Dynamics of Classical and Quantum Fields: An Introduction
Prof. Girish S. Setlur
Department of Physics
Indian Institute of Technology, Guwahati

Lattice Models
Lecture - 36
Tight Binding Models - I

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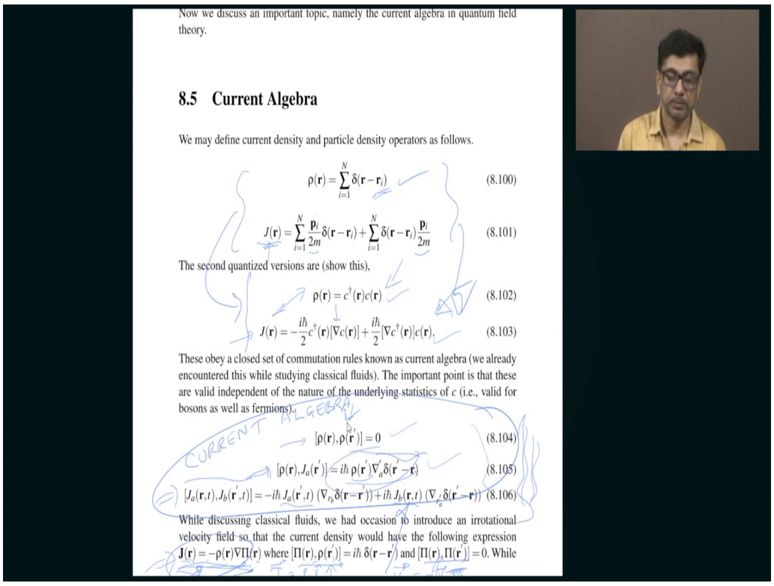

Now we discuss an important topic, namely the current algebra in quantum field theory.

8.5 Current Algebra

We may define current density and particle density operators as follows.

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r}-\mathbf{r}_i) \tag{8.100}$$

$$J(\mathbf{r}) = \sum_{i=1}^{N} \frac{\mathbf{p}_i}{2m}\delta(\mathbf{r}-\mathbf{r}_i) + \sum_{i=1}^{N} \delta(\mathbf{r}-\mathbf{r}_i)\frac{\mathbf{p}_i}{2m} \tag{8.101}$$

The second quantized versions are (show this),

$$\rho(\mathbf{r}) = c^{\dagger}(\mathbf{r})c(\mathbf{r}) \tag{8.102}$$

$$J(\mathbf{r}) = -\frac{i\hbar}{2}c^{\dagger}(\mathbf{r})[\nabla c(\mathbf{r})] + \frac{i\hbar}{2}[\nabla c^{\dagger}(\mathbf{r})]c(\mathbf{r}). \tag{8.103}$$

These obey a closed set of commutation rules known as current algebra (we already encountered this while studying classical fluids). The important point is that these are valid independent of the nature of the underlying statistics of c (i.e., valid for bosons as well as fermions).

$$[\rho(\mathbf{r}), \rho(\mathbf{r}')] = 0 \tag{8.104}$$

$$[\rho(\mathbf{r}), J_a(\mathbf{r}')] = i\hbar\, \rho(\mathbf{r}')\nabla'_a\delta(\mathbf{r}'-\mathbf{r}) \tag{8.105}$$

$$[J_a(\mathbf{r},t), J_b(\mathbf{r}',t)] = -i\hbar\, J_a(\mathbf{r}',t)\,(\nabla_{r_b}\delta(\mathbf{r}-\mathbf{r}')) + i\hbar\, J_b(\mathbf{r},t)\,(\nabla_{r'_a}\delta(\mathbf{r}'-\mathbf{r})) \tag{8.106}$$

While discussing classical fluids, we had occasion to introduce an irrotational velocity field so that the current density would have the following expression $\mathbf{J}(\mathbf{r}) = -\rho(\mathbf{r})\nabla\Pi(\mathbf{r})$ where $[\Pi(\mathbf{r}), \rho(\mathbf{r}')] = i\hbar\,\delta(\mathbf{r}-\mathbf{r}')$ and $[\Pi(\mathbf{r}), \Pi(\mathbf{r}')] = 0$. While

So today let us discuss a new topic basically that involves studying a matters which are of importance and interest to condensed metaphysics, but before I do that let me recollect where I had left off. That means, I had stopped right here which where I discussed something called current algebra.

So, in current algebra means, I showed that the density and current of a collection of a particles can be written in the so called second quantized notation, so where you write it in terms of creation and annihilation of particles.

So, you have operators that correspond to creating and annihilating particles at some point in space. So, that will enable you to rewrite the density of particle and current density in this way so, 8.102 and 8.103. Now, I had also a convinced you that these operators obey something called the current algebra, which is a closed commutation role between the components of current and the density.

So that means, the density commutes amongst themselves and the density and appropriate component of the current density commutes commutator is also proportional again to the density it is self. So, similarly here two different components of the density the commutator of them is also proportional to the appropriate components of the current.

So, these are closed commutation rules in the sense that the so if you look at density and current components of current as members of some family. The commutator, the mutual commutators between them at equal times of course. They are themselves expressible in terms of the same family; that means, you do not have to again invoke something new. So, that is why it is called current algebra. So, it is interesting for that reason.

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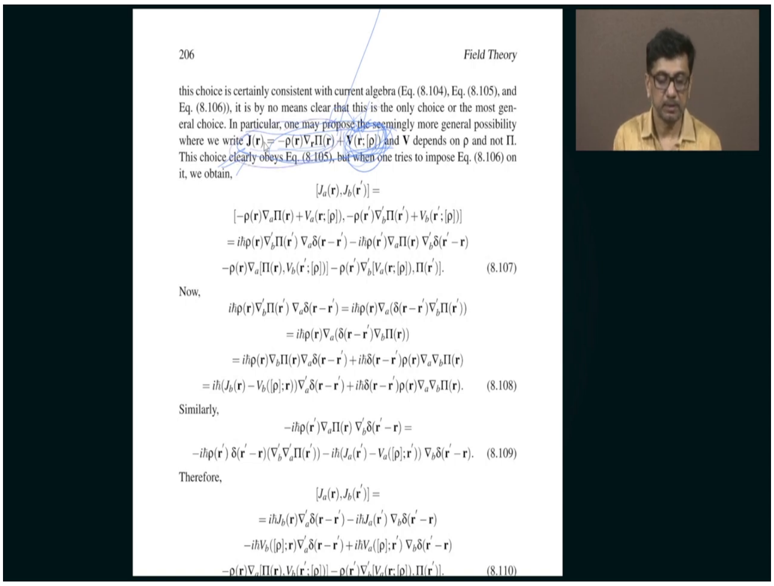

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this choice is certainly consistent with current algebra (Eq. (8.104), Eq. (8.105), and Eq. (8.106)), it is by no means clear that this is the only choice or the most general choice. In particular, one may propose the seemingly more general possibility where we write $\mathbf{J}(\mathbf{r}) = -\rho(\mathbf{r})\nabla_{\mathbf{r}}\Pi(\mathbf{r}) + \mathbf{V}(\mathbf{r};[\rho])$ and $\mathbf{V}$ depends on ρ and not Π. This choice clearly obeys Eq. (8.105), but when one tries to impose Eq. (8.106) on it, we obtain,

$$\begin{aligned}
&[J_a(\mathbf{r}), J_b(\mathbf{r}')] = \\
&[-\rho(\mathbf{r})\nabla_a\Pi(\mathbf{r}) + V_a(\mathbf{r};[\rho]), -\rho(\mathbf{r}')\nabla'_b\Pi(\mathbf{r}') + V_b(\mathbf{r}';[\rho])] \\
&= i\hbar\rho(\mathbf{r})\nabla'_b\Pi(\mathbf{r}')\,\nabla_a\delta(\mathbf{r}-\mathbf{r}') - i\hbar\rho(\mathbf{r}')\nabla_a\Pi(\mathbf{r})\,\nabla'_b\delta(\mathbf{r}'-\mathbf{r}) \\
&-\rho(\mathbf{r})\nabla_a[\Pi(\mathbf{r}), V_b(\mathbf{r}';[\rho])] - \rho(\mathbf{r}')\nabla'_b[V_a(\mathbf{r};[\rho]), \Pi(\mathbf{r}')].
\end{aligned} \tag{8.107}$$

