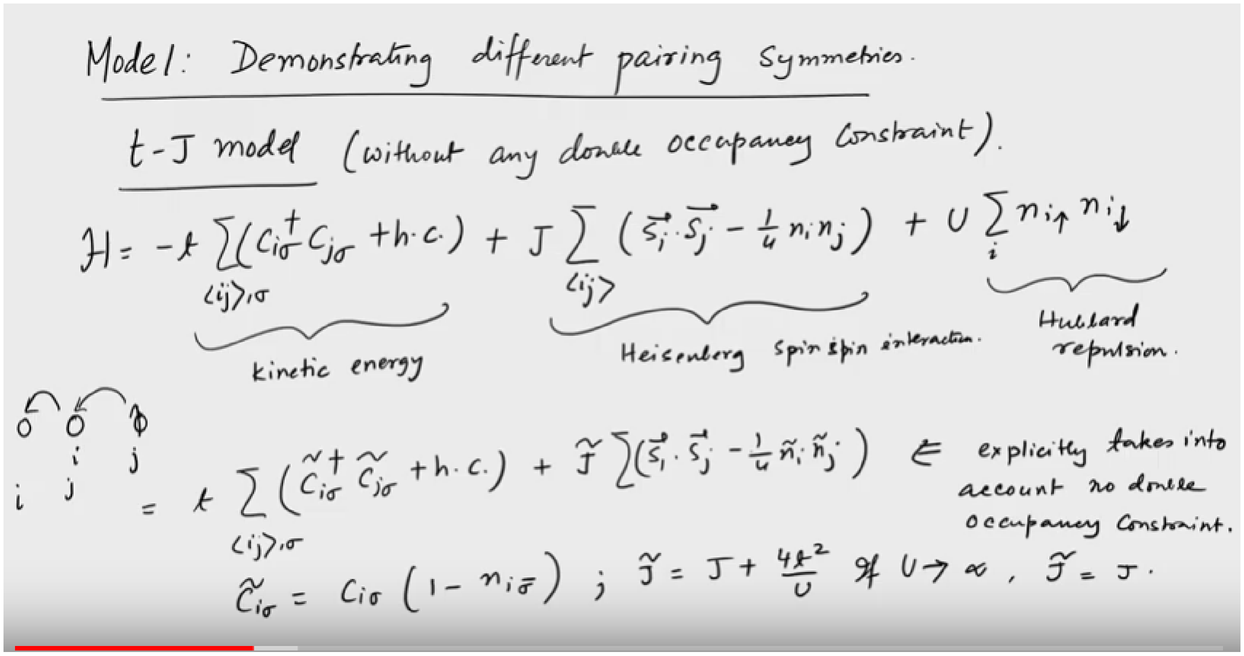

And we introduced this model, as a TJ model so we say that, demonstrating different pairing, symmetries and we write down what is called as a,' T-J Model'. And at this moment we write down, without any double occupancy, constraint, let's first write down, the model and then we'll discuss various issues related to it. So, the Hamiltonian is written as H equal, to minus T and a see I Sigma dagger, C J's Sigma plus a Hermitian conjugate, which is a usual kinetic energy term, the sum is over the nearest neighbor I and J sites, Sigma refers to the spin and we have spin-spin coupling, which is known as the Heisenberg coupling, we have seen that, how this spin-spin coupling, can actually arise, maybe we'll see it in, a tutorial how one can actually get a spin-spin coupling and we write this as si dot s J minus 1/4 ni NJ this is just a constant term, that's added and we also add, on site, repulsion term, which is given by ni up and ni down. So, just to tell you about the various terms in this Hamiltonian, this is called as the,' Kinetic Energy', which is the hopping, of electrons. So, this the one with, not a dagger so, this is called as a,' Destruction Operator'. So, it destroys a particle with spin Sigma at a site J, particle means of a muon and creates the particle at site I with a spin Sigma. So, basically it so, there are two sites, I and J and there was a spin says Sigma, let's call Sigma to be enough spin here and this operator operates on such a state and moves the spin to here and then in the next step this is considered as, J and this is considered as, I and then, one has well I mean I would be probably here and so on. So, maybe this is not, let's not write this as I. Okay? So, I would be a site which is here then, in the next thing and then it will keep moving it by again application of this operator and so on. So, this keeps moving, the electron from one site to another and this is called as a,' Hopping Term 'or the,'Kinetic Energy Term'. And the Hermitian conjugate is mandatory to add to give us a real eigenvalue, for the Hamiltonian, the next term, which is Heisenberg like term, spin-spin interaction. So, this term, is not written in terms, of the Fermion operators. But later on it will be written in terms, of the Fermion operators, it's been written in terms of the spin operators, at site I and J again I and J are nearest neighbors and these are the d**e**nsities at site I and J. So, there's a spin-spin coupling, between the spin vector at I and the spin vector at j and these are vectors. So, this they have components x y and z; and that's why it's called as a, 'Heisenberg Spin-Spin interaction'. We could write it in the Ising sense that is this has only y component and still can write down a similar Hamiltonian, which is what will show in a tutorial and this is called as the,' Hubbard Repulsion', please take a note as this term, this is a term that involves density, of an up spin, with which is an up spin density is interacting, with a down spin density, at a given site I.

