Dynamics of Classical and Quantum Fields: An Introduction

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Lattice Models
Lecture - 37
Tight Binding Models - II

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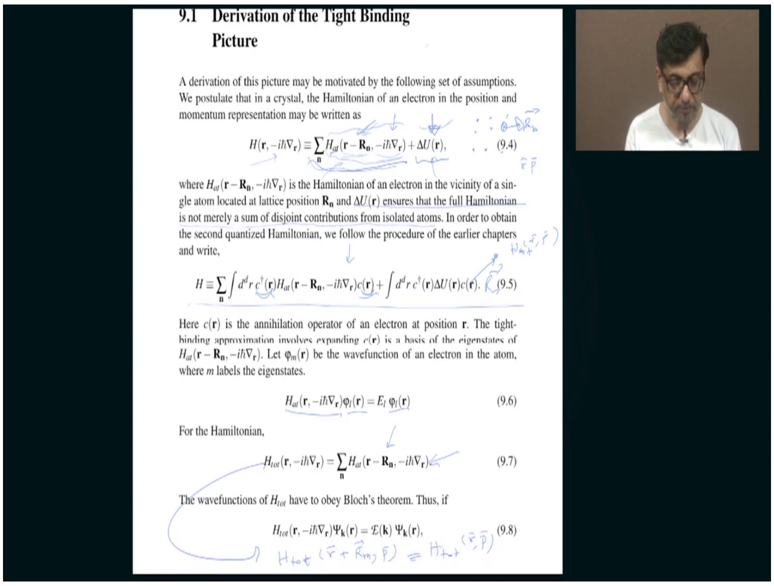

9.1 Derivation of the Tight Binding Picture

A derivation of this picture may be motivated by the following set of assumptions. We postulate that in a crystal, the Hamiltonian of an electron in the position and momentum representation may be written as

$$H(\mathbf{r},-i\hbar\nabla_{\mathbf{r}}) \equiv \sum_{\mathbf{n}} H_{at}(\mathbf{r}-\mathbf{R_n},-i\hbar\nabla_{\mathbf{r}}) + \Delta U(\mathbf{r}), \qquad (9.4)$$

$\vec{R}_n$

$\vec{r}\ \vec{p}$

where $H_{at}(\mathbf{r}-\mathbf{R_n},-i\hbar\nabla_{\mathbf{r}})$ is the Hamiltonian of an electron in the vicinity of a single atom located at lattice position $\mathbf{R_n}$ and $\Delta U(\mathbf{r})$ ensures that the full Hamiltonian is not merely a sum of disjoint contributions from isolated atoms. In order to obtain the second quantized Hamiltonian, we follow the procedure of the earlier chapters and write,

$H_{tot}(\vec{r},\vec{p})$

$$H \equiv \sum_{\mathbf{n}} \int d^d r\, c^{\dagger}(\mathbf{r}) H_{at}(\mathbf{r}-\mathbf{R_n},-i\hbar\nabla_{\mathbf{r}}) c(\mathbf{r}) + \int d^d r\, c^{\dagger}(\mathbf{r}) \Delta U(\mathbf{r}) c(\mathbf{r}). \qquad (9.5)$$

Here $c(\mathbf{r})$ is the annihilation operator of an electron at position $\mathbf{r}$. The tight-binding approximation involves expanding $c(\mathbf{r})$ is a basis of the eigenstates of $H_{at}(\mathbf{r}-\mathbf{R_n},-i\hbar\nabla_{\mathbf{r}})$. Let $\varphi_m(\mathbf{r})$ be the wavefunction of an electron in the atom, where m labels the eigenstates.

$$H_{at}(\mathbf{r},-i\hbar\nabla_{\mathbf{r}})\varphi_l(\mathbf{r}) = E_l\, \varphi_l(\mathbf{r}) \qquad (9.6)$$

For the Hamiltonian,

$$H_{tot}(\mathbf{r},-i\hbar\nabla_{\mathbf{r}}) = \sum_{\mathbf{n}} H_{at}(\mathbf{r}-\mathbf{R_n},-i\hbar\nabla_{\mathbf{r}}) \qquad (9.7)$$

The wavefunctions of H_{tot} have to obey Bloch's theorem. Thus, if

$$H_{tot}(\mathbf{r},-i\hbar\nabla_{\mathbf{r}})\Psi_{\mathbf{k}}(\mathbf{r}) = \mathcal{E}(\mathbf{k})\, \Psi_{\mathbf{k}}(\mathbf{r}), \qquad (9.8)$$

$H_{tot}(\vec{r}+\vec{R}_m, \vec{p}) = H_{tot}(\vec{r},\vec{p})$

Ok. So, today, let us continue our discussion of trying to write down the Tight Binding Hamiltonian in terms of Creation and Annihilation Operators. So, if you recall, in the last class, I started off with this example in terms of position and momentum description that is more familiar to us. So, the idea is that you have a crystal where the atoms are located at this capital letter R n. So, these are the locations of all the atoms.

Now, an electron moving in such a crystal will have a Hamiltonian which is specific to that particular atom, so that means, if, so r is the position of the electron inside the crystal, r minus R n is the position of the electron relative to that particular atom at R n. So, if you are talking only about that particular atom at R n, then the Hamiltonian of the electron will be dependent on the distance of the electron from that particular atom which is r minus R n.

But, it will also clearly depend upon the momentum of the electron which is an operator which is minus i h bar grad r. So, so this is for electron which is experiencing forces from that particular atom. So, then you have to add up over all the atoms. But then you see the point is that it is not true that only, so that means, that the potential energy of an electron is not necessarily only due to that particular atom. So, that there will be other atoms that will also exert forces on this particular electron.

So, the point is that you should also take into account the possibility that there are additional potential energies that are not part of this, right. So, it is not always that you can express the potential energy as the sum of, something due to this particular atom and then that atom and then you it is just a linear sum of that. So, there may be something additional over and above that. So, that is what we call delta U of r, ok.

So, that if you read this sentence it says delta U of r ensures that the full Hamiltonian is not merely a sum of disjoint contributions from isolated atoms. So, you see whatever it is, you can now write the second quantized Hamiltonian in terms of creation and annihilation operator because we have it in terms of position and momentum. So, now, what we did was we said that let us assume that this particular Hamiltonian as a set of completes eigenstates labelled by phi l. So, l is some kind of a shorthand for the orbitals.

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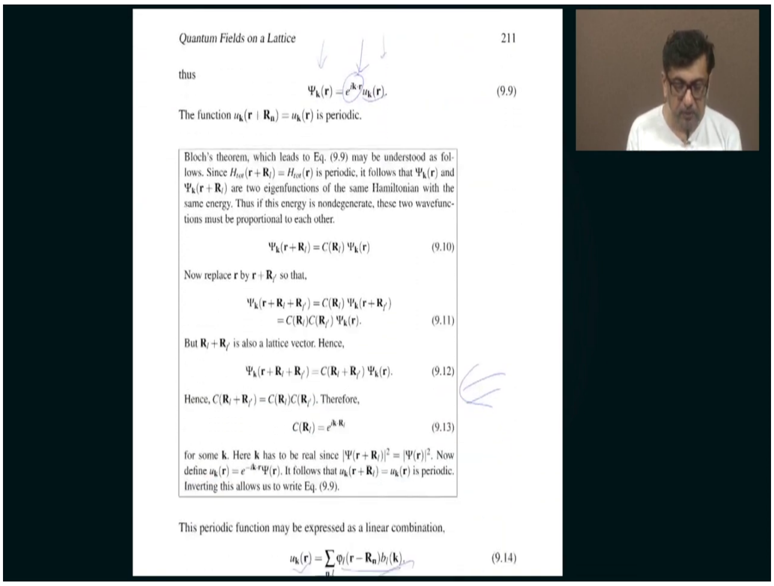

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thus

$$\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}). \quad (9.9)$$

The function $u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_{\mathbf{n}}) = u_{\mathbf{k}}(\mathbf{r})$ is periodic.

Bloch's theorem, which leads to Eq. (9.9) may be understood as follows. Since $H_{tot}(\mathbf{r}+\mathbf{R}_l) = H_{tot}(\mathbf{r})$ is periodic, it follows that $\Psi_{\mathbf{k}}(\mathbf{r})$ and $\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l)$ are two eigenfunctions of the same Hamiltonian with the same energy. Thus if this energy is nondegenerate, these two wavefunctions must be proportional to each other.

$$\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l) = C(\mathbf{R}_l)\,\Psi_{\mathbf{k}}(\mathbf{r}) \quad (9.10)$$

Now replace $\mathbf{r}$ by $\mathbf{r}+\mathbf{R}_{l'}$ so that,

$$\begin{aligned}\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l+\mathbf{R}_{l'}) &= C(\mathbf{R}_l)\,\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_{l'})\\ &= C(\mathbf{R}_l)C(\mathbf{R}_{l'})\,\Psi_{\mathbf{k}}(\mathbf{r}).\end{aligned} \quad (9.11)$$

But $\mathbf{R}_l+\mathbf{R}_{l'}$ is also a lattice vector. Hence,

$$\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l+\mathbf{R}_{l'}) = C(\mathbf{R}_l+\mathbf{R}_{l'})\,\Psi_{\mathbf{k}}(\mathbf{r}). \quad (9.12)$$

Hence, $C(\mathbf{R}_l+\mathbf{R}_{l'}) = C(\mathbf{R}_l)C(\mathbf{R}_{l'})$. Therefore,

$$C(\mathbf{R}_l) = e^{i\mathbf{k}\cdot\mathbf{R}_l} \quad (9.13)$$

for some $\mathbf{k}$. Here $\mathbf{k}$ has to be real since $|\Psi(\mathbf{r}+\mathbf{R}_l)|^2 = |\Psi(\mathbf{r})|^2$. Now define $u_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\Psi(\mathbf{r})$. It follows that $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l) = u_{\mathbf{k}}(\mathbf{r})$ is periodic. Inverting this allows us to write Eq. (9.9).