Now,

$$\begin{aligned}
i\hbar\rho(\mathbf{r})\nabla'_b\Pi(\mathbf{r}')\,\nabla_a\delta(\mathbf{r}-\mathbf{r}') &= i\hbar\rho(\mathbf{r})\nabla_a(\delta(\mathbf{r}-\mathbf{r}')\nabla'_b\Pi(\mathbf{r}')) \\
&= i\hbar\rho(\mathbf{r})\nabla_a(\delta(\mathbf{r}-\mathbf{r}')\nabla_b\Pi(\mathbf{r})) \\
&= i\hbar\rho(\mathbf{r})\nabla_b\Pi(\mathbf{r})\nabla_a\delta(\mathbf{r}-\mathbf{r}') + i\hbar\delta(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r})\nabla_a\nabla_b\Pi(\mathbf{r}) \\
&= i\hbar(J_b(\mathbf{r}) - V_b([\rho];\mathbf{r}))\nabla'_a\delta(\mathbf{r}-\mathbf{r}') + i\hbar\delta(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r})\nabla_a\nabla_b\Pi(\mathbf{r}).
\end{aligned} \tag{8.108}$$

Similarly,

$$\begin{aligned}
&-i\hbar\rho(\mathbf{r}')\nabla_a\Pi(\mathbf{r})\,\nabla'_b\delta(\mathbf{r}'-\mathbf{r}) = \\
&-i\hbar\rho(\mathbf{r}')\,\delta(\mathbf{r}'-\mathbf{r})(\nabla'_b\nabla'_a\Pi(\mathbf{r}')) - i\hbar(J_a(\mathbf{r}') - V_a([\rho];\mathbf{r}'))\,\nabla_b\delta(\mathbf{r}'-\mathbf{r}).
\end{aligned} \tag{8.109}$$

Therefore,

$$\begin{aligned}
&[J_a(\mathbf{r}), J_b(\mathbf{r}')] = \\
&= i\hbar J_b(\mathbf{r})\nabla'_a\delta(\mathbf{r}-\mathbf{r}') - i\hbar J_a(\mathbf{r}')\,\nabla_b\delta(\mathbf{r}'-\mathbf{r}) \\
&-i\hbar V_b([\rho];\mathbf{r})\nabla'_a\delta(\mathbf{r}-\mathbf{r}') + i\hbar V_a([\rho];\mathbf{r}')\,\nabla_b\delta(\mathbf{r}'-\mathbf{r}) \\
&-\rho(\mathbf{r})\nabla_a[\Pi(\mathbf{r}), V_b(\mathbf{r}';[\rho])] - \rho(\mathbf{r}')\nabla'_b[V_a(\mathbf{r};[\rho]), \Pi(\mathbf{r}')].
\end{aligned} \tag{8.110}$$

But then, in fact this current algebra enables us to rewrite the current density in a very powerful simple way. So, you rewrite current density as. So, normally density current density is defined as particle density times the velocity of the fluid.

So, it is rho time’s V J s rho time’s V, but then in order for current algebra to be valid you can convince yourself, so it is not that easy because you have to show that this is the only way of doing it. So, in other words you can convince yourself that rho J is rho time's V is by definition you can always write a V which is J by rho.

So, long as you only focus on points where rho is not 0, then I can always think of V as J by rho, but now the question is what is the property of V I mean is V simply related in some way to rho and the answer is yes. So, you can in fact, you can show that current algebra implies that V should be expressible.

Whenever, at all points where rho does not become 0, V is irrotational; that means, the velocity which is defined as J by rho is basically the velocity is expressible as the negative gradient or basically the gradient of some scalar which typically use it as negative gradient.

So, we think of it as negative gradient. So, I showed first of all that this is consistent with current algebra, but that is not good enough, but you have to show that this is the only way of doing it. So, in order to show that I assume the more general possibility and I showed that the more general possibility is not consistent with our requirements. That basically it is not consistent with current algebra. So, in other words the simpler option is the only one, ok.

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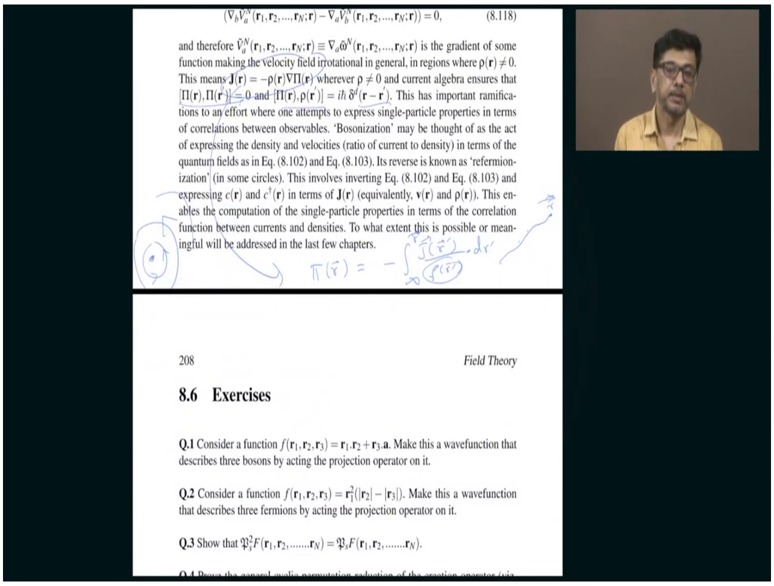

$$(\nabla_b \tilde{V}_a^N(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N;\mathbf{r}) - \nabla_a \tilde{V}_b^N(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N;\mathbf{r})) = 0, \tag{8.118}$$

and therefore $\tilde{V}_a^N(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N;\mathbf{r}) \equiv \nabla_a \tilde{\omega}^N(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N;\mathbf{r})$ is the gradient of some function making the velocity field irrotational in general, in regions where $\rho(\mathbf{r}) \neq 0$. This means $\mathbf{J}(\mathbf{r}) = -\rho(\mathbf{r})\nabla\Pi(\mathbf{r})$ wherever $\rho \neq 0$ and current algebra ensures that $[\Pi(\mathbf{r}),\Pi(\mathbf{r}')] = 0$ and $[\Pi(\mathbf{r}),\rho(\mathbf{r}')] = i\hbar\,\delta^d(\mathbf{r}-\mathbf{r}')$. This has important ramifications to an effort where one attempts to express single-particle properties in terms of correlations between observables. 'Bosonization' may be thought of as the act of expressing the density and velocities (ratio of current to density) in terms of the quantum fields as in Eq. (8.102) and Eq. (8.103). Its reverse is known as 'refermionization' (in some circles). This involves inverting Eq. (8.102) and Eq. (8.103) and expressing $c(\mathbf{r})$ and $c^\dagger(\mathbf{r})$ in terms of $\mathbf{J}(\mathbf{r})$ (equivalently, $\mathbf{v}(\mathbf{r})$ and $\rho(\mathbf{r})$). This enables the computation of the single-particle properties in terms of the correlation function between currents and densities. To what extent this is possible or meaningful will be addressed in the last few chapters.

$$\Pi(\vec{r}) = -\int_{\infty}^{\vec{r}} \frac{\vec{J}(\vec{r}')}{\rho(\vec{r}')} \cdot d\vec{r}'$$

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8.6 Exercises

Q.1 Consider a function $f(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \mathbf{r}_1.\mathbf{r}_2 + \mathbf{r}_3.\mathbf{a}$. Make this a wavefunction that describes three bosons by acting the projection operator on it.

Q.2 Consider a function $f(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \mathbf{r}_1^2(|\mathbf{r}_2| - |\mathbf{r}_3|)$. Make this a wavefunction that describes three fermions by acting the projection operator on it.

