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

## **Lattice Models Lecture - 38 Order Parameters**

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This potential energy and the hopping te<br>Hubbard model. It is usually written as,  $H\alpha$  $(9.47)$  $H = -t \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}.$ Many variants of this exist. One may include next-nearest neighbor hopping and<br>even more through a hopping term such as  $t_{ij}$ . One may also consider next-nearest<br>neighbor interactions in the case of interactions.  $H=-\sum \widehat{u_{ij}} c^\dagger_{i\sigma} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow} + V \sum n_i n_j$  $(9.48)$ 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.  $H=-t\ \sum_{\alpha} \ c^\dagger_{i\alpha}c_{j\alpha}+\xi\sum_{\alpha} (c^\dagger_{i\alpha}d_{i\alpha}+d^\dagger_{i\alpha}c_{i\alpha})+U\sum_{\alpha}(d^\dagger_{i\uparrow}d_{i\uparrow})(d^\dagger_{i\downarrow}d_{i\downarrow}) \eqno(9.49)$ 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 retent regions in this space are usefunded, separated from each other by surfaces.<br>Each of these regions corresponds to a particular phase. The surface represents a boundary across which a phase transition happens. A phas of two such operators (at equal times) has the property,  $\label{eq:4.1} Lim_{|i-j|\rightarrow\infty}<\mathfrak{O}^{\dagger}(i)\mathfrak{O}(j)>=<\mathfrak{O}^{\dagger}(i)><\mathfrak{O}(j)>.$  $(9.50)$ In other words, the average of two  $\hat{\mathfrak{D}}$ 's factor into two independent nonvanishing quantities (which, in a translationally invariant system, would be independent of the

So, in this class let us continue our discussion of Lattice Models. So, if you remember in the last class I had stopped here where, I had explained how to derive something called the extended Hubbard model starting from the description of a solid as being composed of localized positive charges where, negative charges namely the electrons are free to move.

So, the lattice model by contrast is a model where electrons are not free to move especially, but they are confined to specific points in the lattice. So, but then they are allowed to quantum tunnel through space. So, that they can find themselves on the neighboring lattice point without passing through any intermediate special locations.

So, that means, in a lattice system an electron is either at some lattice point or it is found at a neighboring lattice point etcetera. So, that means, space itself has now been discretized into a collection of lattice points.

So, the lattice description basically the tight binding description of a solid involves converting what was initially a homogeneous space into a space containing discrete collection of points. So, that means that an electron can either be at this point or at say some other point etcetera. It cannot be at any continuously in between it cannot be in any other location ok.

So, so that is the lattice description of a solid that is the tight binding approach. So, in the tight binding approach the kinetic energy of an electron manifests itself as a hopping. So, that means, the electron can hop from one lattice site to a neighboring lattice site which is described by this t ij which refers to the hopping amplitude. So, it is the energy it gains by deciding to hop. So, that is why there is a minus sign and i bracket j ij within brackets basically means that you are looking at nearest neighbor.

So, usually you confine yourself to nearest neighbors. But of course, like I told you earlier that it is important to include higher order neighbors; that means, the next nearest neighbors and so on. Just to make sure that your results of that you are interested in. Do not change qualitatively when you make those modifications.

So, that means, there is some physical quantity that vanishes identically because you chose a model with the nearest neighbor hopping. There is some chance that quantity may not vanish identically if you include the next nearest neighbor hopping.

So, if that physical quantity is interesting it is very critical that you also include the next nearest neighbor hopping. So, similarly with coulomb interactions of electrons so; that means, usually when you have a coulomb interaction you obviously, look because it is a lattice model an electron can actually sit on top of another electron on the same lattice point provided one has up spin the other has down spin because of Pauli principle.

Now, when they do they certainly will have a strong coulomb repulsion which is described by this parameter called U, but then you can also have next nearest neighbor coulomb interaction and that is described by the next nearest neighbor interaction. So, this is called the extended Hubbard model.