So, if u is large, it will not allow or rather it is becoming energetically, unfavorable to have a spin down, when there is already a spin up at a given site, I or the vice-versa. So, this actually brings, in the electron correlation, strong electron correlation, that is if the electrons are strongly interacting, this site will not allow, double occupy occupancy and so on. So, basically what we mean to do is that, by we want to solve this Hamiltonian and this Hamiltonian, does not have an exact solution, at least for two dimensions that we are looking for and we need to sort of make simplification, but at this moment in order to show the wave pairing we don't really need to solve this Hamiltonian, we can just write this Hamiltonian and explain as I have explained various terms to you. So, this is a model, for an interacting Fermionic system, in principle in any dimension we are only interested in dimension equal, to 2 D equal to 2 because, of the reason that these high TC or the high temperature superconductors are actually found, in 2 dimensions or rather the, the plains, which are responsible for superconductivity are two dimensional plane, which are copper oxide planes, in order to simplify this Hamiltonian to get to a more meaningful form, we'll have to do a Fourier transform of this, but before that, let us write down the TJ model which one is familiar with, where we can write down this as T and C I Sigma dagger, with a tilde and a C J Sigma and a plus a j, SI dot SJ minus ¼ ni NJ that's it. So, what we have done is that we have replaced, this these operators, we can also replace these operators and so on, by their Tilda's and have neglected the last term, which is the Hubbard repulsion, means that this is implicit taking, into account or rather this is explicit if we do it so, explicitly and no double occupancy constraint. So, the definition is that, the CI Sigma, tilde is equal to CI Sigma, 1 minus ni Sigma bar. So, that automatically says that if there is a spin of Sigma bar at a given site, I so this CI Sigma will be equal to 0, which means that you cannot have another spin, coming there with, with a spin Sigma or with an electron with a spin Sigma and so, on and this j is equal to j plus 4 T Square over u, where you in the limit u going to infinity, then I mean this J tilde is equal to J. So, in order to, do for the simplification to this model, let us write it down in the momentum space.

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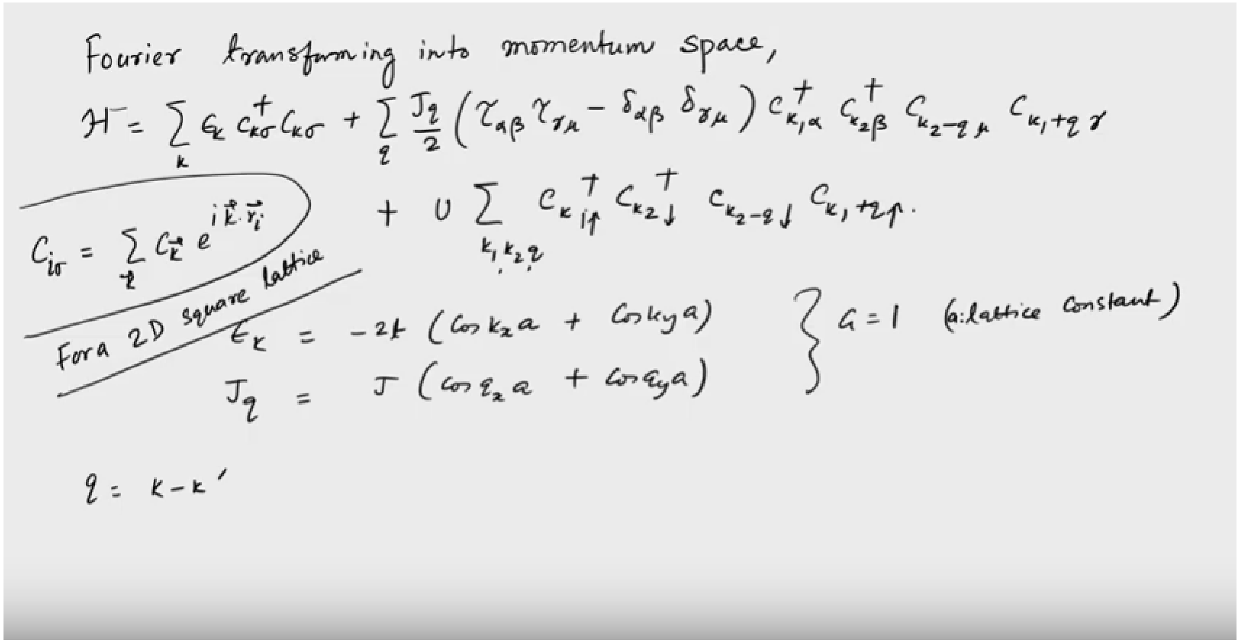