This periodic function may be expressed as a linear combination,

$$u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{n},l} \varphi_l(\mathbf{r}-\mathbf{R}_{\mathbf{n}})b_l(\mathbf{k}), \quad (9.14)$$

So, now, the idea is that you can then having written down for one atom, you can then construct for all the atoms put together. Because then for all the atoms put together the Hamiltonian becomes specially periodic, where the period is determined by the latest vector R n. So; that means, it obeys Bloch's theorem, so that means, the wave functions need not be periodic, but they are related to periodic functions.

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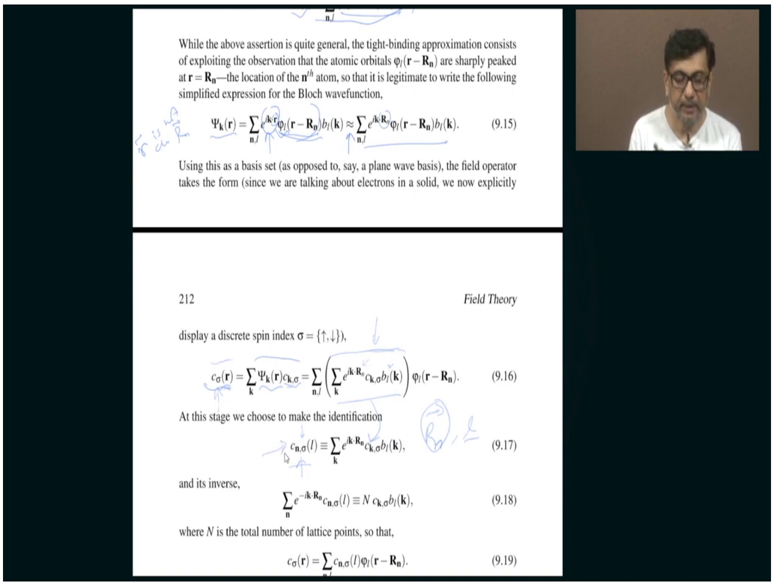

While the above assertion is quite general, the tight-binding approximation consists of exploiting the observation that the atomic orbitals $\varphi_l(\mathbf{r}-\mathbf{R_n})$ are sharply peaked at $\mathbf{r}=\mathbf{R_n}$—the location of the $\mathbf{n}^{th}$ atom, so that it is legitimate to write the following simplified expression for the Bloch wavefunction,

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{n},l} e^{i\mathbf{k}\cdot\mathbf{r}}\varphi_l(\mathbf{r}-\mathbf{R_n})b_l(\mathbf{k}) \approx \sum_{\mathbf{n},l} e^{i\mathbf{k}\cdot\mathbf{R_n}}\varphi_l(\mathbf{r}-\mathbf{R_n})b_l(\mathbf{k}). \tag{9.15}$$

Using this as a basis set (as opposed to, say, a plane wave basis), the field operator takes the form (since we are talking about electrons in a solid, we now explicitly

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display a discrete spin index $\sigma = \{\uparrow,\downarrow\}$),

$$c_\sigma(\mathbf{r}) = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{r})c_{\mathbf{k},\sigma} = \sum_{\mathbf{n},l}\left(\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R_n}}c_{\mathbf{k},\sigma}b_l(\mathbf{k})\right)\varphi_l(\mathbf{r}-\mathbf{R_n}). \tag{9.16}$$

At this stage we choose to make the identification

$$c_{\mathbf{n},\sigma}(l) \equiv \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R_n}}c_{\mathbf{k},\sigma}b_l(\mathbf{k}), \tag{9.17}$$

and its inverse,

$$\sum_{\mathbf{n}} e^{-i\mathbf{k}\cdot\mathbf{R_n}}c_{\mathbf{n},\sigma}(l) \equiv N\, c_{\mathbf{k},\sigma}b_l(\mathbf{k}), \tag{9.18}$$

where N is the total number of lattice points, so that,

$$c_\sigma(\mathbf{r}) = \sum_{\mathbf{n},l} c_{\mathbf{n},\sigma}(l)\varphi_l(\mathbf{r}-\mathbf{R_n}). \tag{9.19}$$

So, so bottom line is that you can then rewrite your wave functions of the combined Hamiltonian of all the atoms put together in terms of these Bloch states. And we said that these Bloch state because the tight binding method assumes that the wave functions of an electron for particular atom are strongly localized near that particular atom.

So, that is what tight binding means. So, tight binding means the electron is typically tightly bound to an a given atom. So, then it can occasionally there is a small probability that it can then hop to the neighbouring one. So, that is the mental picture that we have.

So, now, you see the second quantized annihilation operator can always be; so, because now we have a complete basis here in terms of the Bloch states which are then in turn constructed from the orbitals of the individual atom wave functions. So, having done that, we can now re express the annihilation operator in terms of the Bloch states. So, when you do that you encounter this operator.

So, this operator basically tells you that there is a linear combination of the annihilation operator written in terms of the momentum states which rather has the interpretation of being the coefficient of that particular corresponding atoms annihilation operator. So, you see this is the annihilation operator for an electron in the entire crystal, but this after having summed over k, so once you sum over k the free labels are n and l.

So, what that means, is basically this particular summation is basically this. So, which represents the annihilation of an electron at the atom labelled by R n, so the that means, it represents the annihilation of an electron at the atom labelled by R n and being present in the orbital labelled by s. So that means, this operator what it does is it annihilates that specific electron which happens to belong to the atom labelled by R n.

So, there is an atom sitting at R n and there is there are electrons associated with that. So, the electron that is in orbital l is being annihilated, ok. And then that to that specific l. So, this for kind of uniquely pins down the electron because once you, so then there is a spin projection also, so you have a spin projection, you have the orbital index. So, that orbital can be, you know some say if you are thinking of hydrogen atom, it will be n, l and m.

That means, it will be principal orbital angle, I mean orbital quantum number, principal quantum number and the magnetic quantum number. So, that l can be shorthand for 3 numbers like n, l and m. But I have just written n, l, does not mean it is that only that orbital quantum number. l is shorthand for any discrete set of indices that uniquely and completely specifies the orbital that is we are thinking of, ok. So, it is not necessarily one number. It can be a bunch of numbers.

So, basically, that l put together with the spin projection sigma which is up or down, together with n, which is the nth atom at which you are annihilating the electron, you see uniquely specifies what it means to annihilate an electron with those qualities, so with those properties.

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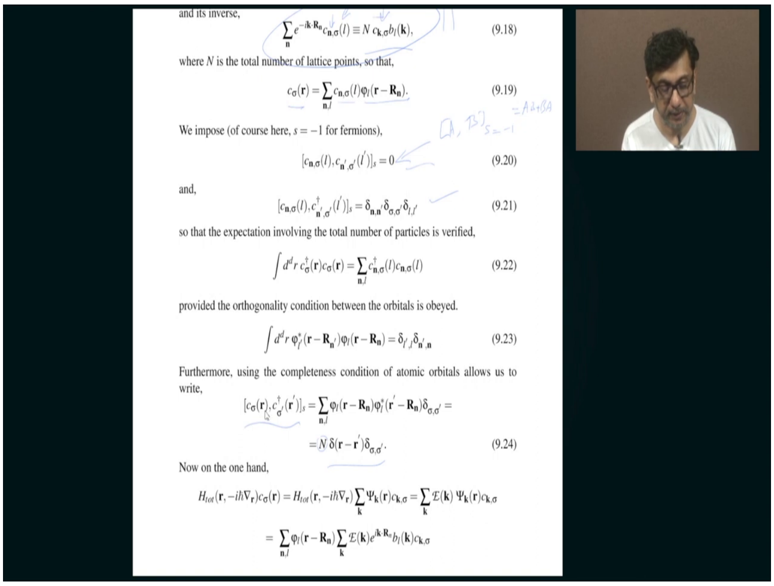

and its inverse,

$$\sum_{\mathbf{n}} e^{-i\mathbf{k}\cdot\mathbf{R_n}} c_{\mathbf{n},\sigma}(l) \equiv N\, c_{\mathbf{k},\sigma} b_l(\mathbf{k}), \tag{9.18}$$

where N is the total number of lattice points, so that,

$$c_\sigma(\mathbf{r}) = \sum_{\mathbf{n},l} c_{\mathbf{n},\sigma}(l)\varphi_l(\mathbf{r}-\mathbf{R_n}). \tag{9.19}$$

$[A, B]_{s=-1} = AB+BA$

We impose (of course here, $s = -1$ for fermions),

$$[c_{\mathbf{n},\sigma}(l), c_{\mathbf{n}',\sigma'}(l')]_s = 0 \tag{9.20}$$

and,

$$[c_{\mathbf{n},\sigma}(l), c^\dagger_{\mathbf{n}',\sigma'}(l')]_s = \delta_{\mathbf{n},\mathbf{n}'}\delta_{\sigma,\sigma'}\delta_{l,l'} \tag{9.21}$$

so that the expectation involving the total number of particles is verified,

$$\int d^d r\, c^\dagger_\sigma(\mathbf{r}) c_\sigma(\mathbf{r}) = \sum_{\mathbf{n},l} c^\dagger_{\mathbf{n},\sigma}(l) c_{\mathbf{n},\sigma}(l) \tag{9.22}$$

provided the orthogonality condition between the orbitals is obeyed.

$$\int d^d r\, \varphi^*_{l'}(\mathbf{r}-\mathbf{R}_{\mathbf{n}'})\varphi_l(\mathbf{r}-\mathbf{R_n}) = \delta_{l',l}\delta_{\mathbf{n}',\mathbf{n}} \tag{9.23}$$

Furthermore, using the completeness condition of atomic orbitals allows us to write,

$$[c_\sigma(\mathbf{r}), c^\dagger_{\sigma'}(\mathbf{r}')]_s = \sum_{\mathbf{n},l} \varphi_l(\mathbf{r}-\mathbf{R_n})\varphi^*_l(\mathbf{r}'-\mathbf{R_n})\delta_{\sigma,\sigma'} =$$

$$= N\,\delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}. \tag{9.24}$$

Now on the one hand,

$$H_{tot}(\mathbf{r}, -i\hbar\nabla_{\mathbf{r}})c_\sigma(\mathbf{r}) = H_{tot}(\mathbf{r}, -i\hbar\nabla_{\mathbf{r}})\sum_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{r})c_{\mathbf{k},\sigma} = \sum_{\mathbf{k}} \mathcal{E}(\mathbf{k})\,\Psi_{\mathbf{k}}(\mathbf{r})c_{\mathbf{k},\sigma}$$

$$= \sum_{\mathbf{n},l} \varphi_l(\mathbf{r}-\mathbf{R_n})\sum_{\mathbf{k}} \mathcal{E}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}_n} b_l(\mathbf{k})c_{\mathbf{k},\sigma}$$

So, having said that, now we can also ask the inverse question, suppose, I want to know how to annihilate an electron with momentum k, right. So, then how would you do that? So, I will simply invert this relation. So, you see any transform has no value unless I know how to invert it also. So, inversion is extremely critical. So, no transform is useful unless you know how to invert. So, the claim is that the way to invert this transform is to do this.