Q.3 Show that $\mathfrak{P}_s^2 F(\mathbf{r}_1,\mathbf{r}_2,.......\mathbf{r}_N) = \mathfrak{P}_s F(\mathbf{r}_1,\mathbf{r}_2,.......\mathbf{r}_N)$.

So, that is important because later on we will be using this in something called bosonization. So, after all you see once you write in terms of density and this velocity potential called pi. So, the pi commutes with other pis; that means, pi of r commutes with pi of r dash and rho of r commutes with rho of r dash. But then, pi at commutator rho is actually proportional to Dirac delta function.

So in that sense, they are actually bosons because, that they canonically conjugate objects. So, that can be used to re express fermions in terms of these what are now bosons. They bosons because they are very closed I mean the commutators are proportional to identity rather than anti commutators.

So, the commutators are proportions, the commutators of rho and rho and pi and pis are identically 0, but the commutator of rho and rho pi is proportional to the Dirac delta function which is basically the identity time sum number.

So bottom line is that, once you identify canonical bosons in the theory see this way of writing V in terms of the gradient of pi with a minus sign is always valid regardless of whether the underlying particles are bosons of fermions, ok. So, the distinction comes somewhere else which I will get to somewhat later, ok.

So, at that level it is the currents and density have the same form regardless of whether the underlying particles of fermions and bosons, ok. So, that is pretty much where I had left off I showed you that current algebra implies the existence of an irrotational velocity, ok.

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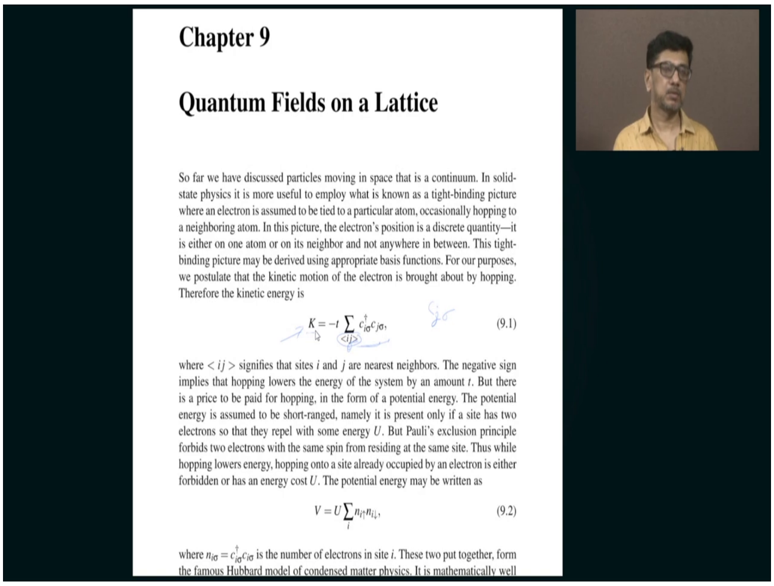

Chapter 9

Quantum Fields on a Lattice

So far we have discussed particles moving in space that is a continuum. In solid-state physics it is more useful to employ what is known as a tight-binding picture where an electron is assumed to be tied to a particular atom, occasionally hopping to a neighboring atom. In this picture, the electron's position is a discrete quantity—it is either on one atom or on its neighbor and not anywhere in between. This tight-binding picture may be derived using appropriate basis functions. For our purposes, we postulate that the kinetic motion of the electron is brought about by hopping. Therefore the kinetic energy is

$$K = -t \sum_{<ij>} c^{\dagger}_{i\sigma} c_{j\sigma}, \qquad c_{j\sigma} \tag{9.1}$$

where $< ij >$ signifies that sites i and j are nearest neighbors. The negative sign implies that hopping lowers the energy of the system by an amount t. But there is a price to be paid for hopping, in the form of a potential energy. The potential energy is assumed to be short-ranged, namely it is present only if a site has two electrons so that they repel with some energy U. But Pauli's exclusion principle forbids two electrons with the same spin from residing at the same site. Thus while hopping lowers energy, hopping onto a site already occupied by an electron is either forbidden or has an energy cost U. The potential energy may be written as

$$V = U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{9.2}$$

where $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the number of electrons in site i. These two put together, form the famous Hubbard model of condensed matter physics. It is mathematically well

So now, I am going to switch gears and discuss something else and that something else is basically quantum fields on a lattice. So till now, I had described creating and annihilating particles in basically empty space. That means, you can create particle at some position r and that r is continuously anything. So, you could create fermions or bosons wherever you want. But then, for applications in solid state physics typically what happens is that, we think of the interesting dynamical objects in a solid as being the electrons.

The ion I mean basically the positive charges in the solid are actually very they are very inert. In the sense that, it is much easier for the electrons to participate in dynamical phenomena due to their lightness and due to the fact that they are very mobile and light and they are also charged, right.

So, they are electrically charged and their light. Whereas the positive charges are several 1000 times heavier and they are stuck at their lattice positions. So, that is typically what a solid is. So, in the most idealized situation we only focus on the electrons and more or less think of the positive charges as providing a pre defined background potential.

So, in other words the implication is that solid state physics is the study of the theoretical solid state physics is the study of the properties of the electrons in a solid typically by assuming the crystal structure which is gleaned from experimental data. So that means, we assume that a solid has a certain stoichiometry; that means, we know what it is made of and we not only know what it is made of, we also know where all the atoms are sitting.

So, that is an important assumption. So, that you might think that is bit of an anticlimax in the sense that is a like assuming pretty much a whole lot, which is in fact true. It is somewhat like I always like to give this example. It is like running the marathon 10 meters before the finish line. If you are asked to run a marathon you know you should honestly start exactly where everybody else is starting.

But this way of doing solid state physics is like running marathon 10 meters below the finish line. But, a surprising amount of physics has been done using this sort of an approach and for reasons that are somewhat mysterious in many times these types of approaches seem to suffice.

In the sense that, a lot of important insights about the nature of the solid can be gleaned just by starting that way and perhaps augmenting that type of an approach with some more ad hoc assumptions about the dynamics of the lattice. So, that is typically for example, you introduce lattice vibrations.

So, rather than first predicting where all the atom are sitting you assume where the atoms are sitting from experimental data like x ray crystallography. And then, you work out the vibrational modes of the atoms and then, and then you try and study the I mean the dynamics of the lattice that way.

And that sort of thing is already quite complicated and so that is not really fair to think of that as starting from the finish line. It is still not starting honestly starting from the starting point, but still it is somewhere midway.

So, but that is still quite challenging and that is how solid state physics has been progressing till now. So, it is important therefore for us to learn how to study the dynamics of electrons specifically in a solid given the fact that the thus those electrons move around in a pre existing lattice of positive charges, whose locations are known beforehand, ok.

So, that is precisely this chapter 9 which is quantum fields on a lattice ok, the fields I am referring to is the electron field I mean the fermion field. So you will see that, it actually makes more sense in to now stop thinking of the space as being a continuum. Rather it makes more sense now; see now that you have resigned yourself to the fact that you will not inquire about the origin of the lattice it is self, that somebody has already told you that there is a lattice and the electrons just go from one point on the lattice to the other.

So, in that if you accept that starting point then it stands to reason that you would it makes more sense to think of this underlying space as not being continuous at all, but rather made of these discrete points, which whose locations are determined beforehand we already know where all the points are on the lattice. So now, the thing is that our space it is self has now been discretized. So, now the electrons the fermion fields that live on the lattice.

So; that means, if I want to create or annihilate. Now, I have to rather than creating and annihilating at some particular point like I was doing earlier. So, and that point can be anywhere so, instead of doing that now I am forced to create and annihilate at exactly one of the lattice points not anywhere in between. So, creating and annihilating fermions basically in between has no meaning in this lattice picture.