One gets so, H is a function of K now, it becomes, a slum or slim, the kinetic energy becomes somewhat simpler and the terms, which are the other terms, we are still writing the original Hamiltonian and not the Hamiltonian that we have written down, in the form of TJ model. So, we still have a u term there, there's a gamma, alpha beta, gamma mu nu minus Delta alpha beta, delta gamma mu and there's a CK, 1 alpha dagger c, k 2 beta and CK 2 minus Q mu C K 1 plus Q gamma. So, this is the second term, this you have to do it very carefully, where each of those C I Sigma, is converted into sum over, K this is CK exponential, I K dot RI and so on. So, use this and I use those momentum conservation and you'll be arriving at this so, this is something that needs to be used and there is a U and then there is a k1, K2 and Q. So, these are the three momentum indices that are required here, CK 1 dagger, c k2 down, dagger and CK 2 minus Q down and CK 1 plus Q up now it's, it's very easy to see that, there are only singlet pairings available, because the pairing, if this is a model for superconductivity, that is if this model can give rise to superconductivity, in for some parameter range, TJ and you then this is this as only, the singlet pairing is only encoded in this model and there's no triplet pairing and neither we are interested in triplet pairing as we have told, in the last discussion, we are we only want to concentrate on the singlet pairing and only finite momentum singlet pairing and that to the d-wave pairing, which is L equal to two and in order to do that, let us write down, the definitions of epsilon K, for a so, in for a two dimensional square lattice. So, this is equal to a minus two T, where T is the strength of the hopping and cosine KX a plus a cosine, KY a and a J Q is equal to, a J plus cosine Q X a plus a cosine qy a, we can take a equal to one, which is a lattice constant, and then can in principle, forget about so, a is equal to the lattice constant, a is the lattice constant and we can simply ignore that, from later on. Now here of course the Q is equal to K minus K prime or which is here, I mean there is a K 1 and K 2 and then K 2 minus Q and K 1 K 1 plus Q and there is of course a key one and a K 2 so, it's basically either you call it a K 1 minus K 2 or you call it a K minus K prime, we could write in principle in terms of, you know in terms of K and K prime, we just wanted to write it in terms of K 1 and K 2, but in any case the Q the momentum index Q, is actually for the transferred momentum and this one, now we need to understand a few things, how to resolve, this according to the symmetries of the 2d square lattice, and write the interaction, in a more meaningful fashion, such that we can get the d-wave super conductivity out. So, I reiterate, that having Fourier transform, the Hamiltonian which is a TJ model, we have still kept that T U, which is a tunable parameter, if u is very large then of course, it won't allow W occupied sites. So, they'll project all the W occupied sites, from the Hilbert space, which is what the TJ model is, which is written in the last slide and having written the Fourier transformed, Hamiltonian and these definitions of the, the spin dispersions or spin wave dispersions and the electronic dispersions, we need to understand, that how to get the interaction term, which can cause superconductivity. So, in order to do that, let us, look at a little bit of group theory and since, this study of group theory will be outside them it of this course, neither we want to do it very elaborately, we will give you the basic, things and basic ingredients, that are required for our purpose and write down, the interaction term, in terms of various symmetries or various basis functions, which come from the irreducible representations, of a symmetric group or discrete symmetric group, that is relevant, for a 2d square lattice.

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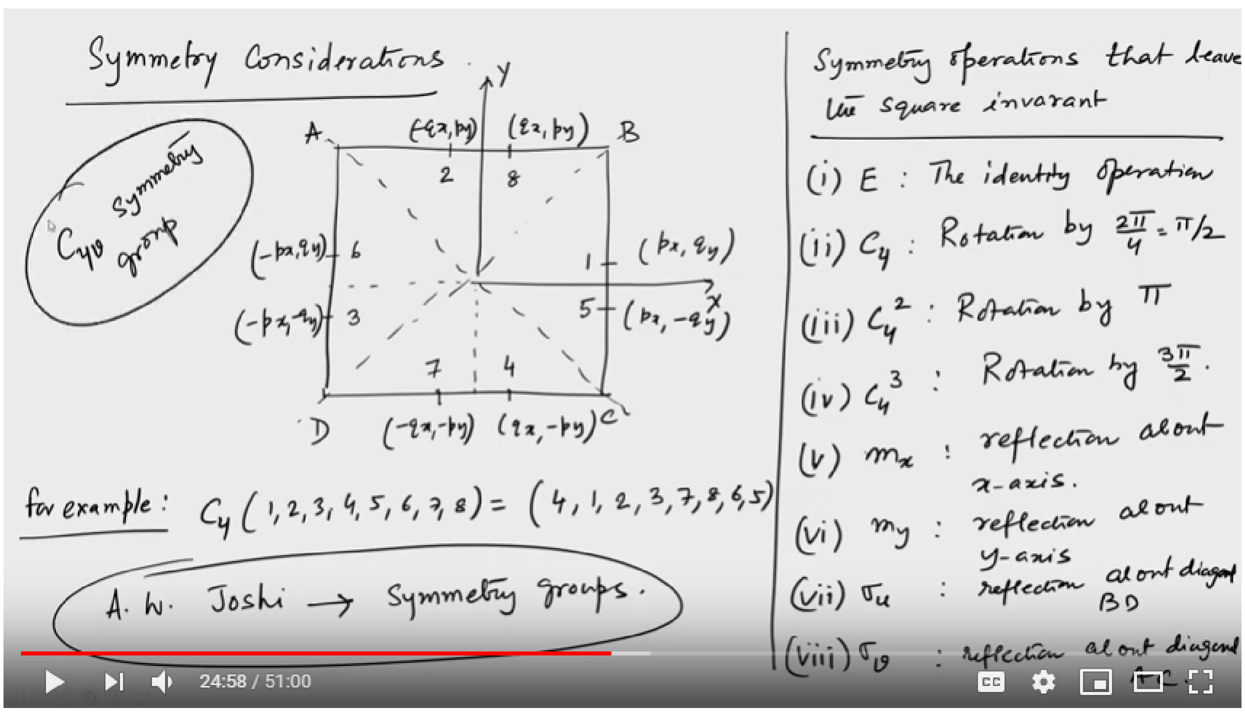