So, you can easily convince yourself this is correct by you know just take; see you have this formula here in change this k to k dash because then it will become a dummy index where you are summing over. Then, insert this formula here, right. And then, you sum over n you will get this result, ok. So, you can see that this is an identity. So, this tells you how to annihilate an electron with momentum k with spin projection sigma, ok.

So, bottom line is that, so this is I just pointed this out that you can do this, but now let us get back to this. So, this c sigma r which annihilates an electron at some point r in the entire crystal can now be written in terms of the basis functions of the individual atoms times localized annihilation operator. That means, an annihilation which annihilates an electron in a particular atom in a certain orbital with a certain spin projection, ok.

So, now the claim is that if I impose, so now, I want to understand the commutation rules obeyed by; that means, I want to ensure that the anti-commutation rules for the electrons are properly obeyed. So, that is guaranteed because we are going to assume that the basis functions are orthonormal and complete. So, if the basis functions phi l are orthonormal and complete the that is both necessary and sufficient to ensure the fermion commutation rules of these annihilation operators.

So, we can just go ahead and impose these commutation rules. And these are the s; remember that if s is minus 1 A commutator B with a s equal to minus 1, means it is AB plus BA, right. Otherwise it is AB minus BA for Bosons. So, bottom line is that this is we are going to impose this. Suppose, you impose this, then you can convince yourself that the s anti-commutation rules for the fermions are correctly given as being proportional to the Dirac delta function, ok.

So, you can choose to divide by 1 by square root of n if you do not want this n sitting there, ok. You can redefine your sigma with a 1 by square root of n, maybe we should have done that. So, if I had defined it in terms of 1 by square root of n, this would not have come. So, then it would be clearly anti-commutation of c c dagger is exactly Dirac delta.

You see the that is why it is you might think that I am being bit sloppy. But it is not sloppiness, if I tell you how to do the forward transform and the inverse transform both. So, when I do both and things are mutually consistent and if I insert one into the other, if it leads to an identity, then it is certainly not sloppy because it is absolutely rigorously correct.

It becomes sloppy only if I show you one only the forward transform and then I do not tell you what the reverse is, and then I just proceed. Then, it becomes ambiguous because then somebody will pick up some other convention from some other book and it will lead to an inconsistency. But here that is the reason why I have taken the trouble to show you both the forward transform and the inverse transform, so that the chances of me going wrong are absolutely 0, alright.

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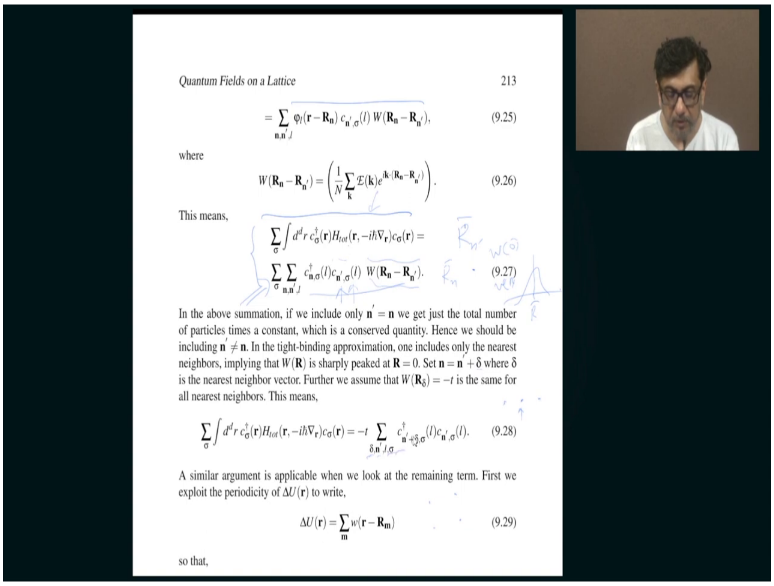

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$$= \sum_{\mathbf{n},\mathbf{n}',l} \varphi_l(\mathbf{r}-\mathbf{R}_\mathbf{n})\, c_{\mathbf{n}',\sigma}(l)\, W(\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'}), \qquad (9.25)$$

where

$$W(\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'}) = \left(\frac{1}{N}\sum_{\mathbf{k}} \mathcal{E}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'})}\right). \qquad (9.26)$$

This means,

$$\sum_\sigma \int d^d r\, c^\dagger_\sigma(\mathbf{r}) H_{tot}(\mathbf{r},-i\hbar\nabla_\mathbf{r}) c_\sigma(\mathbf{r}) =$$
$$\sum_\sigma \sum_{\mathbf{n},\mathbf{n}',l} c^\dagger_{\mathbf{n},\sigma}(l) c_{\mathbf{n}',\sigma}(l)\; W(\mathbf{R}_\mathbf{n}-\mathbf{R}_{\mathbf{n}'}). \qquad (9.27)$$

In the above summation, if we include only $\mathbf{n}' = \mathbf{n}$ we get just the total number of particles times a constant, which is a conserved quantity. Hence we should be including $\mathbf{n}' \neq \mathbf{n}$. In the tight-binding approximation, one includes only the nearest neighbors, implying that $W(\mathbf{R})$ is sharply peaked at $\mathbf{R} = 0$. Set $\mathbf{n} = \mathbf{n}' + \delta$ where δ is the nearest neighbor vector. Further we assume that $W(\mathbf{R}_\delta) = -t$ is the same for all nearest neighbors. This means,

$$\sum_\sigma \int d^d r\, c^\dagger_\sigma(\mathbf{r}) H_{tot}(\mathbf{r},-i\hbar\nabla_\mathbf{r}) c_\sigma(\mathbf{r}) = -t \sum_{\delta,\mathbf{n}',l,\sigma} c^\dagger_{\mathbf{n}'+\delta,\sigma}(l) c_{\mathbf{n}',\sigma}(l). \qquad (9.28)$$

A similar argument is applicable when we look at the remaining term. First we exploit the periodicity of $\Delta U(\mathbf{r})$ to write,

$$\Delta U(\mathbf{r}) = \sum_\mathbf{m} w(\mathbf{r}-\mathbf{R}_\mathbf{m}) \qquad (9.29)$$

so that,

So, the point is that now we can go ahead and calculate the Hamiltonian the second quantized form namely this. So, for that I have to first understand how the total Hamiltonian for all the atoms put together acts on the annihilation operator for the electrons in the crystal.

So, if this H total acting on the Bloch states gives you the energy of energy of the electron in the crystal, so which depends on the momentum. And then, notice that I have then re-express the Bloch states in terms of the original orbitals and I have used the fact that it is tightly bound.

So, I have replaced r by R n here and so on and so forth. So, then I end up with this result. Then, I use the completeness orthonormality, and then I do this integral, ok. So, once I do this integral, so I will I will leave you to verify some of these steps on your own because it is really pointless for me to explain all the steps. Because it is also your responsibility to ensure that you are following all the steps. Because you see quite a number of steps are displayed and it is really important for you to fill in the small remaining number of steps.

So, the bottom line is that once you integrate, you end up with this new interpretation for the Hamiltonian of the entire crystal. So, what is this interpretation? You see it has this interpretation that it is given by; so, the total energy of the system. So, we will come to that delta U later. So, remember it is not really still the total energy because there is a delta U that is talks about the extra you know it is not merely a disjoint sum of the Hamiltonians from all the different atoms. There could be something extra.

But the analysis of that extra term is also very analogous to what I have already done here because even the extra term is also going to be specially periodic, because after all it has to represent an electron moving in a periodic crystal. So, because anything that is periodic will have a very similar mathematical consequence. So, bottom line is that as far as the term that corresponds to the total energy of the atoms put together is concerned it can certainly be written in this way. And what is this way? So, what does it say?

So, it basically says that the energy of the electrons, the total energy of all the electrons of all the atoms when you add them all up, it is going to consist of, so it amounts to annihilating an electron at some other location R n dash, ok. And then creating it at some other location R n, and then you multiply that, so that means, that when you do that you see, so what this is doing is that the Hamiltonian of the system now in this language corresponds to annihilating an electron which belongs to some atom sitting at R n dash, ok.

And so that means, you remove an electron from an atom that sitting at R n dash, and then you insert that electron into an atom that is sitting at R n. So, that is pretty much what this says. So, it says that it amounts to doing that. And there is an energy cost or gain or whatever it is depending on the sign, associated with doing that. And that energy is determined by or we have taken that to be W of R n minus R n dash because clearly it depends on the distance between the two atoms.

So, you can see already here that it has this interpretation of hopping. So, what was originally a Hamiltonian consisting of you know position and momentum operator. So, remember there was this H a t which was the starting point. So, this had position and momentum. So, the position and momentum description has given way to this hopping description. So, now, we have re-expressed the entire Hamiltonian in terms of processes that correspond to hopping. So, the kinetic energy of the system in some sense now represents the hopping of an electron from one atom to another, ok.