So, the inclusion of next nearest neighbor hopping next nearest neighbor coulomb interaction all those things they are called extended versions of the original simpler models. So, now it is possible you see once you allow for the possibility of introducing these parameters such as t ij and U and V and so on. Nothing prevents you from becoming a little more adventurous and trying to you know write down models, which do not necessarily have a derivation systematic derivation the way I have derived this extended Hubbard model starting from you know r and p s you know description.

That means starting from the momentum and position descriptions of the electrons I used tight binding bases and all that and then derive this. So, it is not in condensed matter what one does is that one typically postulates certain Hamiltonian that we can intuitively feel are likely to capture certain phenomena that are of interest to us. So, one such seemingly ad hoc lattice model, which is of immense interest in condensed metaphysics it is called the Anderson lattice model.

So, that is the Anderson this periodic Anderson model. So, the idea is that there are two types of fermions one is what is called the itinerant fermions. Itinerant means mobile electrons that move throughout the crystal. So, they are the ones who have prominent hopping amplitudes. So, that means, they hop around from one side to another. So, itinerarium basically when you travel from one city to another you make an itinerary. That means, you for tell yourself you know how you are going from say Guwahati to Bangalore.

So, what are the stops in between? So, itinerary means a journey. So, itinerant electrons means electrons that perform a certain journey. So, the journey is that of hopping. They hop from one side to another and so those are the itinerant electrons. So, they are denoted by c i and c dagger i for annihilation and creation. So, now there is another unrelated species, which are not it itinerant which are exact the exactly the opposite of itinerant which is localized.

That means these electrons denoted by symbol small letter d in this Hamiltonian. They are actually localized to the lattice sites. So, they are actually the usually the d orbitals of the atoms. That means, if you look at the you know if you remember your hydrogen atom orbital's you have spdf. So, that d has something like a meaning of a d orbital you can think of it like that if you want or you can think of it as some orbital which is somewhat localized.

So, basically the idea is that there is some localized orbital and the localized orbital will actually hybrid. So, that means that the idea is that the itinerant electron can undergo something called hybridization. Hybridization basically means it kind of trades places with this localized electron. So, that means the mobile electron can trade places with the localized electron.

So, that means, it can dislodge a localized electron and make it itinerant or it can itself become localized. So, that means, there is a possibility of that you know it is somewhat like you know there are some fictional stories where, like Jekyll and Hyde where you know there is the scientist who is a scientist by day and a monster by night. So, it is some something like that. So, this electron can be itinerant and then it can choose to change its character completely and become localized. So, that is achieved through something called hybridization.

So, you might be wondering why people invoke such models. So, basically you will see that these models actually are very useful in describing what are called itinerant magnetism. That means, magnets where electrical conduction also takes place. So, that means, it exhibits magnetic properties, but it is also exhibits electrical conductions. If a typical example is iron, iron is strongly ferromagnetic, but it is also electrically conducting.

So, that is an example of an itinerant magnet. So, generally speaking people use these models in an ad hoc way to describe various realistic physical systems ok. So, but the key word here is ad hoc; that means, that ad hoc means for that purpose in Latin. So, it may basically means it has just been invented for that particular purpose. So, there is no more fundamental derivation.

So, this type of an point of view was advocated by this great physicist condensed what many people consider as father of condensed metaphysics which is Philip Anderson of Princeton. He is no more, but he was very influential in this subject and he is the one who gave a lot of prominence to these ad hoc lattice models and many of them are named after him and the thing is that they do capture a lot of interesting physics, but; however, none of them are easy to solve.

So, it is easy to write. So, basically in condensed matter physics if you adopt this ad hoc lattice approach you can write down a large number of very interesting models that seemingly capture a plethora of very important interesting phenomena that you see in actual solids. However, sadly that is the extent to which you can go because most of these models are exceedingly hard to solve especially in more than one dimension where those materials actually exist.