So, let's write as, symmetry considerations, let us write a square and let's just mark some points so, this is your Y and this is your X and these is the square ABCD, we know that it has certain symmetry properties, that is if you rotate it by 90 degree, in the clockwise direction then a will go to, B, B will go to C, C will go to, D and D will go to, a however the square remains, invariant is just renaming, of this vertices that will take place. So, we are going to take 8 points, which are these we'll call them as, so, these are the eight points, which are taken, on either side of this the axis that is that that are marked here. So, let's call this as, one this as two, will tell you the reason for writing this 8, this is 6, this is 3, this is 7 and this is 4. So, this has well this is 3, I'm sorry this 5 so, this is a P, X, Q, Y that's the coordinate of this, where P and Q are some numbers and this is PX minus qy this is QX minus py, this is minus QX minus py, this is P X minus PX minus qy, this is minus PX q y and this is minus QX and py and this is a QX and py. So, this is how the eight points are labeled or their mark and so, there are these one to eight points, shown in the above figure, they correspond to certain basis functions, which we'll see, now, let us look at the symmetry operations, that sleeve this, square invariant. So, one is called as,' E ', the identity operation, which of course leaves anything invariant you just multiply it by one, number two is c4 so, rotation by 2 pi by 4. So, this if it becomes C n it becomes 2 pi by N's and its 4 so, which is equal to PI by 2. So, that's another operation, which have already seen C 4 square, which is rotation twice, so rotation, by PI rotation thrice so, it's rotation by 3 PI by 2 rotation C. So, now it's a reflection about the x-axis, let's call it as M X, reflection about x-axis, six, my it's a reflection about, y-axis seven, Sigma u, let's call this Sigma you to be the diagonal, which is a BD and a Sigma V to be a diagonal AC so, the reflection or inversion, reflection, about diagonal, say BD and finally, the last one, Sigma V. so, reflection about, diagonal AC. Okay? so, these are the eight symmetry operations, that leaves the square, the two dimensional square, unchanged it will simply be you know, probably one will go to two, to three will go to, 4 and 4 will go to, 7 and, and things like that, let me show that one operation, which so, for example, you can test it yourself, a c4 on one, two, three, four, five, six, seven, eight. So, if you apply the c-4 operations, then what happens is that? A 1 becomes, 4 and then, 2 becomes 1 and then it becomes 2 and then it becomes 3 and then it becomes 7 then it becomes 8 and then it becomes 6 and then it becomes PI. So, and then you can you can work out that what happens when you apply a c4 square or C 4 cube or AMX my or Sigma U or Sigma V. So, these are the symmetry operations, which leaves the square unchanged. Now this is quite arbitrarilym we are writing down, character table and a full knowledge of group theory, is required at least for limited knowledge, discrete groups and which you can get in this book, by A W Joshi which talks about, the symmetric groups. So, let us write down. The character table, of so, this is called as a c4v symmetric room so we are going to write down.

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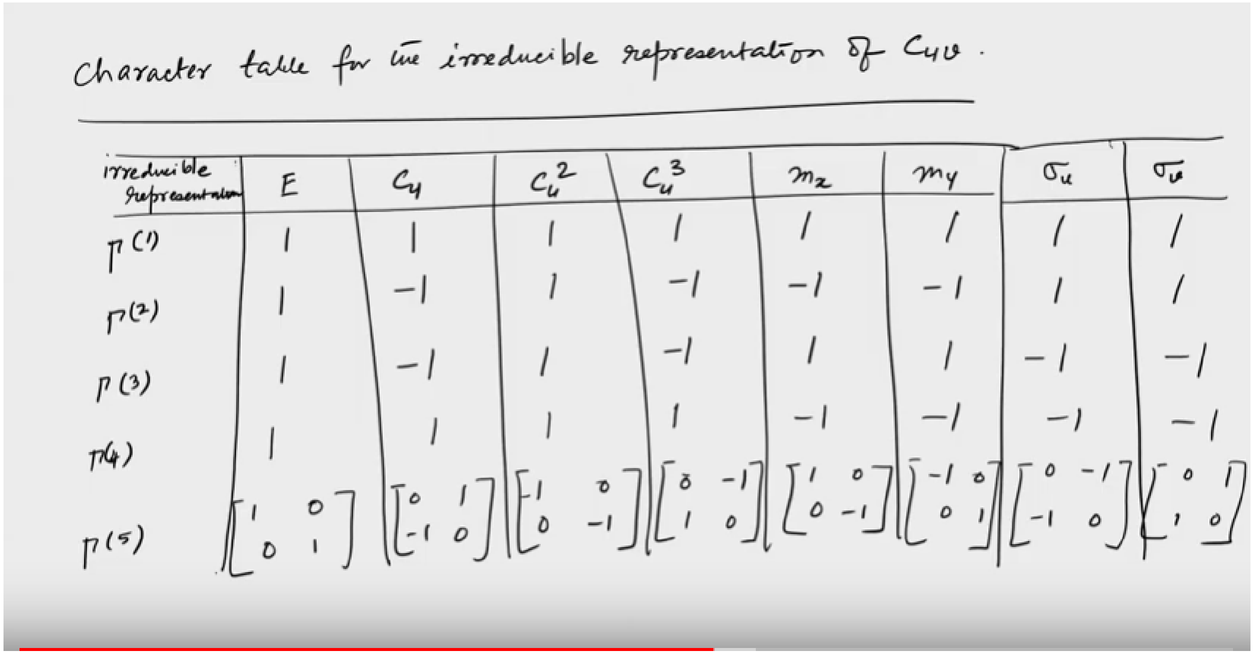