So, the idea is that, so we are going to assume that this w n is sharply peaked at 0. So, that means, W 0 is the maximum. So, it is sharply peaked W R will be sharply peaked at R equal to 0, ok. So, if that is the case then clearly n dash equals n is the dominant contribution, but that is uninteresting because that corresponds to the total number of particles, ok.

So, the interesting term comes from the next term. So, the next most important contribution to this summation comes when R n is, R n dash is not close not equal to R n, but is as close to R n as possible. So, that is called the nearest neighbor. So, we are going to assume therefore, that the most dominant contribution which is not proportional to an identity comes from the nearest neighbors. So, that means, the n dash is a nearest neighbor to n. So, that means, n is equal to n dash plus delta where delta is the distance between nearest neighbors.

So, remember, I told you that already in one dimension there are two nearest neighbors one to the left, one to the right. So, if this is your atom of interest, its nearest neighbor there is one to the left, one to the right. So, in two-dimension it can be even more interesting. So, that means, you can have many nearest neighbors. So, the whole idea is that whatever it is that you have to sum over all the nearest neighbors. So, you have to sum over them.

So, we are going to assume that n is n dash plus delta and then you sum over all the nearest neighbour, then you sum over all n dash and then you of course, sum over the orbitals and the spin projections.

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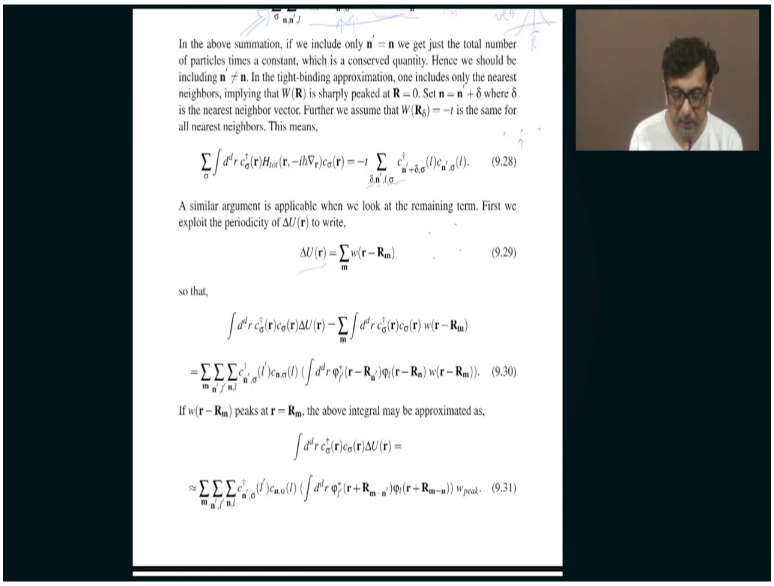

In the above summation, if we include only $\mathbf{n}' = \mathbf{n}$ we get just the total number of particles times a constant, which is a conserved quantity. Hence we should be including $\mathbf{n}' \neq \mathbf{n}$. In the tight-binding approximation, one includes only the nearest neighbors, implying that $W(\mathbf{R})$ is sharply peaked at $\mathbf{R} = 0$. Set $\mathbf{n} = \mathbf{n}' + \delta$ where δ is the nearest neighbor vector. Further we assume that $W(\mathbf{R}_\delta) = -t$ is the same for all nearest neighbors. This means,

$$\sum_{\sigma} \int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) H_{tot}(\mathbf{r}, -i\hbar\nabla_{\mathbf{r}}) c_{\sigma}(\mathbf{r}) = -t \sum_{\delta, \mathbf{n}', l, \sigma} c^{\dagger}_{\mathbf{n}'+\delta,\sigma}(l) c_{\mathbf{n}',\sigma}(l). \qquad (9.28)$$

A similar argument is applicable when we look at the remaining term. First we exploit the periodicity of $\Delta U(\mathbf{r})$ to write,

$$\Delta U(\mathbf{r}) = \sum_{\mathbf{m}} w(\mathbf{r} - \mathbf{R}_{\mathbf{m}}) \qquad (9.29)$$

so that,

$$\int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) c_{\sigma}(\mathbf{r}) \Delta U(\mathbf{r}) = \sum_{\mathbf{m}} \int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) c_{\sigma}(\mathbf{r})\, w(\mathbf{r} - \mathbf{R}_{\mathbf{m}})$$

$$= \sum_{\mathbf{m}} \sum_{\mathbf{n}', l'} \sum_{\mathbf{n}, l} c^{\dagger}_{\mathbf{n}',\sigma}(l') c_{\mathbf{n},\sigma}(l) \left(\int d^d r\, \varphi^{*}_{l'}(\mathbf{r} - \mathbf{R}_{\mathbf{n}'}) \varphi_l(\mathbf{r} - \mathbf{R}_{\mathbf{n}})\, w(\mathbf{r} - \mathbf{R}_{\mathbf{m}}) \right). \qquad (9.30)$$

If $w(\mathbf{r} - \mathbf{R}_{\mathbf{m}})$ peaks at $\mathbf{r} = \mathbf{R}_{\mathbf{m}}$, the above integral may be approximated as,

$$\int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) c_{\sigma}(\mathbf{r}) \Delta U(\mathbf{r}) =$$

$$\approx \sum_{\mathbf{m}} \sum_{\mathbf{n}', l'} \sum_{\mathbf{n}, l} c^{\dagger}_{\mathbf{n}',\sigma}(l') c_{\mathbf{n},\sigma}(l) \left(\int d^d r\, \varphi^{*}_{l'}(\mathbf{r} + \mathbf{R}_{\mathbf{m}-\mathbf{n}'}) \varphi_l(\mathbf{r} + \mathbf{R}_{\mathbf{m}-\mathbf{n}}) \right) w_{peak}. \qquad (9.31)$$

So, you see it so happens that even the extra term that we had omitted till now; that means, that what is that extra term basically it corresponds to the possible including the possibility that the energy of the electron may not be merely a disjoint sum of the energy of all the individual atoms. It can be due to something else. So, I mean it can be due to all the atoms put together can you know contribute to the energy or the potential energy of the electron in a different way. So, even if that is the case you will see that it similarly leads to the same type of hopping, ok.

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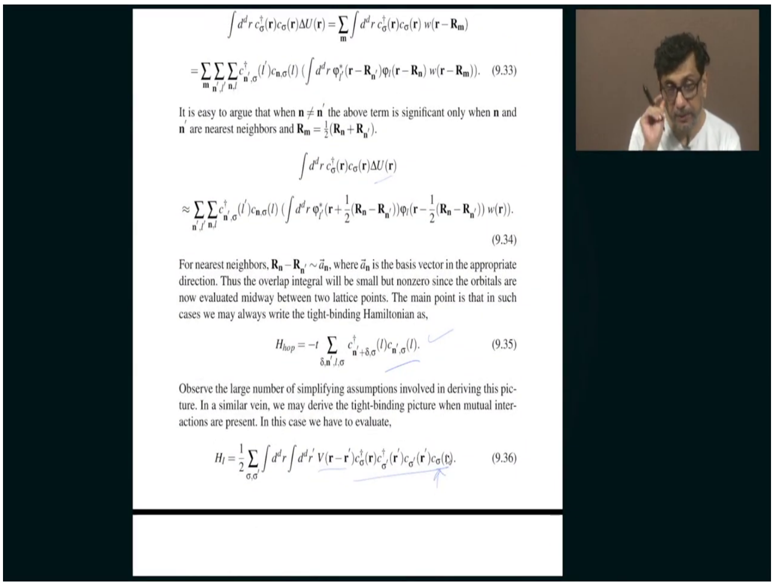

$$\int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) c_{\sigma}(\mathbf{r}) \Delta U(\mathbf{r}) = \sum_{\mathbf{m}} \int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) c_{\sigma}(\mathbf{r})\, w(\mathbf{r} - \mathbf{R}_{\mathbf{m}})$$

$$= \sum_{\mathbf{m}} \sum_{\mathbf{n}', l'} \sum_{\mathbf{n}, l} c^{\dagger}_{\mathbf{n}',\sigma}(l') c_{\mathbf{n},\sigma}(l) \left(\int d^d r\, \varphi^{*}_{l'}(\mathbf{r} - \mathbf{R}_{\mathbf{n}'}) \varphi_l(\mathbf{r} - \mathbf{R}_{\mathbf{n}})\, w(\mathbf{r} - \mathbf{R}_{\mathbf{m}}) \right). \qquad (9.33)$$

It is easy to argue that when $\mathbf{n} \neq \mathbf{n}'$ the above term is significant only when $\mathbf{n}$ and $\mathbf{n}'$ are nearest neighbors and $\mathbf{R}_{\mathbf{m}} = \frac{1}{2}(\mathbf{R}_{\mathbf{n}} + \mathbf{R}_{\mathbf{n}'})$.

$$\int d^d r\, c^{\dagger}_{\sigma}(\mathbf{r}) c_{\sigma}(\mathbf{r}) \Delta U(\mathbf{r})$$

$$\approx \sum_{\mathbf{n}', l'} \sum_{\mathbf{n}, l} c^{\dagger}_{\mathbf{n}',\sigma}(l') c_{\mathbf{n},\sigma}(l) \left(\int d^d r\, \varphi^{*}_{l'}(\mathbf{r} + \frac{1}{2}(\mathbf{R}_{\mathbf{n}} - \mathbf{R}_{\mathbf{n}'})) \varphi_l(\mathbf{r} - \frac{1}{2}(\mathbf{R}_{\mathbf{n}} - \mathbf{R}_{\mathbf{n}'}))\, w(\mathbf{r}) \right). \qquad (9.34)$$

For nearest neighbors, $\mathbf{R}_{\mathbf{n}} - \mathbf{R}_{\mathbf{n}'} \sim \vec{a}_{\mathbf{n}}$, where $\vec{a}_{\mathbf{n}}$ is the basis vector in the appropriate direction. Thus the overlap integral will be small but nonzero since the orbitals are now evaluated midway between two lattice points. The main point is that in such cases we may always write the tight-binding Hamiltonian as,

$$H_{hop} = -t \sum_{\delta, \mathbf{n}', l, \sigma} c^{\dagger}_{\mathbf{n}'+\delta,\sigma}(l) c_{\mathbf{n}',\sigma}(l). \qquad (9.35)$$

Observe the large number of simplifying assumptions involved in deriving this picture. In a similar vein, we may derive the tight-binding picture when mutual interactions are present. In this case we have to evaluate,

$$H_I = \frac{1}{2} \sum_{\sigma, \sigma'} \int d^d r \int d^d r'\, V(\mathbf{r} - \mathbf{r}') c^{\dagger}_{\sigma}(\mathbf{r}) c^{\dagger}_{\sigma'}(\mathbf{r}') c_{\sigma'}(\mathbf{r}') c_{\sigma}(\mathbf{r}). \qquad (9.36)$$

So, if you redo the analysis for that delta U it also leads to hopping. So, bottom line is this hopping interpretation is extremely generic and natural when you re-express your Hamiltonian which was originally in terms of position and momentum, you re-express it in terms of the tight binding picture.