And because they are very hard to solve you have to make a large number of approximations then it becomes less and less obvious whether those. So, if you encounter a discrepancy between theory and experiment it becomes less and less obvious whether those discrepancies or the fact that theory and experiment do not agree very well, is that a result of the failure of the model or an inadequacy of the approximations.

So, that becomes very hard to disentangle and very hard to judge. So, that is the reason why condensed matter physics continues to challenge physicists even now and still there is no clear idea of how to. So, there is no actually a kind of a unified theory of condensed matter systems. Ideally that would be nice see this ad hoc approach has the exact opposite effect intentionally that it advocates the proliferation of unrelated models to describe a physical system.

In fact, the same material is often described by unrelated different unrelated models because the implication is there are phenomena which do not influence other phenomena even if they happen in the same material.

So, it is prudent according to this philosophy to describe this these different phenomena using different models even though this these phenomena occur in the same material, but that would be at odds with the (Refer Time: 13:22) issue or the first principles description of a material as being composed of just the fundamental constituents.

So, that would really constitute a unified description of the substance from which all other phenomena that you see in that material should emerge. So, there are these completely divergent viewpoints that physicists often grapple with and it is very hard to know which one will finally, succeed if any will at all ok. The point is that at this stage I have nothing more to add as far as lattice models are concerned.

Because as I told you that once you accept this philosophy of writing down ad hoc models then you can write a bunch of them with relative ease and they seemingly capture interesting phenomena, but they are impossible to solve very easily. In fact, you have to make a whole bunch of approximations.

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But; however, you know it is important to understand that suppose by some accident you are able to solve some of these models. Maybe you will reach a stage where there might be a quantum computer in the future that can simulate these lattice models exactly and that would pretty much take care of everything.

So, in that eventuality it is important for us to know what are the interesting questions to ask and answer with regard to these models. So, the idea is that so I am just going to read of this paragraph, which is reasonably well written. So, it says having derived the latest version of the Hamiltonian of mutually interacting particles we are now faced with the prospect of deducing its properties ok.

So, 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 side; that means, total number of fermions, the total number of electrons divided by total number of sites.

And then there is lastly the ratio which describes the strength the relative strength of the coulomb repulsion versus the copping. So, basically it tells you whether kinetic energy is more important or potential energy is more important. So, u by t is basically the ratio of the potential versus kinetic energy. So, that means, you see that the phase diagram consists firstly of three axis.

So, these are the three axis and within this so that means, in this octant or whatever. So, there are regions which are identified and these are regions are called phases and these regions are separated by surfaces and the surfaces represent a boundary across which a phase transition takes place. A phase is characterized by a set of non vanishing order parameters. So, an order parameter is an operator that has a non vanishing expectation value in that phase ok. So, it is more convenient to use the following definition.

So, imagine the script O bracket i; that means, basically it is some operator which is made of creation and annihilation operator of the electrons. So, imagine something like c dagger i c i plus 1 something like that. So, c i up into c i down c i dagger up into c i down something like that so that sort of thing. So, these are typical I mean you can have many such operators, but bottom line is something like that. So, that operator and i is basically a lattice point.

So, now the idea is that if some operator deserves to be called an order parameter it had better obey this property namely it has to obey this property. That is if you take the average of o dagger i into o j and you make i and j far apart. So, remember that i and j are the lattice points. So, I am talking about the lattice model. So, if i and j are far apart the idea is that they become O i and O j are uncorrelated.

So; that means, the average of the product is same as a product of the averages. So, in the in that case we say that the system possesses long range order with respect to this order parameter ok. And typically what happens is that so in other words if the system is in some well defined phase you will always be able to identify such an order parameter ok. So, whereas, when it is not in that phase the average between O i and O i dagger O i dagger and O j will actually not separate out that way.