So, the lattice picture forces us to create and annihilate exactly at the lattice points. So, you will see the so you might think that is a rather radical departure from what you are accustomed to and it becomes hard to swallow that until at least for somebody like me it is really impossible for me to accept that unless somebody shows me that there is a smooth logical link between my you know p squared by 2 m plus V of r picture which forces I mean which basically tells me the particle can be anywhere it wants and then, going from there to the so called tight binding model.

So, what I described are just now this sort of an assumption of that the electrons can either live on one lattice point or the other and nothing in between that is called the tight binding model ok, because it is tightly bound to one of those lattice sites.

So, it is tightly bound to one lattice site or the other. So, it can so typically what happens is that conduction takes place when the electron that is tightly bound to one of the lattice sites kind of tunnels across and finds it is self on the next one or the neighboring one so, so that is called hopping.

So, these are the kind of this is a sort of jargon that people use in this field is called hopping. Hopping is kind of what is called kinetic energy for a continuum system is hopping in a lattice system, ok. So, we will be able to, so the point is that I have to you know for the skeptical minded audience who is listening to this lecture, it is really important that I should be able to establish a logical link between the traditional way of thinking about electrons.

Namely that it has a kinetic energy and it has a potential energy due to the surrounding positive charges that are there. So, from there so we see that way of looking at it electron can be anywhere; there is no restriction that it cannot be here or there.

But then, from there I have to be able to systematically make a sequence of approximations or assumptions simplifying assumptions and get to a stage. Where I can justify the lattice model which mandates that every electron is either stuck to one lattice point or the other and it cannot possibly found anywhere else. So, I have to justify that transition. Basically the remaining part of this lecture and perhaps the next lecture also will be devoted to explaining this connection, ok. So, I am going to try and derive this, ok.

So, but before that let me tell you what the lattice or the hopping term looks like. So, the so what we normally associate as kinetic energy of electron, the kinetic motion of electrons due to basically p squared by 2 m type of term. So, if you rewrite that for the lattice it would correspond to something like this.

So, what this is saying. So, let me tell you what these symbols mean. c j sigma is optional so, so I have to sum over sigma i i omitted that. So, sigma is just a spin projection which is uninteresting it can I mean, because it is an electron it can have up or down spin, but the important index here is j or i.

So, j basically tells you the lattice point in question. So, I have used lowercase Latin letters it does not mean I am looking at 1 dimension. j can refer to some point in the lattice and the a lattice can be either 1 dimensional lattice, 2 dimensional, 3 dimensional lattice. It can be any one of those.

So, basically j refers to some point on some given lattice. And similarly, I also refers to some other point on the same lattice. So now, I have to sum over i and j, but then there is some funny symbol here that I have put i and j in between you know two angular brackets.

So, what does that mean? What that means is basically the so the implication is that the kinetic energy of the electrons are due to what is called hopping; and hopping is I am going to show you that the simplest version of the tight binding model, which can be derived systematically from the p squared by 2 m plus V of r starting point.

So, the simplest version of the tight binding model requires that I should only consider hopping between nearest neighbors. So that means, if j is some point on a lattice on the given assumed lattice. So, then this i is supposed to be another point which is not j, but which is closest to j.

And there can be more than one point that are equally close to j and typically more than 1 by already in 1 dimension you have two points, one to the left one to the right. But, in higher dimensions you can have more number of points that are closest to j. So, I am supposed to sum over all such pairs of points that are as close to each other as possible without being the same points, ok. So, then I am describing what is called hopping.

So, the implication is that an electron can hop only to the nearest neighbor and the chances that it will hop to the next nearest driver are overwhelmingly suppressed. That means, the chance the probability of that happening is very less and to a first approximation may be ignored.

So, this is called the nearest neighbor hopping. And this can be derived you know that this is not like an assumption that you can actually derive this from the traditional p squared by 2 m plus V of r language, ok.

So now, you see now the point is that this only describes hopping only is like a substitute is a lattice version of the kinetic energy; it is a lattice equivalent of the kinetic energy there is a kinetic energy. It is just p squared because, particle can be anywhere so, it can have any p any r whatever it is. But, here the particle can only be on lattice points.

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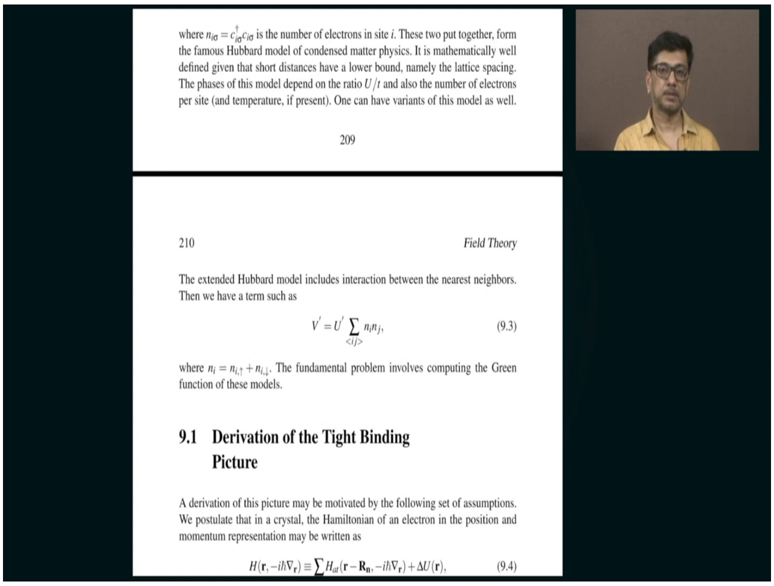

where $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number of electrons in site i. These two put together, form the famous Hubbard model of condensed matter physics. It is mathematically well defined given that short distances have a lower bound, namely the lattice spacing. The phases of this model depend on the ratio U/t and also the number of electrons per site (and temperature, if present). One can have variants of this model as well.

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The extended Hubbard model includes interaction between the nearest neighbors. Then we have a term such as

$$V^{'} = U^{'} \sum_{<ij>} n_i n_j, \tag{9.3}$$

where $n_i = n_{i,\uparrow} + n_{i,\downarrow}$. The fundamental problem involves computing the Green function of these models.

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

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

So now, what about potential energy? So, what is the lattice equivalent of potential energy? So, of course if you have some external field that is a separate matter, but I am talking about say the coulomb interaction between particles, means between electrons the repulsion.

So, if there is one electron you see if another electron tries to sit on the same lattice site. Then, first of all Pauli principle says that you cannot do that unless one of them has up spin, the other has down spin.

So, which is why I have said this. So, this is the number of particles on site i with up spin, this is the number of particles on site i with down spin. So, what this says is that this potential energy is 0 unless there is exactly 1 fermion with up spin and 1 fermion with down spin at site i in which case the potential energy is U so, that is the repulsion term, but then in all other cases it 0.

So, if there is only one if say up spin is 1 ni up is 1 and ni down is 0; that means, there is only one electron and that electron has up spin then, it does not have anything to repel it mean nothing can repel it. Because, I told you know far away they do not repel, they only repel. So, that is again the nearest neighbor. So, if they since they are allowed to sit on top of each other when one is up one is down, clearly that is the dominant term, right

So, it is only when both are up or both are down right, then it is not allowed to sit on top of each other then, so there is something called the extended model which where you have to include that also. Typically that is important, because these see this model ignores the possibility that if two spins come and both are up then, even though they cannot sit on top of each other they can at least repel sitting nearby.

So, that is not included in this. So, that is the next order term, which should logically be included. So, bottom line as you see this approach has this following drawback which you have probably already noticed. That it is a whole bunch of ad hoc assumptions that. This nearest neighbor hopping, nearest neighbor coulomb interactions these are all ad hoc assumptions because, see there is no a priori valid reason for ignoring next nearest neighbor next to next nearest neighbor.

So in fact, lots and lots of papers are published by including one after another successively and there is a kind of I mean at least you know you know the community is inundated with papers of this sort and you know there is an implication that somehow this constitutes progress, but I personally have a different view. So, I feel that this way of thinking about solids has actually done a disservice to the subject, because it is ad hoc in the extreme.