So, here the assumption is that each electron is tightly bound to a given atom. So that means, the all the wave functions sharply peaked around the atoms. And so the natural description is in terms of the, so the kinetic motion through the crystal is possible only through this mechanism of hopping.

So, that to hopping into the to the nearest neighbors. So, there is a small chance that an atom I mean electron tied to a certain atom will kind of quantum mechanically tunnel through and cross the barrier and reach the neighboring atom. And the chance is that it will go further are very slim. So, that is the whole idea about when you are talking about hopping of nearest neighbors. So, now we had restricted ourselves only to studying atom, I mean electrons that do not interact with each other.

They only interact with their atoms. So, that means, they interact with the positive charges, they do not interact with each other. But we can also include the idea that they interact with each other.

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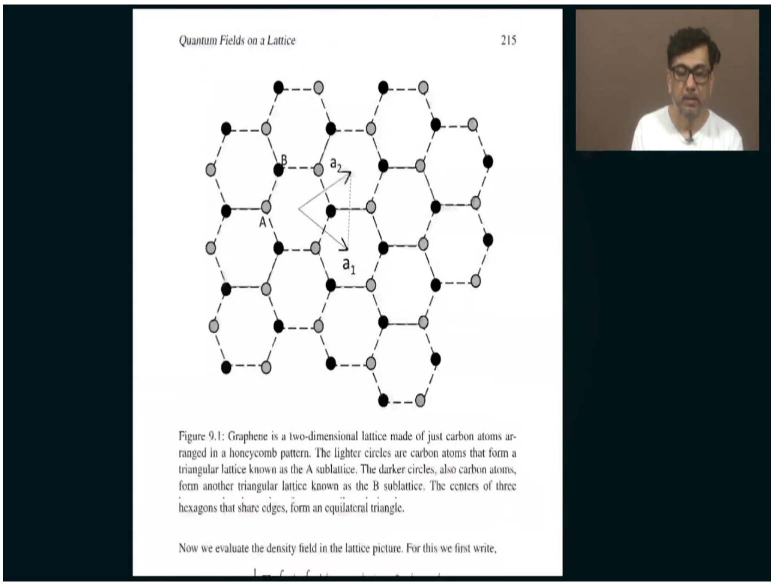

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Figure 9.1: Graphene is a two-dimensional lattice made of just carbon atoms arranged in a honeycomb pattern. The lighter circles are carbon atoms that form a triangular lattice known as the A sublattice. The darker circles, also carbon atoms, form another triangular lattice known as the B sublattice. The centers of three hexagons that share edges, form an equilateral triangle.

Now we evaluate the density field in the lattice picture. For this we first write, So, how do you do that? You simply introduce this type of two body interaction term. So, usually if the charged particles you expect this to be the coulomb term that is e squared by r types.

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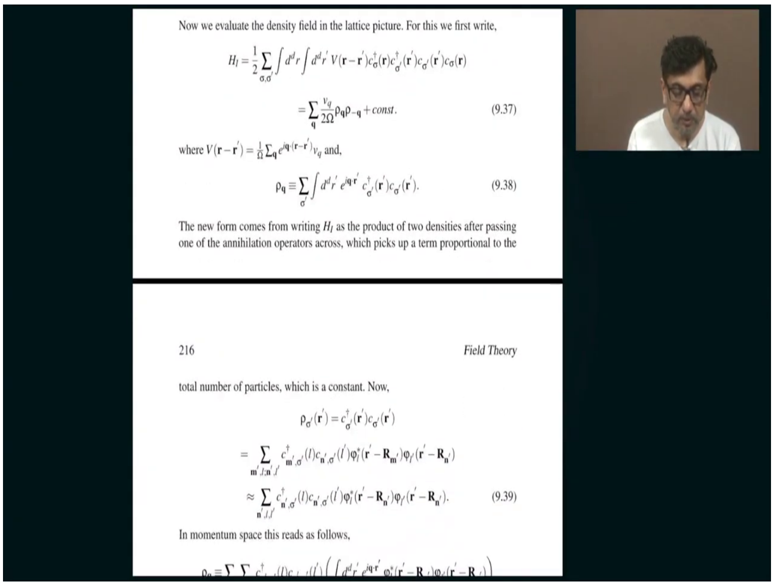

Now we evaluate the density field in the lattice picture. For this we first write,

$$H_I = \frac{1}{2}\sum_{\sigma,\sigma'}\int d^dr\int d^dr'\, V(\mathbf{r}-\mathbf{r}')c^{\dagger}_{\sigma}(\mathbf{r})c^{\dagger}_{\sigma'}(\mathbf{r}')c_{\sigma'}(\mathbf{r}')c_{\sigma}(\mathbf{r})$$

$$= \sum_{\mathbf{q}}\frac{v_q}{2\Omega}\rho_{\mathbf{q}}\rho_{-\mathbf{q}} + const. \tag{9.37}$$

where $V(\mathbf{r}-\mathbf{r}') = \frac{1}{\Omega}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}v_q$ and,

$$\rho_{\mathbf{q}} \equiv \sum_{\sigma'}\int d^dr'\, e^{i\mathbf{q}\cdot\mathbf{r}'}\, c^{\dagger}_{\sigma'}(\mathbf{r}')c_{\sigma'}(\mathbf{r}'). \tag{9.38}$$

The new form comes from writing H_I as the product of two densities after passing one of the annihilation operators across, which picks up a term proportional to the

total number of particles, which is a constant. Now,

$$\rho_{\sigma'}(\mathbf{r}') = c^{\dagger}_{\sigma'}(\mathbf{r}')c_{\sigma'}(\mathbf{r}')$$

$$= \sum_{\mathbf{m}',l;\mathbf{n}',l'} c^{\dagger}_{\mathbf{m}',\sigma'}(l)c_{\mathbf{n}',\sigma'}(l')\varphi^{*}_{l}(\mathbf{r}'-\mathbf{R}_{\mathbf{m}'})\varphi_{l'}(\mathbf{r}'-\mathbf{R}_{\mathbf{n}'})$$

$$\approx \sum_{\mathbf{n}',l,l'} c^{\dagger}_{\mathbf{n}',\sigma'}(l)c_{\mathbf{n}',\sigma'}(l')\varphi^{*}_{l}(\mathbf{r}'-\mathbf{R}_{\mathbf{n}'})\varphi_{l'}(\mathbf{r}'-\mathbf{R}_{\mathbf{n}'}). \tag{9.39}$$

In momentum space this reads as follows,

So, but whatever it is you can re-express, so just like we did with the hopping, the kinetic term, we can re-express this in terms of the Bloch states, the Bloch wave functions and rewrite this whole thing in terms of the Bloch states.

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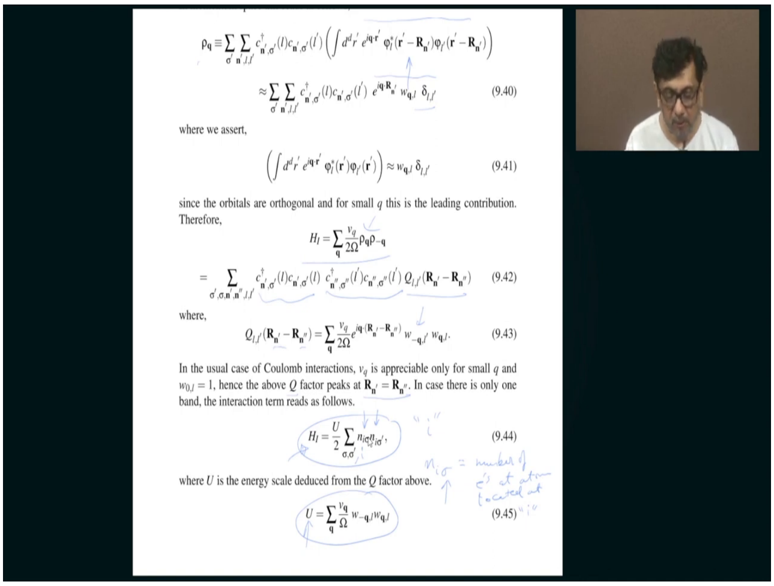

$$\rho_{\mathbf{q}} \equiv \sum_{\sigma'}\sum_{\mathbf{n}',l,l'} c^{\dagger}_{\mathbf{n}',\sigma'}(l)c_{\mathbf{n}',\sigma'}(l')\left(\int d^dr'\, e^{i\mathbf{q}\cdot\mathbf{r}'}\,\varphi^{*}_{l}(\mathbf{r}'-\mathbf{R}_{\mathbf{n}'})\varphi_{l'}(\mathbf{r}'-\mathbf{R}_{\mathbf{n}'})\right)$$

$$\approx \sum_{\sigma'}\sum_{\mathbf{n}',l,l'} c^{\dagger}_{\mathbf{n}',\sigma'}(l)c_{\mathbf{n}',\sigma'}(l')\, e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}'}}\, w_{\mathbf{q},l}\,\delta_{l,l'} \tag{9.40}$$

where we assert,

$$\left(\int d^dr'\, e^{i\mathbf{q}\cdot\mathbf{r}'}\,\varphi^{*}_{l}(\mathbf{r}')\varphi_{l'}(\mathbf{r}')\right) \approx w_{\mathbf{q},l}\,\delta_{l,l'} \tag{9.41}$$

since the orbitals are orthogonal and for small q this is the leading contribution. Therefore,

$$H_I = \sum_{\mathbf{q}}\frac{v_q}{2\Omega}\rho_{\mathbf{q}}\rho_{-\mathbf{q}}$$

$$= \sum_{\sigma',\sigma,\mathbf{n}',\mathbf{n}'',l,l'} c^{\dagger}_{\mathbf{n}',\sigma'}(l)c_{\mathbf{n}',\sigma'}(l)\; c^{\dagger}_{\mathbf{n}'',\sigma''}(l')c_{\mathbf{n}'',\sigma''}(l')\; Q_{l,l'}(\mathbf{R}_{\mathbf{n}'}-\mathbf{R}_{\mathbf{n}''}) \tag{9.42}$$

where,

$$Q_{l,l'}(\mathbf{R}_{\mathbf{n}'}-\mathbf{R}_{\mathbf{n}''}) = \sum_{\mathbf{q}}\frac{v_q}{2\Omega}e^{i\mathbf{q}\cdot(\mathbf{R}_{\mathbf{n}'}-\mathbf{R}_{\mathbf{n}''})}\, w_{-\mathbf{q},l'}\, w_{\mathbf{q},l}. \tag{9.43}$$