But, however, the correlation actually vanishes. So, that means, this product basically vanishes as the separation between i and j increase. So, what; that means, is that this O this particular operator certainly does not describe any particular order. So, the system is not ordered in any ordered phase according to that particular operator. So, you can cook up many such operators O i from by combining c dagger i up and c i plus 1 down or whatever it is you can cook up many such operators.

So, the question is you have to find one such operator or several such operators which obeys equation 9.50. So, only then you can say that the system is has an order described by that order parameter. So, when you are successful only you can when you are successful in verifying 9.50 only you can say the system as a well defined order and you can write down you can label that phase as that by that particular order parameter.

But, when you are unsuccessful in finding such an order so; that means, any random O that you construct will typically obey not 9.50. It will typically obey 9.51. So, what it basically will say is that there is no relation between O i and O j unless they are pretty much i and j are pretty much the same things.

So; that means so they are completely uncorrelated, but in one dimension what will happen is that. So, this 9.50 is typical in for systems in three dimensions, but what will happen if there is a theorem called Mermin Wagner theorem which says that you can never have something like 9.50 in one dimension. So, in one dimension the next best thing you can have is this. So, that means, that instead of being a constant.

So, you see these are constants because in a translationally invariant system O i average will be independent of i. So, instead of being a constant it will actually become some power law. So, this is the best you can manage. So, remember that you might think that how are these two more or less the same. Well there of 9.50 and 9.52 are closer to each other compared to 9.50 and 9.51.

See 9.51 tells you that the correlation between i and j exponentially decays as you move away as i moves away from j whereas, 9.50 says that pretty much they are always correlated. That means, regardless of so; that means, if i and j's far apart they will or then close by they are more or less close by or far apart makes no difference they are all equally correlated.

So, these are diametrically opposite properties. So, if an operator obeys 9.50; that means, you are stumbled upon an order in the system, but when you are unsuccessful in finding such an operator invariably you will be repeatedly verifying that 9.51 is the valid statement. That means, any random O that you construct typically you will obey 9.51 very rarely you will stumble upon an O that will obey 9.50 in which case you are in luck.

So, you can go ahead and label that particular phase by that operator, but; however, in one dimension you will never be able to stumble upon any operator which obeys 9.50.

The best you will do is end up with something called 9.52. Of course, you will always be able to I mean any random thing you come across will always obey 9.51 in any dimension. But occasionally in one dimension you might stumble upon something that obeys 9.52 in which case you have to be content at that, because you will never be able to verify anything resembling 9.50 in one dimension because of Mermin Wagner theorem ok.

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So, I kept on very mysteriously talking about order parameters or operators without telling you how to construct them. So, here are some concrete examples of orders. So, there is something called the charge density wave order. So, where basically what you do is the psi is the fermion annihilation. So, you create total number of up and down spins at some lattice point i. So, that is basically the total density of fermions.

So, that is called the charge density wave because it sums over all the spins. So, that; that means, if you see now if O i and O j if you take averages what will happen is that if i and i if you make them far apart they are still correlated what that means, is that there is a kind of an O; that means, the electrons have decided to order themselves spatially.

See remember that this represents the dense total density of electrons at site i. So, if i and j if the density of electrons at i is correlated with density of electrons at j even when i and j are very far apart what does that mean? So, that would be the case if 9.50 is verified using this construction. So, if that is the case what that means, physically is that the electrons have decide to spatially order themselves.

That means that there is a so there is some spatial periodicity for example, in the density of the electron. So, that is why it is called as charge density wave right. So, it is charged as opposed to spin. So; that means, you are summed over all the spins. So, it describes a charge. So, now, you could also describe a spin density wave where you stick in your poly matrix, which now describes spins in various directions spin components in various directions and that would describe your spin density wave.

So, if you are able to verify 9.50 using this order parameter then it means that there is some sort of a magnetic order in your system. So, the electrons have kind of the their spins have arranged themselves in some orderly fashion, but; however, you do not have to necessarily first destroy and then create; that means, your order parameter does not have to conserve the number of electrons.