Because, there are infinitely many adjustable parameters; because you can include the next nearest neighbor which is another see this t and U are already adjustable parameters. It is extremely hard to derive them a priori, right. Already the existing lattice structure is an assumed structure from experimental data. On top of that this t and U are also fitted from experiment typically. Then, next nearest neighbor terms are also sometimes fitted from experiment.

Yeah, you can use something called density functional theory and all that to try and derive this from what are called Ab initio methods, but those are very ambiguous and far from being successful. So, bottom line is that this sort of an approach gives you a model with infinitely many adjustable parameters and you know there is this famous mathematician Von Neumann who is known to have said also very famously that you give me 3 parameters I can draw an elephant; you give me one more I can make him wiggle his tail.

So, bottom line is that you can describe any organism, any system you want if you have sufficient number of parameters in your model. So, that does not mean anything. So, it is just an exercise in curve fitting. So, those are not explanations they are just wishful thinking.

Unfortunately a lot of condensed matter physics is mostly wishful thinking and disguise, ok. But then, given that physics I mean the literature is filled with such approaches we are forced to discuss them. But I am making these disclaimers, because I feel that it is important for me to express my personal opinion as well, ok.

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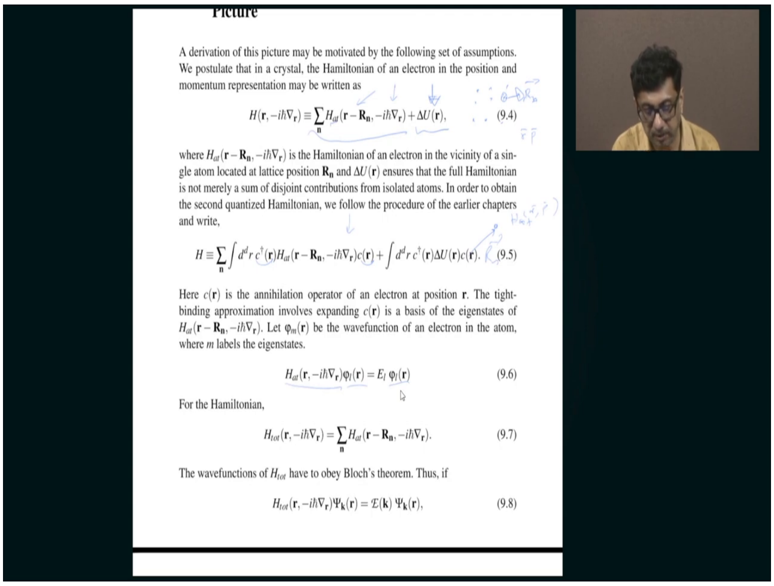

Picture

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

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

where $H_{at}(\mathbf{r}-\mathbf{R}_{\mathbf{n}},-i\hbar\nabla_{\mathbf{r}})$ is the Hamiltonian of an electron in the vicinity of a single atom located at lattice position $\mathbf{R}_{\mathbf{n}}$ 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,

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

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 $H_{at}(\mathbf{r}-\mathbf{R}_{\mathbf{n}},-i\hbar\nabla_{\mathbf{r}})$. Let $\varphi_m(\mathbf{r})$ be the wavefunction of an electron in the atom, where m labels the eigenstates.

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

For the Hamiltonian,

$$H_{tot}(\mathbf{r},-i\hbar\nabla_{\mathbf{r}}) = \sum_{\mathbf{n}} H_{at}(\mathbf{r}-\mathbf{R}_{\mathbf{n}},-i\hbar\nabla_{\mathbf{r}}). \tag{9.7}$$

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

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

So, question is how do you that apart I mean it is true that it has a whole bunch of parameters, but is it true that we can at least derive that whole bunch of parameters from first principles we can know what they are right, the next the hopping coefficient t, the onsite repulsion U, the next I mean nearest neighbor repulsion V.

So, can all these be derived from some atomic calculations of the you know the atomic structure of the atom that sitting at the lattice sites, the answer is yes, but it is not easy. So, the question is how do you do that? So, it is a long story and I do not know if you have the stomach for it or the patience for it, but those of you are somewhat unnerved and skeptical about this lattice approach to solids would probably be better off in paying attention to this.

But, those of you who just want to get on with it, who just want to learn how to use the lattice method to do practical calculations, who could not care less just want publications can just go ahead and skip this section.

But then, let me just get to this method. So, the idea is that you see. So, imagine you have a collection of atoms sitting at some positions called Rn. So, you have these so there is a given lattice ok and this is some typical Rn, n is some discrete index which tells you where that lattice point is, ok.

So now, the thing is that what is sitting here is an actual atom. So, that is why it is called at, at means atom. So, this atom has it is own Hamiltonian. So, this atom will have a nucleus which is positively charged it will have a bunch of electrons that are going round and round that positive charge.

So, it will have it is own Hamiltonian. So, that Hamiltonian is basically a function of r and p. Well, it is a function of several rs and several ps, but then I am now going to think of some typical r and typical p. Because, remember in the second quantized notation I will just have to pre multiply by c dagger r and post multiply by c r and integrate over r and I would have accounted for all the electrons that are there in the atom.

So, at stage I am going to just select some typical electron that happens to be in that particular atom. So, if that is the case then you see the Hamiltonian of so, if that atom is sitting at the origin the Hamiltonian of the electron is basically H at bracket r comma p so, if that atom is at the origin; but if it is not at the origin, but if it is at some R n. So, if the atom is at the origin the Hamiltonian is of the electron which is you know tied to this particular atom is H at within brackets r comma p.

But, if that atom it is self is at some other location called R n instead of being at the origin. Then, clearly the Hamiltonian for an electron you know going round and round that particular atom is this one where r is getting shifted by R n, ok.

So now, if you add up all the locations of all the atoms you will necessarily get the Hamiltonian of all the atoms put together but then, this ignores an important facet and namely that you know the total Hamiltonian is not necessarily the sum of the Hamiltonians of all the atoms put together.

Because, that assumes that the atoms do not talk to each other, that is that there is no interaction energy between atoms. See the atoms are electrically neutral, because they are the equal number of positive and negative charges that is fine.

But then, they can still interact with each other. Say for example, if one of them if they all have dipole moments, then clearly they will interact pretty strongly with closer neighbors. But even if they do not have dipole moments, they can induce dipole moments on one another.

So, that is called polarizability of polar. So, they can polarize each other and still interact. So, all those possibilities are there and that is what causes bonding. See the chemical bond is because, if you place atoms on a lattice. If they strictly remain inert they do not the electrons just interact with the nucleus of the it is own atom, it does not even acknowledge the existence of any other atom, then clearly there is no concept of hopping or there is no concept of chemical bonds or anything of that sort.

So, but in nature we do expect all that. So, which is why you need a we need to postulate that there is a further energy which is over and above whatever you see here. So, this further energy is basically a function of the position of the electron alone and that basically tells you so the implication here is that the kinetic part is already taken care of by the atomic Hamiltonian.

So, the rest of it basically is tells you that the electron is electron of one atom can actually feel the presence of the neighboring atoms. And that leads to an excess different I mean correction to the potential energy of the system and that is I have denoted that by delta of U of r.

So, that r is the location of my typical electron in the system and delta of U is basically the extra potential energy which that electron feels due to the fact that the atoms kind of do not influence only their own electrons, but they also influence the electrons of their neighbors.

So, that is the reason why you have this extra term. So now, that I have written down the Hamiltonian of a typical electron in such a solid. Now, I can go ahead and write down my second quantized version of all the electrons put together in the solid. So, that is the beauty of the second quantized approach. So, I do not have to do sigma i equal to 1 to some n where n is 10 raise to 36.

So, I can just do it for one typical atom and then, pre multiply by creation, post multiply by annihilation and integrate over all the locations of all the electrons and then I will end up getting the Hamiltonian of the all the electrons in the solid, ok. So now, I mean this is still looks very far from my tight binding model. So, this still looks like p squared y 2 m. In fact, that is what this is still I mean there is p squared by 2 m hidden here.