In the usual case of Coulomb interactions, v_q is appreciable only for small q and $w_{0,l} = 1$, hence the above Q factor peaks at $\mathbf{R}_{\mathbf{n}'} = \mathbf{R}_{\mathbf{n}''}$. In case there is only one band, the interaction term reads as follows.

$$H_I = \frac{U}{2}\sum_{\sigma,\sigma',i} n_{i\sigma}n_{i\sigma'}, \tag{9.44}$$

"i"

$n_{i\sigma}$ = number of e's at atom located at "i"

where U is the energy scale deduced from the Q factor above.

$$U = \sum_{\mathbf{q}}\frac{v_{\mathbf{q}}}{\Omega}\, w_{-\mathbf{q},l}w_{\mathbf{q},l} \tag{9.45}$$

So, the idea is that you see, again it is a lot of tedious algebra and I will allow you to go over the details. So, the idea is that you rewrite this in terms of the dense. So, it is a density interaction, ok. So, the density now can be written in terms of the orbitals. So, in terms of creating and annihilating electrons that are sitting in different orbitals. So, here clearly you are going to be, because it you see you are creating and annihilating. So, at the same point in space, so that is c dagger r c r, ok. So, those things are same; so, that the dominant terms will already be.

So, you see remember that we ignored the m dash equal to n dash term in the case of hopping because that led to a trivial additive term proportional to the total number of particles, but here it is not going to do that. So, it is not going to trivially lead to, so that that itself will contribute. So, we can actually first try out the most obvious dominant contribution where m dash is equal to n dash, ok. So, in the case of hopping that led to a trivial additive constant which was uninteresting. But here it will not lead to something, it will not be very trivial.

So, the idea is that you re-express your rho q which is your Fourier transform density in terms of these integrals which involve the overlap between the orbitals l and l dash, ok of this particular atom. So, the idea is that; so, when you do that you get this sort of I mean; so, not surprisingly you will of course, be forced to conclude these orbitals also have to be equal. I could have easily assumed that right from the start, but then I have made it slightly more general by not assuming that.

So, bottom line is that you see when you rewrite this in terms of these operators, you will end up getting this sort of an idea. So, that means, you will get this result. So, what this implies is that you are actually, so this Q factor peaks at R n minus R n dash equals R n double dash. So, I know that there is a whole lot of unnecessary, seemingly unnecessary notation here. It is just that I want to get to this result as quickly as possible and perhaps I am not doing a very good job.

But you see it this is this procedure is necessary because, remember that originally the description is in terms of position and momentum operators. So, I have to gradually transform those that description. So, that I end up with a description in terms of electrons hopping from a lattice point to another and not; so, the idea that an electron can reside in between two lattice points is meaningless in this tight binding picture.

So, the electron is either at one lattice point or at some other lattice point. So, it simply hops from one to the other. So, it there is no concept of an electron being somewhere in between. So, the idea is that we have to arrive at that sort of a picture systematically from because that picture is a priori not obvious. So, if you look at space as a continuous set of points then there is no reason to believe that an electron can be somewhere in between two lattice points.

But now given that it; so how do we arrive at the lattice description from a continuum description is the fundamental question we are trying to address. So, it is achieved through a series of approximations. So, the most important of them being that the tight binding approximation; that means, an electron is tightly bound to a given atom. It occasionally hops, so there is a small probability for it to tunnel through and increase the other atom.

So, if you accept that sort of a progression of ideas, then you can easily convince yourself that the interaction between electrons, so the potential energy between, so the coulomb potential energy for example, can be rewritten in terms of a certain integral. So, that means, it can be re-expressed in terms of an integral over the, so, you can re-express it. So, this is your w q. So, that is an that is an overlap between the orbitals if you like. So, it tells you how the what is the energy cost to putting one electron on top of the other. So, that is pretty much what this is.

So, basically this U is therefore, that energy cost to putting one electron on top of the other. So, the idea is that here this is the number of electrons sitting at position i, so that means, is the number of electrons sitting at atom which is located at some location i, ok. So, this is the number of electrons. So, n i sigma is the number of electrons at atom located at i. So, and that electron has a spin projection sigma, so that means, so it can be either up or down.

So, the what this is saying is that this potential energy, the coulomb potential energy of all the electrons put together, now has this new interpretation in the tight binding picture.

And what is that new interpretation? The new interpretation is that that potential energy is simply the energy cost is the sum of all the energy cost to putting one electron on top of another in a given atom summed over all atoms. So, I forgot to sum over i. So, that summation over i is implied, ok. So, you have to sum over i also. So, summed over all i's, ok. So, that is the whole idea.

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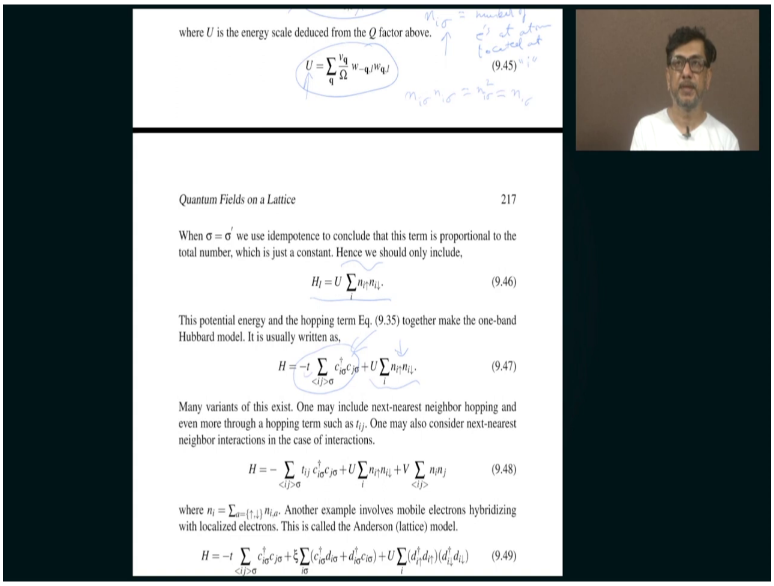

where U is the energy scale deduced from the Q factor above.

$$U = \sum_{\mathbf{q}} \frac{v_{\mathbf{q}}}{\Omega} w_{-\mathbf{q},l} w_{\mathbf{q},l} \tag{9.45}$$

$n_{i\sigma}$ = number of e's at atom located at "i"

$n_{i\sigma} n_{i\sigma} = n_{i\sigma}^2 = n_{i\sigma}$

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When $\sigma = \sigma'$ we use idempotence to conclude that this term is proportional to the total number, which is just a constant. Hence we should only include,

$$H_I = U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{9.46}$$

This potential energy and the hopping term Eq. (9.35) together make the one-band Hubbard model. It is usually written as,

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{9.47}$$

Many variants of this exist. One may include next-nearest neighbor hopping and even more through a hopping term such as t_{ij}. One may also consider next-nearest neighbor interactions in the case of interactions.

$$H = -\sum_{<ij>\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{<ij>} n_i n_j \tag{9.48}$$

where $n_i = \sum_{a=\{\uparrow,\downarrow\}} n_{i,a}$. Another example involves mobile electrons hybridizing with localized electrons. This is called the Anderson (lattice) model.

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \xi \sum_{i\sigma} (c^{\dagger}_{i\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} c_{i\sigma}) + U \sum_i (d^{\dagger}_{i\uparrow} d_{i\uparrow})(d^{\dagger}_{i\downarrow} d_{i\downarrow}) \tag{9.49}$$

So, that you see you might think that why did I; so, finally, the interpretation is that you see because you cannot put one or two electrons with the same spin on top of another, that is you know that that violates Pauli principle. So, strictly speaking you should only include this term. So, mathematically, you might think that why is that, because here sigma dash equals sigma is also possible. Because here finally, I am saying that sigma dash equals minus sigma is the only one you have to include.

So, it is possible I mean mathematically also you can see that; so, if I put sigma dash equals sigma this will become n i sigma squared, but then remember n i is either 0 or 1, n i sigma is either 0 or 1. So, because what is n i sigma? It is the number of electrons at position i with spin projection sigma. So, that is clearly either 0 or 1. So, in that case this is n i sigma itself; n i.

So, if 0 square, if some number is either 0 or 1 its square is also either 0 or 1, so that means, n i sigma squared is n i sigma. So, if that is the case then if sigma dash equals sigma it will become n i sigma squared which is n i sigma, but then when you sum over all i and sigma you will get you will basically get total number of particles which is an uninteresting constant.