A character table, for the irreducible representation, of c4v so, if we so, this is the irreducible, representation and this is the identity, this is c4 as, we have discussed this is C 4 square is C 4 cube MX my and we need 2 more for Sigma U and Sigma B. Okay? So, so the so, the different reducible representations, they, they are these representations are gamma 1, gamma 2, gamma 3, gamma 4, which are sorry this is gamma 4 and there's a all these are one dimensional representations, gamma 5 is the only 2 dimensional representation, So, these representations under these symmetry operations, they this the values they acquire, in the character table are as I told that you need to look at, the C 4 V symmetric group in, either in any book or in this book by A W Joshi which has which presents a very clear, description of this symmetric group and many others actually. So, this is these are all ones and there is a 1 minus 1, 1 minus 1, minus 1 ,minus 1, 1 ,1 this is 1 minus 1, 1 minus 1, 1, 1 minus 1 and a minus 1 and 1, 1, 1 ,1 minus 1, minus 1, minus 1, minus 1 and these are the two dimensional representations, 1, 0, 0, 1, 0, 1 minus 1, 0 ,1 0 ,0 minus 1, sorry this is minus 1, 0 this 0 minus 1, 1, 0, 1, 0, 0 minus 1, minus 1 ,0 0 1 & 0 minus 1, minus 1, 0 & 0, 1, 1 ,0 and so on. So, these are this is the character table, for this symmetric group, but what is more important to us is the following.

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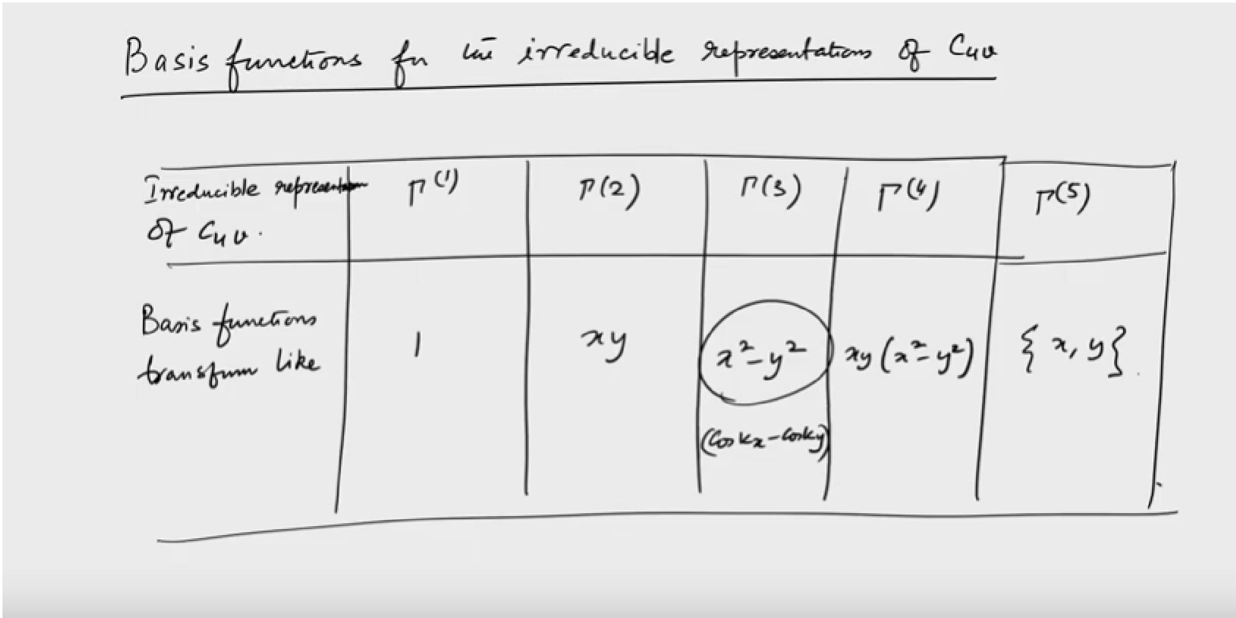

The basis functions, of c4v and so, these are the irreducible representations and then we have, two, three, four irreducible presentation, of this c4v the basis functions transform like, gamma one, this is one this, gamma two, it goes like X Y, gamma three, this is what is important to us the X s square, minus y square, this what was told yesterday that, FX y was taken as X square minus y square, a gamma 4, which is XY X square minus y square and this gamma 5 is written as, this in fact it's not important, the two-dimensional representations are not important, what is important for us is gamma 3, which is related to this, the d-wave what we have seen earlier, now let's go back to this ongoing discussion, on this and in fact if you do a case based representation this actually looks like, a cos KX minus, cos KY and of course these the this, there are other two-dimensional representations, rather there are the singlet representations, which we'll be talking about. So, let us look at, the term that comes with, so, so the singlet.