So, the question is how would I reach there? So, I am going to now make some assumptions about the nature of the wave functions of this H at. So, first of all let me postulate that this H at has some stationary states, right.

So, the stationary states of H at are let us assume that they are labeled by some index called l which could be your orbital's, ok. So, it will have some values. So, now the point is that if I define H total as the sum over all the. So, remember I told you that this H at r comma p, p means this one minus i h bar grad.

So, H at r comma p is the Hamiltonian of an electron tied to this particular atom assuming that particular atom is sitting at the origin, but if it is not sitting at the origin it is sitting at R n it is this one. But then, you can have R n is like some particular lattice point, but you can have a whole bunch of lattice points and each lattice point has an atom sitting there.

So, if you want to take into account the Hamiltonian of all of them, you have to add up all the lattice points. So, which is what I have done here? So now, having done this, you see now the important point is that this Hamiltonian has a periodicity.

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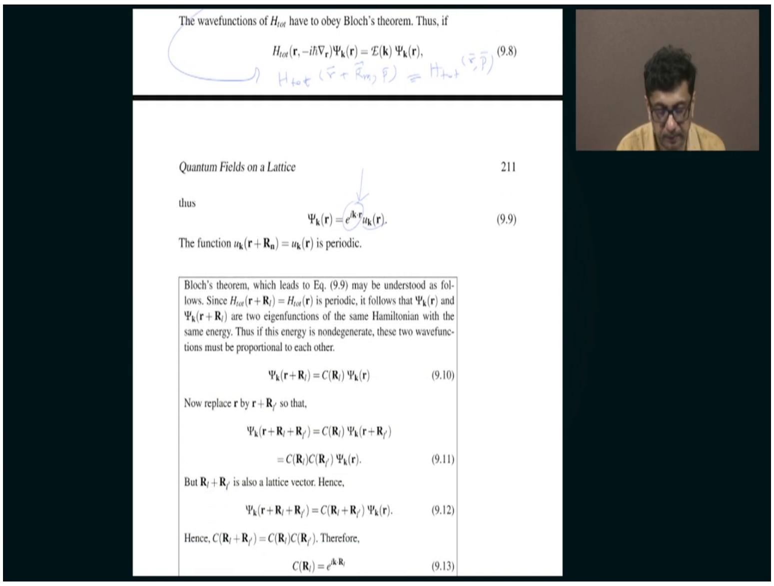

The wavefunctions of H_{tot} have to obey Bloch's theorem. Thus, if

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

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

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thus

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

The function $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R_n}) = u_{\mathbf{k}}(\mathbf{r})$ 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.

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

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

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

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

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

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

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

That means, if I take H total and take r and you just translate it by some lattice vector, this is going to be exactly same as earlier. So, this is going to be periodic in r. So, the Hamiltonian is periodic, because I have added up all the atoms locations.

So, now if I shift my point of view from one atom to the next the system still looks the same because, I am taken into account all of them and I infinitely many of them so, ok. So, it is a kind of a boundary less system there is no boundary. So, this Hamiltonian is strictly periodic in space.

So, if it is periodic in space we know from solid state physics which is sort of a prerequisite for this course, but maybe I mentioned this earlier also. So, basically the wave function the Hamiltonian periodic does not mean the wave function is also periodic, but it means that the wave function can be related to something periodic, ok.

So, the Hamiltonian periodic means you can actually rewrite the wave function as something which is very simple like a plane wave multiplied by a periodic function. So, that is what Bloch's theorem says. Bloch's theorem says that if you have a Hamiltonian which is periodic in space, it is eigen functions or stationary states are not necessarily periodic, but they are writable as a plane wave times a periodic function.

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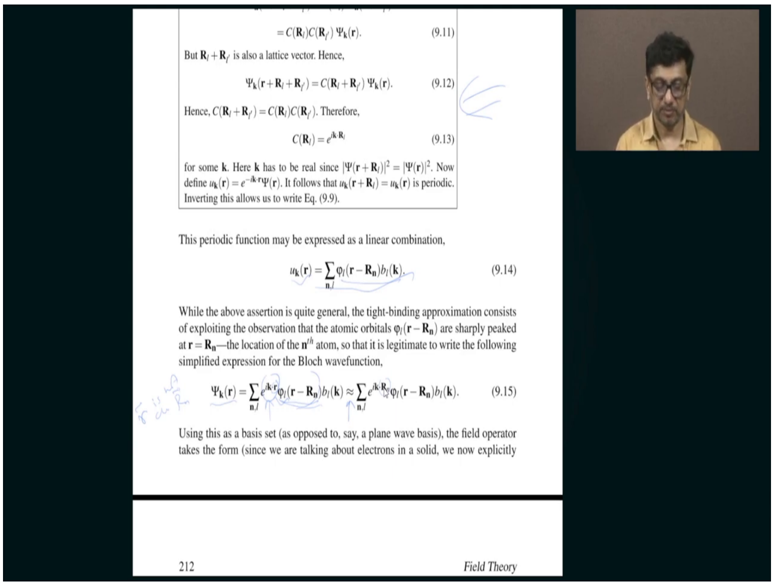

$$= C(\mathbf{R}_l)C(\mathbf{R}_{l'})\,\Psi_{\mathbf{k}}(\mathbf{r}). \qquad (9.11)$$

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

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

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

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

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,

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

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

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

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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So, that is what that is. So, and the Bloch's theorems proof is given in this square here. So, even if you did not know it earlier you can just read this square where the proof is there, ok. Since, we know that from Bloch's theorem that there is such a periodic function. Now, you see I am going to exploit the fact that I can write the periodic function like this, is not it. Because, now I have so it is all related now to the firstly the stationary states of H at form a complete set.

So, I can write any function as a like a linear combination of those stationary states because they form a basis, right. So, if they form a basis I can always write like this, but then I am not necessarily going to stop here because, I have to make sure that this is periodic. So, I have to shift the sum over all the R ns, ok. So, when I do that I get a function which is strictly periodic, ok. So, that is what that is.

So, therefore the Bloch states; that means the wave function of electron in that periodic potential, periodic system can be the plane wave which is this one multiplied by the periodic function, ok. But, because so now is the crucial assumption this is a very crucial step. See, here what I have assumed is that these wave function psi l what is the psi l remember what this is, this is the stationary state of the atom. So, the implication is that these electrons which are tied to this particular atom are very closely bound. So, it is called tight binding.

So; that means, a very tightly bound to this particular atom, they do not necessarily venture out too far away from the atom. So, that tightly bound to that atom. So, if you make the tight binding assumption. So, if you make that assumption then you see what this is saying is that, this function it is self is very small if r is not close to small letter r vector is not close to is not close to this lattice one of the lattice because, that is where the atoms are located.

So, if small letter r is not close to the lattice location this wave function it is self is very very small. So, if that is the case then there is no loss of generality or I am not making a serious mistake by replacing this r by R n, ok.

I mean I know that these are all very crude hand waving yeah. I am just trying to motivate the transition to tight binding picture. I am not implying that this sort of an analysis is particularly rigorous or anything. I am just saying that, this is like a 0th order calculation which is guaranteed to give you the hopping and on site repulsion and all that.

Which kind of sort of motivates the this ad hoc approach to solid state physics. I mean it makes you sort of believe it more, but that does not take away from the fact that it really still remains theory with a large number of adjustable parameter, whose you know I any issue meaning is not at all clear and you have no means of calculating them very easily in a practical system.

So, they are also typically fitted from experiment which kind of dilutes the predictive power of those models enormously, alright.