So, therefore, the only interesting situation is when you have one spin which is up and one which is down sitting on top of each other. So, that is the dominant contribution to the electron electron interaction in a tight binding picture. So, the bottom line is that the end description is that you see, if you have a crystal, so you have a bunch of positive charges sitting at some regular lattice locations and then you have bunch of electrons which are trying to roam around that crystal. So, now two things happen one is that there will be an Hamiltonian.

So, the Hamiltonian description of those electrons can be attributed or described in the following way. One contribution will come from the atoms. So, each atom will contribute a certain Hamiltonian to that electron. So, that means, that there will be an Hamiltonian associated with the interaction of the of an electron with the positive charge sitting at some particular location in the lattice. So, and then summed over all such lattice points. So, that is one contribution.

So, the other contribution will come due to some extra potential energy that may be over and above that. So, it may not be a; so, there could be some residual contributions that is not attributable to a disjoint some of the contribution from all the atoms sitting separately. So, there will be a delta U contribution there, but then both these contributions put together in the tight binding picture can simply be thought of as a hopping term.

So; that means, so the contribution to the Hamiltonian due to the individual atoms the, so that means, the electrons interacting with all the different positive charges is simply lumped and described in the tight binding picture as a hopping term. So, that means, that an electron can hop from one lattice point to its neighbor, ok. So, then there is an energy cost associated with that hopping which we call as t. So, that is the tight binding description of an electron in a lattice. So, but then electron will also interact because it is a charge particle it can they can mutually repel.

So, how do you describe that? So, remember that in the tight binding picture an electron is either at one lattice point or at some other lattice point and it is meaningless to talk about some electron being somewhere in between. So, the idea is that when you want to describe a the repulsion between electrons, so naturally, it will be sensible only if one electron is sitting on top of another. So, that will be the dominant contribution.

So, one electron is at some atom, the other electron is on the same atom. So, then there will be an energy cost associated with that because that is when the repulsion will be the strongest, right. So, you will have to include that. So, that is what this is. So, but then one electron cannot sit on top of another unless one of them is up spin, the other is down spin, ok. So, that is the tight binding approach in the nearest neighbor hopping and the dominant contribution to the coulomb interaction.

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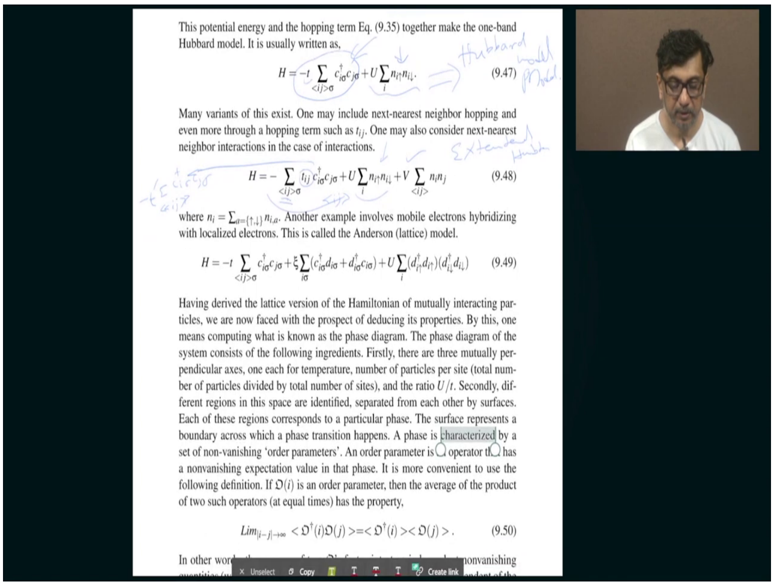

This potential energy and the hopping term Eq. (9.35) together make the one-band Hubbard model. It is usually written as,

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \qquad (9.47)$$

Hubbard model Model.

Many variants of this exist. One may include next-nearest neighbor hopping and even more through a hopping term such as t_{ij}. One may also consider next-nearest neighbor interactions in the case of interactions.

Extended Hubbard

$$H = - \sum_{<ij>\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{<ij>} n_i n_j \qquad (9.48)$$

$-t \sum_{<ij>} c^{\dagger}_{i\sigma} c_{j\sigma}$

where $n_i = \sum_{a=\{\uparrow,\downarrow\}} n_{i,a}$. Another example involves mobile electrons hybridizing with localized electrons. This is called the Anderson (lattice) model.

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \xi \sum_{i\sigma} (c^{\dagger}_{i\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} c_{i\sigma}) + U \sum_{i} (d^{\dagger}_{i\uparrow} d_{i\uparrow})(d^{\dagger}_{i\downarrow} d_{i\downarrow}) \qquad (9.49)$$

Having derived the lattice version of the Hamiltonian of mutually interacting particles, we are now faced with the prospect of deducing its properties. By this, one means computing what is known as the phase diagram. The phase diagram of the system consists of the following ingredients. Firstly, there are three mutually perpendicular axes, one each for temperature, number of particles per site (total number of particles divided by total number of sites), and the ratio U/t. Secondly, different regions in this space are identified, separated from each other by surfaces. Each of these regions corresponds to a particular phase. The surface represents a boundary across which a phase transition happens. A phase is characterized by a set of non-vanishing 'order parameters'. An order parameter is [illegible] operator th[illegible] has a nonvanishing expectation value in that phase. It is more convenient to use the following definition. If $\mathfrak{O}(i)$ is an order parameter, then the average of the product of two such operators (at equal times) has the property,

$$Lim_{|i-j|\to\infty} < \mathfrak{O}^{\dagger}(i)\mathfrak{O}(j) > = < \mathfrak{O}^{\dagger}(i) > < \mathfrak{O}(j) > . \qquad (9.50)$$

In other wor[illegible] nonvanishing

So, but then there are other possibilities. So, that, so this is the although this is the dominant contribution, it is also important to include a subdominant contribution and see if they change the results qualitatively. Because it is possible that there are some effects that vanish identically because of these stringent assumptions. And inclusion of subdominant contributions may actually make a quantity which is 0 suddenly nonzero. See, if the if inclusion of subdominant contributions change a nonzero quantities slightly, that is uninteresting.

So, you might as well not consider the subdominant contributions. So, the interesting situations in physics are when the dominant contribution produces a trivial result. So, that means, there is some physical quantity which is identically 0, if you consider a point of view a certain set of approximations. So, now, then it becomes extremely critical for you to include the things that you have thrown away, especially the leading things that you have thrown away, so you put it back into your analysis.

Then, the quantity that was actually identically 0 because of that over simplifying assumptions are now going to be nonzero. So, that is the reason why it is also important to consider the possibility that you those consider those possibilities. So, that means, in addition to this. So, remember what I told you about this angular brackets. Angular bracket i j is a standard notation in tight binding picture. What it means is i and j are nearest neighbors. So, it is also important to consider the next nearest neighbor and make sure that that does not change anything qualitatively.

So, that is also frequently done. So, and similarly, here also you have to make sure that not only you consider coulomb repulsion for electron sitting on the same atom, one is up, one is down, but you should also consider the possibility that an electron sitting on neighboring atoms will also have a coulomb repulsion, but of significantly less in magnitude. But maybe inclusion of that might change some results qualitatively.

So, we should be wary of those possibilities as well, so which is why I have done that. So, I strictly speaking I should have done for the hopping also. I should have done minus t dash. So, the next nearest neighbor, so the nearest neighbor is angular bracket ij, next nearest neighbor standard notation is two angular brackets, so that means, its one removed from the other, ok. So, I should have done included that also. So, there will be 4 terms t ij. Well, t ij can be thought of as just t typically.

So, then there is a t and at t dash for the next nearest. So, the nearest neighbor hopping is t that is the amplitude, t dash is the next nearest neighbor amplitude. So, the repulsion between electrons sitting on the same lattice point is U and the repulsion on neighboring lattice points is V. So, this is basically, so this is by the way this is the famous Hubbard model, ok. So, this is the famous Hubbard model of solid state physics, ok.

So, this is the famous Hubbard model and this is called the extended Hubbard model. So, the point is that if your lattice is in one-dimension, you can actually solve for the many properties of this Hubbard model in one-dimension exactly, using a technique called Bethe Ansatz, which I will not be discussing in this course.

So, this course is more about exposing you to the interesting models of solid state physics. It is not about teaching you how to solve those models, which are somewhat technical and they require a lot of effort. So, it is not suitable to teach in a course. It is best for self- learning.

But I am offering this course just to alert you to the basics. So, that means, I am making you aware of the existence of all these models that are worth solving. So, it is for you to find out how they are solved in practice. So, in one-dimension they are typically solved using something called Bethe Ansatz and there are other techniques called Bosonization which are also important, which I am going to discuss by the way in this course towards the end, ok. But Bethe Ansatz is also typically used in one-dimension.

So, just to summarize I have successfully hopefully convinced you that it is possible to simplify the description of the motion of an electron in a crystal through this tight binding picture. So, that means, through the tight binding picture, you replace this continuum description, replace it with a lattice description. So, that means, in a lattice description an electron does not have an option of being somewhere wherever it wants to be. It has to be either sitting on one atom or the next atom or the other atom.

It does not have a choice of being somewhere in between. So, the thing is the kinetic motion comes about by when an electron tunnels through and reaches the neighboring atom, right. So, and the coulomb interaction between electron comes if one electron is sitting with up spin on one atom and electron another can come only if it has down spin. And if it sits on that atom, they will repel with some fixed energy called U.

So, this description is called the tight binding description and it enormously simplifies the you know the description of the motion of electrons in a solid, in a crystalline solid. And a lot of effort has been made to understand these simplified models of electrons in a crystalline solid. And a lot is known, a lot is also not known, especially in more than one-dimension. So, I will stop here. And in the next class, I will describe some variants of this Hubbard model, there are something called the Anderson lattice model and so on.