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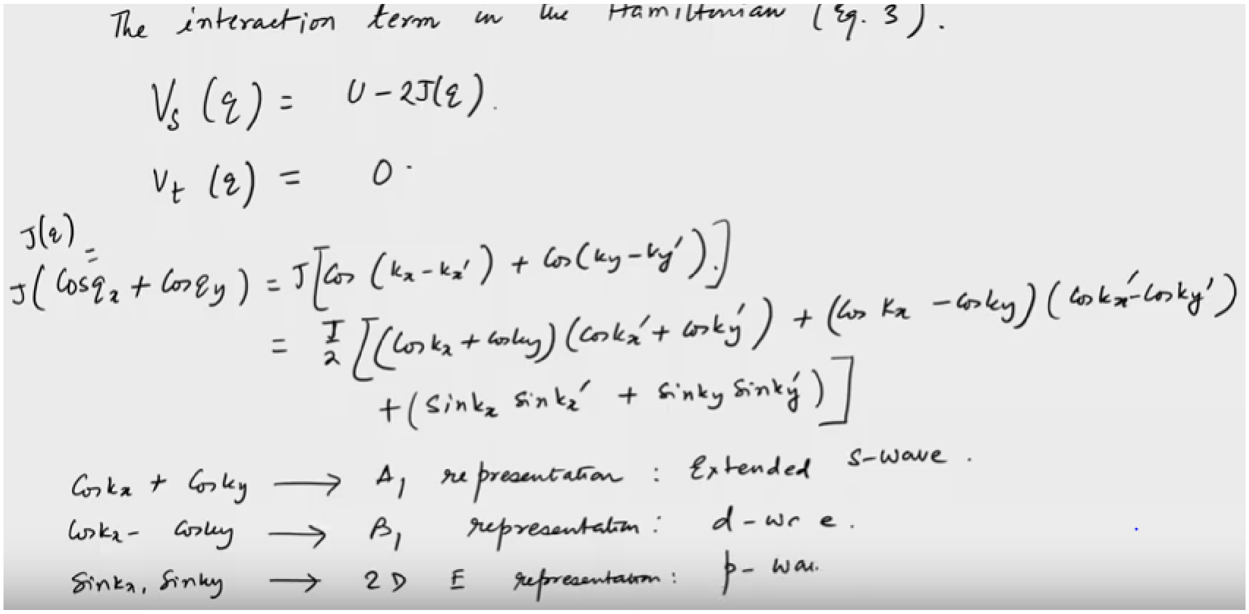

So, the interactions so, we refer to the three slides back, when we wrote down this, this Hamiltonian less, call this as equation 1 and if you want this as equation 2 and this as maybe this as equation 3. So, from Equation 3, we write down the interaction term. Okay? So, the in the singlet channel, we have, Vs and this is equal to 2j Q, it's important to note that as this, this two factor is coming from the sum over all spin indices, there you is the, the onsite term and the other one has a K dependence or Q dependence, this is in the singular channel and in the triplet channel, which of course would promote on up, up or a down, down pairing and nothing in this Hamiltonian that promotes up, up or a down, down pairing, is always a pairing between and up and down up, down spins and hence this is 0 and let's write down the, the term which is a cos of QX plus a cos qy, which is coming from the JQ term. So, this is equal to a cos, of KX minus a K X prime plus a cos KY minus a KY prime. So, this is like, a half of cos K X plus a cos K Y, cos of KX prime. So, basically, this can be expanded, which I skipped one step is cos a minus cos B, cos a minus B plus cos of C minus D and if you combine, all the terms and then do a, sort of simplification, then this thing comes, as told earlier that we have taken, the, the lattice constant to be equal to one and so, there are terms such as, a cos K X minus cos K Y and a cos of KX Prime, and a cos of minus, a cos of K Y Prime and we can also take, of course k x sine, KX sine, KX Prime and assign, KY sine, K Y Prime. So, this is the, the end so, this J Q so, this is nothing but the JQ without that J factor. Okay? We can write down the J factor if you like so, there's a J so, there's a J and this is like the JQ, equal to this so, there's a J there and so on and so we have a J here. So, we have seen these things. So, cos K X plus cos K Y, this transforms according to the a one representation, again you have to refer to the group Theory book by A W Joshi or any other group Theory book, it will give you what the a one representation, is and for our case is known as the extended s-wave, cos KX minus cos, K Y it's a b1 representation and as said earlier this is called as the,'d-wave'. And sine KX sine K Y, this corresponds so, the 2d, E representation and this is called as a,' p-wave'. Okay?