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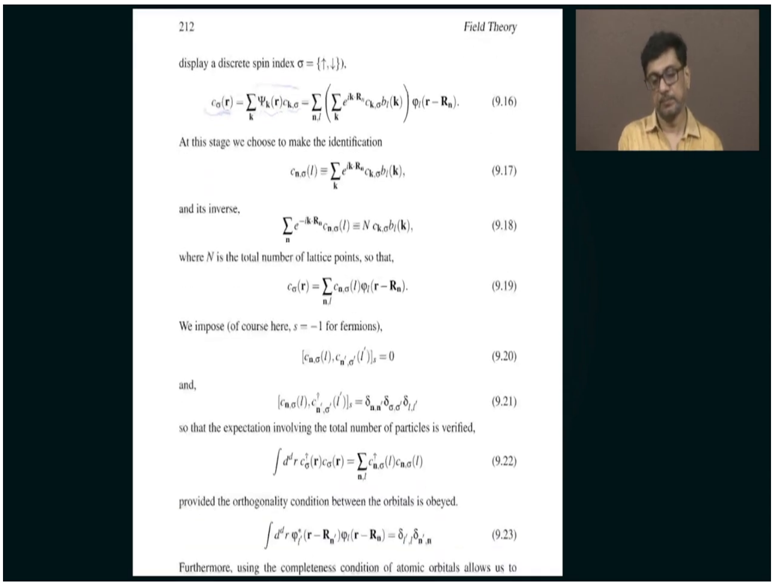

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display a discrete spin index $\sigma = \{\uparrow, \downarrow\}$),

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

At this stage we choose to make the identification

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

and its inverse,

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

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

$$c_\sigma(\mathbf{r}) = \sum_{\mathbf{n},l} c_{\mathbf{n},\sigma}(l) \varphi_l(\mathbf{r} - \mathbf{R}_\mathbf{n}). \quad (9.19)$$

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

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

and,

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

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

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

provided the orthogonality condition between the orbitals is obeyed.

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

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

So, point is that if you accept this then you go ahead and rewrite. So that, now you can you see. So, any so now these Bloch states now the actuals the wave function of the actual electrons in the solid it is self in the periodic solid. So, if that is the case then I can re express any annihilation operator at some point r in terms of these Bloch states.

Now, the coefficients will be the corresponding operators in momentum space, ok. So, I think now I am going to stop because, what I am going to do is that in the next class I will show you how to systematically rewrite. So, remember that the second quantized notation had this. So, I am going to rewrite this cs in terms of the Bloch states. So, which will enable me to then make a transition to the tight binding model, ok.

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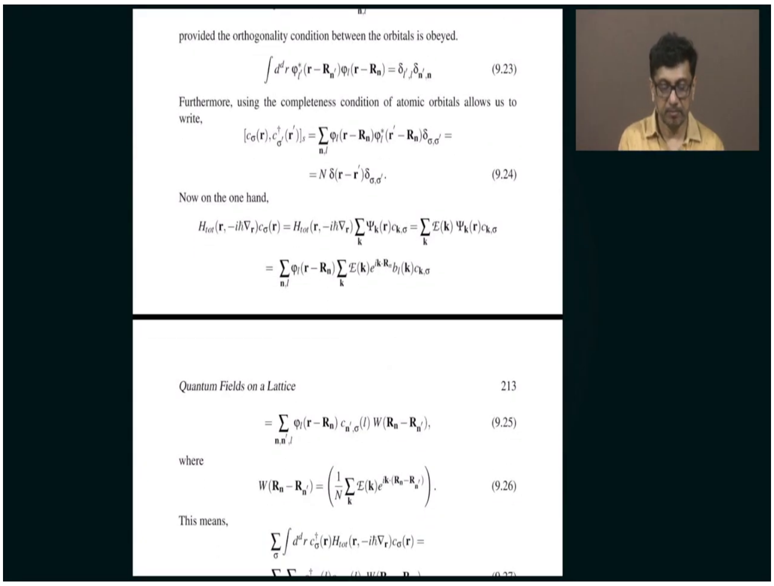

provided the orthogonality condition between the orbitals is obeyed.

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

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

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

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

Now on the one hand,

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

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

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

where

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

This means,

$$\sum_\sigma\int d^dr\, c^\dagger_\sigma(\mathbf{r})H_{tot}(\mathbf{r}, -i\hbar\nabla_{\mathbf{r}})c_\sigma(\mathbf{r}) =$$

How I am going to do that I will tell you gradually ok. So, there is a systematic procedure by which you can do that, ok.

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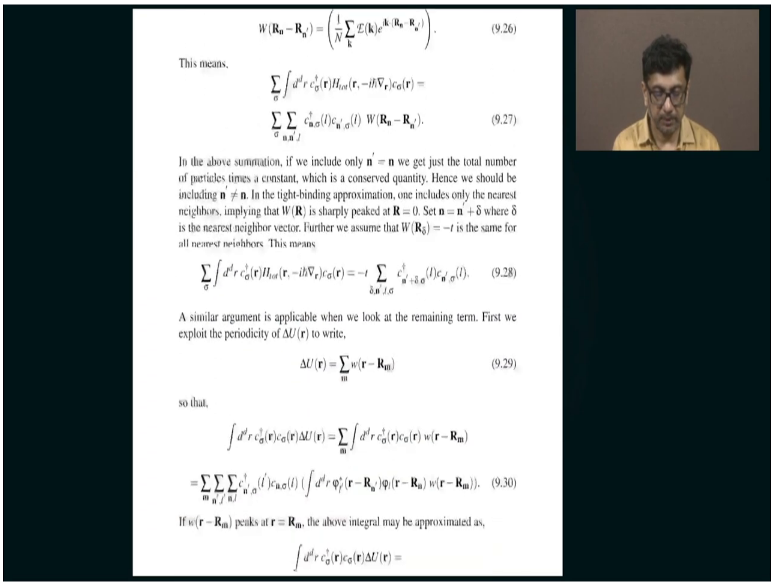

$$W(\mathbf{R}_{\mathbf{n}}-\mathbf{R}_{\mathbf{n}'}) = \left(\frac{1}{N}\sum_{\mathbf{k}}\mathcal{E}(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{R}_{\mathbf{n}}-\mathbf{R}_{\mathbf{n}'})}\right). \tag{9.26}$$

This means,

$$\sum_\sigma\int d^dr\, c^\dagger_\sigma(\mathbf{r})H_{tot}(\mathbf{r}, -i\hbar\nabla_{\mathbf{r}})c_\sigma(\mathbf{r}) =$$

$$\sum_\sigma\sum_{\mathbf{n},\mathbf{n}',l} c^\dagger_{\mathbf{n},\sigma}(l)c_{\mathbf{n}',\sigma}(l)\;W(\mathbf{R}_{\mathbf{n}}-\mathbf{R}_{\mathbf{n}'}). \tag{9.27}$$

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

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

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

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

so that,

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

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

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

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

So, finally, I will just fast forward and tell you where finally, we will end up like this.

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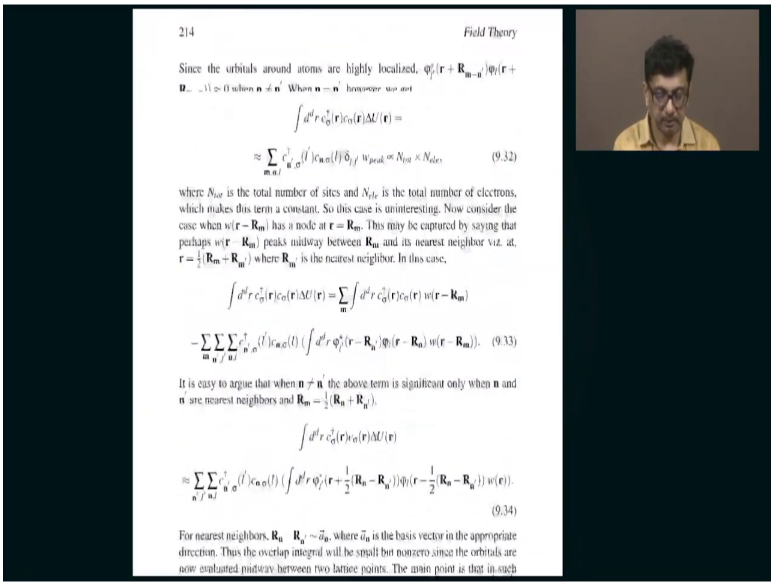