So, in superconductivity there are order parameters that do not conserve the number of electrons. So, as you very well know superconductivity is described by cooper pairs. See in these first two examples you are actually creating an electron hole pair; that means, you are first annihilating an electron then creating an electron.

So, that is basically like saying creating a hole and creating an electron. So, basically you are creating an electron hole pair in the first two examples. So, whereas, here you are actually creating two holes or annihilating two holes creating two electrons and annihilating two electrons.

So, that would be typical in a superconductor because the order parameter there it does not refers to creation of electron and a whole pair, but two electrons themselves form an order per pair. So, that is called a cooper pair. So, cooper pair is where you have one electron with up spin typically and one electron with down spin ok. So, that is called the singlet superconductor, because there is that forces one electron to be up. So, sigma and this is minus sigma because sigma dash equals sigma.

So, you create one electron with up spin and down or annihilate one electron with up spin and i like one electron with down spin. So, you are creating a hole with up spin hole with down spin simultaneously at lattice point i and if that obeys if that operator obeys 9.50. So, what that means, is that there is a phase characterized by this order this peculiar order.

So, this peculiar order is complexity unlike these are real order the expectation values of these quantities are real that the expectation of these superconducting order parameters are typically complex ok. So, the complex numbers have their own peculiar properties, they will have a magnitude and a phase. So, that phase has some important intrinsic physical meanings, which we will not go into, but traditionally those were discovered first historically speaking.

And this is a modern more condensed matter version field theory version of a description of superconductors, but this came later historically speaking the description of that in terms of phases and so on, they came earlier. So, then you have the singlet superconductor where you have up and down spin; that means, you create an and I let two electrons by one with up one with down.

But, you can also have a situation where, you can have other types of superconductors where you can. So, this is called s wave superconductor. You can have p wave superconductors where the where you create two electrons one with up and one with again with up, but then you have to make sure that there are other indices that distinguish otherwise because of Pauli principle that order parameter will be identically 0.

So, you will have to have different say orbital angular momentum states. So, that means, you should be creating one electron with a certain orbital angular momentum the other one with a different orbital angular momentum. So, that is called p wave superconductor you can have s wave p wave singlet triplet superconductivity and so on. So, these are all the different possibilities ok. So, I am not going to of course, finally, verifying 9.50 involves being able to calculate this average which is of course, not at all an easy task because this is a many body problem.

Calculating this sort of average of o dagger i o j for a Hamiltonian such as 9.49 or 9.48 is exceedingly difficult and its nothing much is known ok, but I have at least told you what is worth doing in case somebody comes up with a very effective tool in the future say such as quantum computers typically analytically is quite hopeless ok.

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So, in the next class I will be describing some approximation schemes, which are controlled in the sense that you can justify them somewhat mathematically as a systematic expansion in powers of something. So, we will be able to show that such a systematic expansion one such expansion is called the Schrieffer Wolff transformation.

So, which enables us to show that there is a limit in which this sort of Hubbard type of model can be mapped into something called a tj model which describes anti ferromagnetism ok so; that means, models that describe ferromagnetism anti ferromagnetism and so on that is magnetic insulators can be obtained by studying a suitable limit of the Hubbard model that is interesting to know because you see the Hubbard model describes itinerant electrons and coulomb repulsion.

So, it is nice to know that there is some limit in which electrons which are repelling through coulomb interaction and just moving around kinetically. There is a limit in which they behave like a magnetic material; that means, that how does magnetism ferromagnetism specifically come about or anti ferromagnetism how does it come about. After all everything is finally, made of electrons that are running around here and there and repelling each other.

So, it is nice to know that there is some limit in which magnetism comes out the magnetic material comes out of such a generic description of a solid quite naturally. So, that is worth doing and I am going to do that the first thing next class ok. So, I am going to stop here. I hope to see you in the next class for Schrieffer Wolff Transformation.

Thank you.