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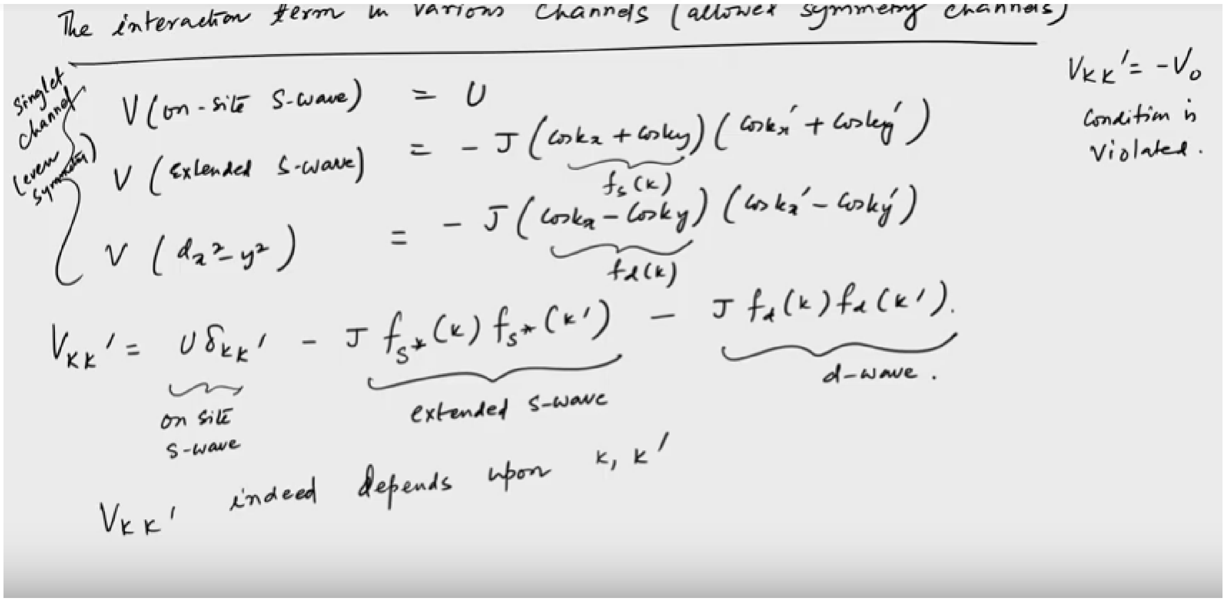

So, the interaction term, in the so less right down, which are allowed symmetry channels, is a V on site, as an s-wave and that's equal to u, V extended, s wave, which is equal to minus J cosine, of KX plus cosine, of K Y cosine of, KX prime, plus cosine, of K Y prime, you remember that when we derive, BCS theory or V KK prime, was taken to be equal to minus V 0 for all K and K prime, provided the energies of the single particle energies, live within a thickness or a energy shell, of H cross Omega D just outside the Fermi field Fermi see here, of course this condition is not, satisfied condition is violated that is we have a K dependence or a key K minus K prime dependence coming in the, in the interaction term and V in the DX square minus, y square channel, as we told that this is what is going to be most important and interesting for RK. So, luckily that comes in this model and that's why we have actually considered this model, it's a cos KX prime minus, cos K Y Prime. So, we can write down the V KK prime, now it's equal to a u Delta KK prime, that is precisely the same as, what we have seen in BCS Theory accepting the fact, that there we needed specifically, an attractive interaction for super conductivity to occur, however this U is purely repulsive and it may actually, come or has it may have a large value, which encodes, strong electron correlation, into the model. So, this is there and we have J F s we are only talking about we are leaving those, P wave representation or two-dimensional, representation, it's only in the so, this is only in the singlet channel, rather and these are even symmetry, if K X goes to minus KX it doesn't change sign. So, this is called,' f s star', we write down so this is with, a just on site, S wave and this is the extended s wave. So, this is your F s K and this is your f DK, minus j, FD k, FD K Prime and that's the that's the interaction team stoled earlier that. So, this is extended s wave and this is a d-wave. Okay? So, VK k prime, indeed, indeed depends upon, k and K and K Prime and eight, luckily it depends, in a product form of, K NK prime. So, they get decoupled and that causes a lot of simplification. So, we'll put this will not solve it further, but we have been able to, show that this model can give rise to D wave correlations and this is probably, a very relevant for the study of, this high TC superconductor ET. So, if we write it down,
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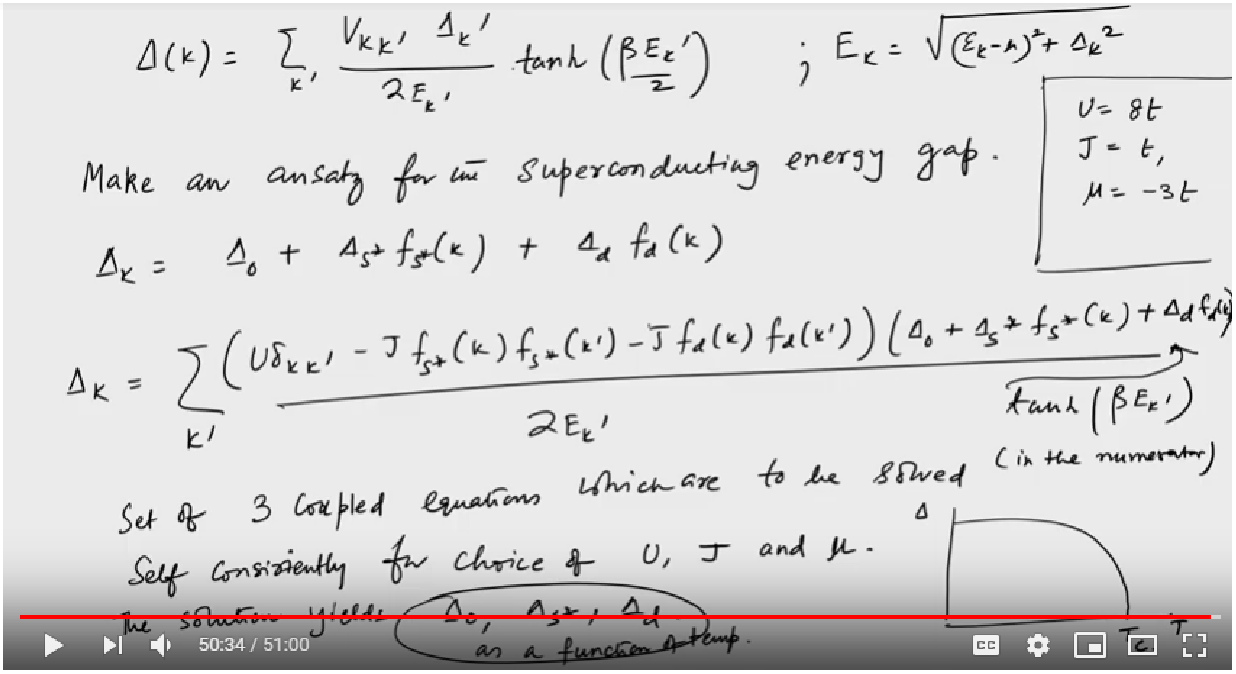