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Since the orbitals around atoms are highly localized, $\varphi^{*}_{l'}(\mathbf{r}+\mathbf{R}_{\mathbf{m}-\mathbf{n}'})\varphi_l(\mathbf{r}+\mathbf{R}_{\mathbf{m}-\mathbf{n}})) \approx 0$ when $\mathbf{n} \neq \mathbf{n}'$. When $\mathbf{n} = \mathbf{n}'$ however we get

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

$$\approx \sum_{\mathbf{m},\mathbf{n},l} c^{\dagger}_{\mathbf{n}',\sigma}(l')c_{\mathbf{n},\sigma}(l)\,\delta_{l,l'}\, w_{peak} \propto N_{tot} \times N_{ele}, \qquad (9.32)$$

where N_{tot} is the total number of sites and N_{ele} is the total number of electrons, which makes this term a constant. So this case is uninteresting. Now consider the case when $w(\mathbf{r}-\mathbf{R_m})$ has a node at $\mathbf{r} = \mathbf{R_m}$. This may be captured by saying that perhaps $w(\mathbf{r}-\mathbf{R_m})$ peaks midway between $\mathbf{R_m}$ and its nearest neighbor viz. at, $\mathbf{r} = \frac{1}{2}(\mathbf{R_m}+\mathbf{R}_{\mathbf{m}'})$ where $\mathbf{R}_{\mathbf{m}'}$ is the nearest neighbor. In this case,

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

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

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 $\mathbf{R_m} = \frac{1}{2}(\mathbf{R_n}+\mathbf{R}_{\mathbf{n}'})$.

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

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

For nearest neighbors, $\mathbf{R_n}-\mathbf{R}_{\mathbf{n}'} \sim \vec{a}_{\mathbf{n}}$, 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

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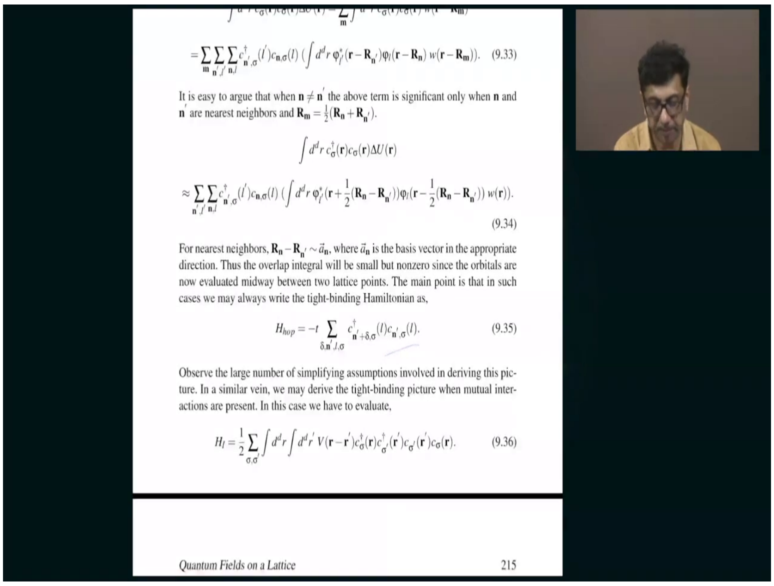

$$=\sum_{\mathbf{m}}\sum_{\mathbf{n}',l'}\sum_{\mathbf{n},l} c^{\dagger}_{\mathbf{n}',\sigma}(l')c_{\mathbf{n},\sigma}(l)\,\Big(\int d^d r\, \varphi^{*}_{l'}(\mathbf{r}-\mathbf{R}_{\mathbf{n}'})\varphi_l(\mathbf{r}-\mathbf{R_n})\, w(\mathbf{r}-\mathbf{R_m})\Big). \qquad (9.33)$$

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 $\mathbf{R_m} = \frac{1}{2}(\mathbf{R_n}+\mathbf{R}_{\mathbf{n}'})$.

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

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

For nearest neighbors, $\mathbf{R_n}-\mathbf{R}_{\mathbf{n}'} \sim \vec{a}_{\mathbf{n}}$, 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,

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

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So, we will actually get that hopping. So, this is the nearest neighbor hopping, ok.

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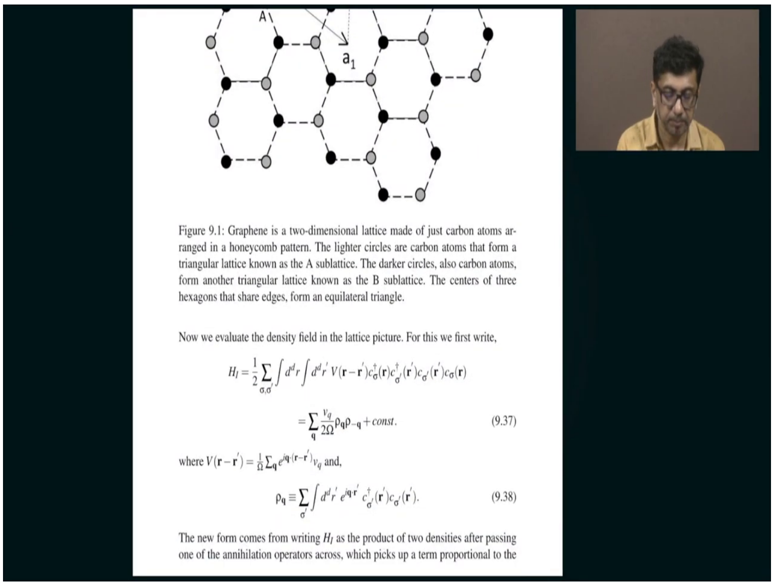

Figure 9.1: Graphene is a two-dimensional lattice made of just carbon atoms arranged in a honeycomb pattern. The lighter circles are carbon atoms that form a triangular lattice known as the A sublattice. The darker circles, also carbon atoms, form another triangular lattice known as the B sublattice.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

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

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

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

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

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

So, this is an example for graphene. So, bottom line is that is some effort and we will get there, but then it is a bit of a disappointment anti climax because, having gotten there all you know is that there is a whole bunch of simplifying assumptions you have to make to go from here to there and it is not clear what you have gained by doing this.

Because, you have ended up with a model that has a whole bunch of adjustable parameters and it is still as hard to solve as before. The only mild advantage is that it already encodes the structure of the existing lattice. So, that means that you do not have to then derive that also. So, somebody has already told you that this is the lattice and then now you are trying to proceed and see how the electrons behave on that lattice.

So, that is the slight advantage but then, the problem remains intractable if you insist on including coulomb repulsion in between electrons on the same lattice sites, ok. And most of the interesting physics happens because of that. I mean, when you ignore those terms then you get results which are entirely predictable. Of course, you know in 2 dimensions like for example, if you have this honeycomb lattice there are some unusual phenomena that take place.

They are theoretically very easy to derive, but they are of importance because experimentally they have been found to be also realized means they have been realized experimentally and the simplest theoretical description seems to suffice and describing say substances like graphene.

So, you do not have to work very hard to describe graphene. So, that is somewhat of a surprise in the sense that, if you think about it the tight binding model has. So, many simplifying assumptions and yet the simplest version of that seems to suffice in describing a whole lot of real systems.

So, yeah, so that is the reason why many physicists simply do not even bother to inquire about what why that is they are quite satisfied they are quite happy that it works and then they go ahead and publish papers that way, ok. Anyway so, that is a matter of taste. So, I am going to stop here in the next class I will proceed and tell you how to finally arrive at the hopping term and the onsite repulsion term starting from this continuum picture.

I will finish that description and after that we will go on to some other topics, ok. Thanks for listening to me and I intend to upload some video lectures on solving problems from my book meaning.

If you if you have noticed the end of every chapter has a large number of problems which I feel you should attempt and in order for me to know facilitate that I am going to solve some of those more difficult ones myself. And I am going to upload those videos and I hope after listening to them you will gain more confidence in solving those assignments at the end of each chapter, ok.

Thanks for listening to me. See you next time.