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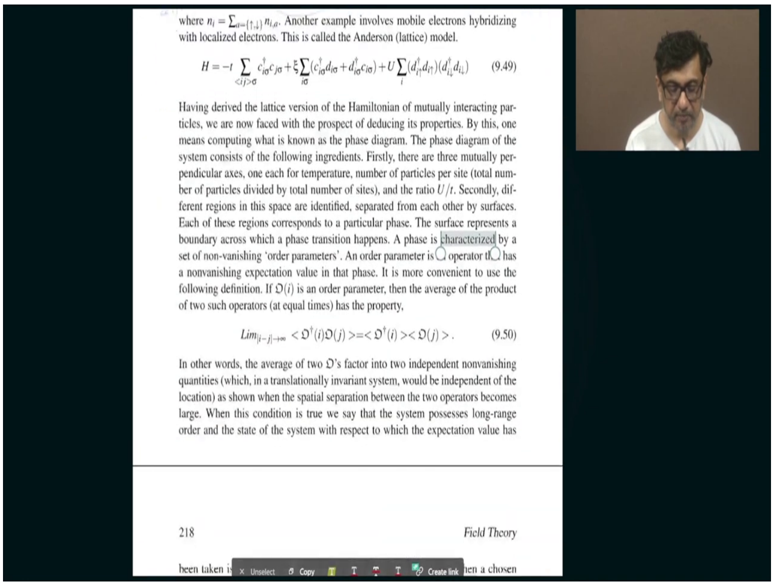

where $n_i = \sum_{a=\{\uparrow,\downarrow\}} n_{i,a}$. Another example involves mobile electrons hybridizing with localized electrons. This is called the Anderson (lattice) model.

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \xi \sum_{i\sigma} (c^{\dagger}_{i\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} c_{i\sigma}) + U \sum_{i} (d^{\dagger}_{i\uparrow} d_{i\uparrow})(d^{\dagger}_{i\downarrow} d_{i\downarrow}) \tag{9.49}$$

Having derived the lattice version of the Hamiltonian of mutually interacting particles, we are now faced with the prospect of deducing its properties. By this, one means computing what is known as the phase diagram. The phase diagram of the system consists of the following ingredients. Firstly, there are three mutually perpendicular axes, one each for temperature, number of particles per site (total number of particles divided by total number of sites), and the ratio U/t. Secondly, different regions in this space are identified, separated from each other by surfaces. Each of these regions corresponds to a particular phase. The surface represents a boundary across which a phase transition happens. A phase is characterized by a set of non-vanishing 'order parameters'. An order parameter is [illegible] operator th[illegible] has a nonvanishing expectation value in that phase. It is more convenient to use the following definition. If $\mathfrak{O}(i)$ is an order parameter, then the average of the product of two such operators (at equal times) has the property,

$$Lim_{|i-j|\to\infty} < \mathfrak{O}^{\dagger}(i)\mathfrak{O}(j) > = < \mathfrak{O}^{\dagger}(i) > < \mathfrak{O}(j) > . \tag{9.50}$$

In other words, the average of two $\mathfrak{O}$'s factor into two independent nonvanishing quantities (which, in a translationally invariant system, would be independent of the location) as shown when the spatial separation between the two operators becomes large. When this condition is true we say that the system possesses long-range order and the state of the system with respect to which the expectation value has

been taken i[illegible]hen a chosen

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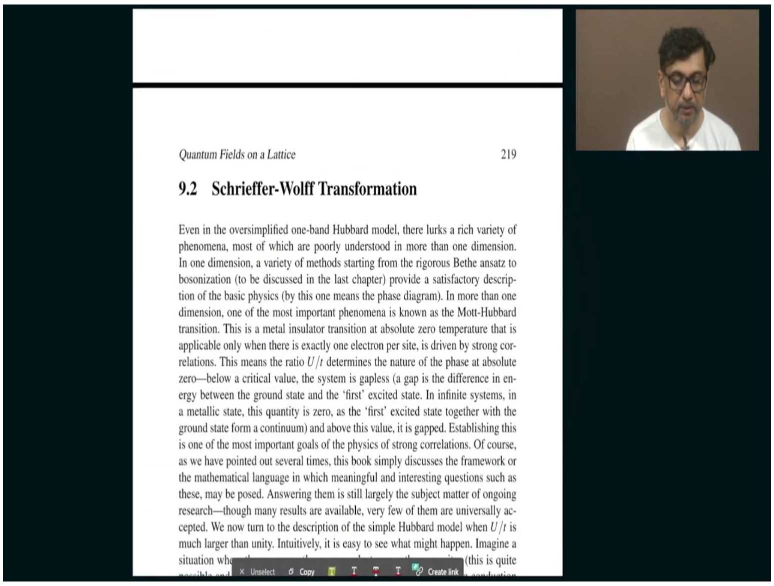

9.2 Schrieffer-Wolff Transformation

Even in the oversimplified one-band Hubbard model, there lurks a rich variety of phenomena, most of which are poorly understood in more than one dimension. In one dimension, a variety of methods starting from the rigorous Bethe ansatz to bosonization (to be discussed in the last chapter) provide a satisfactory description of the basic physics (by this one means the phase diagram). In more than one dimension, one of the most important phenomena is known as the Mott-Hubbard transition. This is a metal insulator transition at absolute zero temperature that is applicable only when there is exactly one electron per site, is driven by strong correlations. This means the ratio U/t determines the nature of the phase at absolute zero—below a critical value, the system is gapless (a gap is the difference in energy between the ground state and the 'first' excited state. In infinite systems, in a metallic state, this quantity is zero, as the 'first' excited state together with the ground state form a continuum) and above this value, it is gapped. Establishing this is one of the most important goals of the physics of strong correlations. Of course, as we have pointed out several times, this book simply discusses the framework or the mathematical language in which meaningful and interesting questions such as these, may be posed. Answering them is still largely the subject matter of ongoing research—though many results are available, very few of them are universally accepted. We now turn to the description of the simple Hubbard model when U/t is much larger than unity. Intuitively, it is easy to see what might happen. Imagine a situation wh[illegible](this is quite

Then, I will explain to you what sort of quantities are worth calculating using this tight binding picture.

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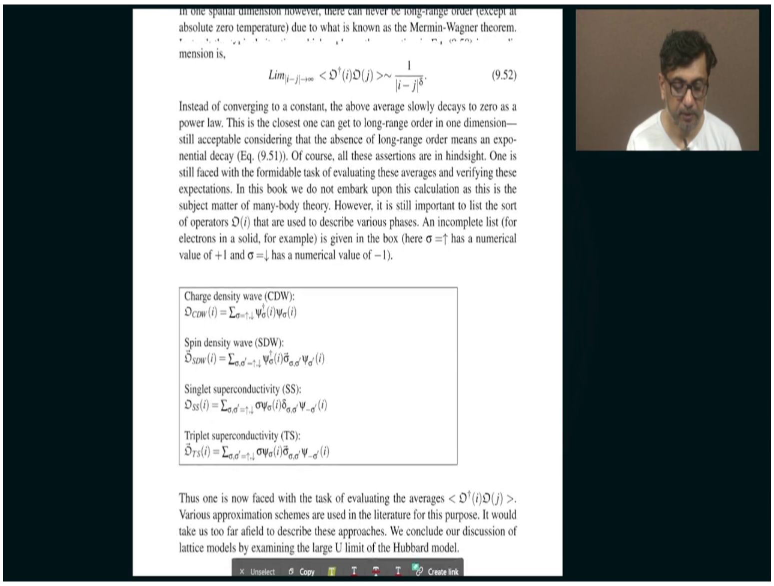

In one spatial dimension however, there can never be long-range order (except at absolute zero temperature) due to what is known as the Mermin-Wagner theorem. [illegible] mension is,

$$Lim_{|i-j|\to\infty} < \mathfrak{O}^{\dagger}(i)\mathfrak{O}(j) > \sim \frac{1}{|i-j|^{\delta}}. \qquad (9.52)$$

Instead of converging to a constant, the above average slowly decays to zero as a power law. This is the closest one can get to long-range order in one dimension—still acceptable considering that the absence of long-range order means an exponential decay (Eq. (9.51)). Of course, all these assertions are in hindsight. One is still faced with the formidable task of evaluating these averages and verifying these expectations. In this book we do not embark upon this calculation as this is the subject matter of many-body theory. However, it is still important to list the sort of operators $\mathfrak{O}(i)$ that are used to describe various phases. An incomplete list (for electrons in a solid, for example) is given in the box (here $\sigma = \uparrow$ has a numerical value of $+1$ and $\sigma = \downarrow$ has a numerical value of -1).

Charge density wave (CDW):
$\mathfrak{O}_{CDW}(i) = \sum_{\sigma=\uparrow,\downarrow} \psi^{\dagger}_{\sigma}(i)\psi_{\sigma}(i)$

Spin density wave (SDW):
$\vec{\mathfrak{O}}_{SDW}(i) = \sum_{\sigma,\sigma'=\uparrow,\downarrow} \psi^{\dagger}_{\sigma}(i)\vec{\sigma}_{\sigma,\sigma'}\psi_{\sigma'}(i)$

Singlet superconductivity (SS):
$\mathfrak{O}_{SS}(i) = \sum_{\sigma,\sigma'=\uparrow,\downarrow} \sigma\psi_{\sigma}(i)\delta_{\sigma,\sigma'}\psi_{-\sigma'}(i)$

Triplet superconductivity (TS):
$\vec{\mathfrak{O}}_{TS}(i) = \sum_{\sigma,\sigma'=\uparrow,\downarrow} \sigma\psi_{\sigma}(i)\vec{\sigma}_{\sigma,\sigma'}\psi_{-\sigma'}(i)$

Thus one is now faced with the task of evaluating the averages $< \mathfrak{O}^{\dagger}(i)\mathfrak{O}(j) >$. Various approximation schemes are used in the literature for this purpose. It would take us too far afield to describe these approaches. We conclude our discussion of lattice models by examining the large U limit of the Hubbard model.

So, there are some quantities called order parameters that are interesting which you have to calculate. So, and the next section will be devoted to understanding how to certain limiting cases of the Hubbard model will describe magnetism. So, I will be describing, I will show you how the models of magnetism that you might be familiar with can be systematically derived as certain limiting cases of the Hubbard model. So, that will be few classes down the road, ok.

So, thanks for listening to me. Hope to see you in the next class.

Thank you.