even without much thought into the, BCS gap equations. Now one can solve, for so this is the gap equation, if you look at your earlier, notes or discussion, you'll see that this is the gap equation, now this gap equation VK k prime, is precisely what you have written here. So, if you put this V KK prime, if you put this VK K Prime, into this equation, this gap equation one can actually solve for each of those symmetries, namely the so one can actually, make an ansatz for the superconducting energy gap, this corresponds to the on-site, s-wave this corresponds, to the extended, s-wave and this corresponds to the d-wave. So, each one of them and according to this irreducible representation so, these are the, the basic functions, in the k space for these representations and each one is actually orthogonal to the other, which can let us write that, Delta K is equal to a sum over K prime, u Delta KK prime, minus J of FS star, k, FS star, K prime, minus j FP k FD case, k prime and so, this and then multiplied by the Delta zero plus the Delta s, star, FS star, K plus a delta d, FD K and so, on and then of course there is a 2EK Prime and a Tran hyperbolic beta e K Prime, where of course your Ek prime, is equal to root over epsilon K minus mu plus a delta K square, now of course this tan hyperbolic could come here, I mean it is not in the denominator, it is in the numerator. So, this is in the numerator, it's a highly nonlinear equation and there is no way, other than resorting to numerical techniques for solving this equation, but the good part, is that you will also have to write this Delta K, in this part of this equation and then I use the Fourier trick, that is you try to, make these each write down these equations, which are coupled equations and set of basically, set of three coupled equations, which are to be solved self consistently, for choice of U J and for UJ and of course, mu and T is of course one, I mean the hopping term T is equal to 1 the solution, yields, a delta 0, Delta s star and Delta D, which are what we want which are the gap functions in this particular, symmetry channels and these give the information, that how this as they fall off as a function of temperature, if you remember, that this is what we wanted to do and in any second order phase transition. So, these are the, the gap parameter or the order parameter, for each of those and these actually fall off as T each one of them, we have seen in the BCS theory that, we had a single delta. So, we didn't have to solve three coupled equation, it was just one equation, because of this emergence, of new symmetry channels, we have three symmetries particularly, which are important, which are s-wave and extended s wave and D wave and then which has to be solved for each one of those Delta 0, Delta s star and Delta D and it has to be solved as a function of T for these choices of you J and mu and this gives the TC Delta as a function of, TC and this actually completes, the problem of finding the gap function and finding, what is T C and as we have emphasized a number of time, that the energy gap is the most important thing, in superconducting problem or in the study, of superconductivity and this is what it aims to do it is true that, we could not solve this problem, like sitting here, because it involves a very highly nonlinear equation solution of nonlinear equation, you could try a Newton Rapson method, but these are coupled equations, they have to be solved self-consistency also, for these choices of UJ j and mu, which are left to you to choose and the values as I told that the U is has a value which is large and J has a value, which is given by, I mean it basically it's typically, much lesser than you, because, there's a form that we have shown, is J equal to some J tilde equal to J plus 40 square by u. So, one good representative, value of this can be shown as, say u equal to twice of bandwidth, it's a square lattice it has a bandwidth ,of 40, because it's 2 T cos KX plus cos K Y. So, it's 48 T. So if we take its to be a bandwidth, then J should be much smaller and J should be maybe, maybe, maybe a tea or even lesser than T maybe, maybe half T or some but of the order of T and mu can be taken to be any value because, this is a solution, that we want to believe that it is true for small electronic densities, it doesn't have to be in fact small, if you take the electronic density to be large, then the solution converges faster. So, you could take it to be you know a value, which is it minus 3t or something, that T can be set equal to 1 and then you have 8 1 and minus 3 as the various parameters and if you wish to try this solution, you could try that and one should get a, behavior like this that these gap functions individually, would vanish at a temperature, which is Demark or rather distinguishes and the temperature, for this particular transition, in this symmetry channel, which is given by this TC.