Advanced Condensed Matter Physics
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Lecture – 05
Second quantized Hamiltonian

So, we started with discussing propagators and a propagators for a for; in the context of quantum mechanics and then we introduced greens function and how the propagator is related to the greens function. And then we have started talking about second quantization. So, which is basically the beginning or start of the course and so, it is a good time to talk about the references which we should be referring to.

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References:

1. Quantum Many Particle systems – J.W. Negele and H. Orland (Levant Books)
2. Quantum Theory of Many Particle Systems – A.L. Fetter and J.D. Walecka (McGRAW Hill)
3. Many Particle Physics – G.D. Mahan (Springer)
4. Condensed Matter Field Theory - A. Altland and B. Simmons (Cambridge University Press)
5. Introduction to Superconductivity – M. Tinkham (Dover Publications)

So, the references are some of the references are I will probably include more references as we go along, some of them are quantum, many particle system by negele and orland it is a Levant books publication and it has an Indian edition; the quantum theory of many particle system which is a classic by Fetter and Walecka, it is a McGraw hill publication, many particle physics by Gerald D Mahan, it is a springer publication and quite a popular book, then it is a condensed matter field theory by Altland and Simmons which is a Cambridge University press publication and then for other things such as super conductivity will mostly refer to Tinkham which is dover publications and in addition to that we will refer to some other scientific articles other than books or may be research papers which we shall a site from time to time.

So, with this let us go back to the issue second quantization that we have been discussing and let us now convince ourselves that the one that the symmetrization of the quantum many particle state which was encoded in a complicated factor and which have to be summed over as we have seen in previous lecture, in equation one to be precise that can be taken care of by using states which are formed by creation and annihilation operators and this symmetrisation is actually taken care by the commutation relations of these will operators the creation and the annihilations operators. So, let us take a simple example.

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Example $\quad a_1^\dagger a_2^\dagger |0\rangle \rightarrow \underset{\substack{\uparrow \\ \text{fermions}}}{-} a_2^\dagger a_1^\dagger |0\rangle$

$$[a_1^\dagger, a_2^\dagger]_+ = 0 \Rightarrow a_1^\dagger a_2^\dagger + a_2^\dagger a_1^\dagger = 0$$

$$\Rightarrow a_1^\dagger a_2^\dagger = -a_2^\dagger a_1^\dagger$$

$\bar{\Psi}$ in terms of $a, a^\dagger$

And where I can write down a quantum state as a 1 dagger, a 2 dagger and acting on 0.

So, this if you change 1 and 2, it would go to a 2 dagger a 1 dagger and we have seen earlier that for bosons, it does not make a difference that that is there is no sign that comes in front of this the second term on your right; however, for fermions, we get a negative sign.

So, this is negative sign comes for fermions and just that this negative sign can also be obtained if we consider the anti-commutation relation of this 2 operators which is written as this which is equal to 0 and this immediately means that the a 1 dagger a 2 dagger plus a 2 dagger a 1 dagger equal to 0 a 1 dagger equal to 0 and the consequence is that that if I change the position, I will get a minus sign as you can see from here.

So, this minus sign that you are getting is actually taking care of the swapping of particle or transposition of the quadrates of the particle and hence we shall pick up a minus sign. So, I think by now, it is clear that how the tremendous work of symmetrizing ten to the power twenty 3 number of particles which is Avogadro number of particles in any system how that huge symmetrisation requirement can be taken care of by writing the many particle state in terms of the creation and the annihilation operators. So, now, we shall go ahead and talk about.

So, the how to write down a single particle operators and may be 2 particle operators or rather many particle operators in this second quantized form in terms of the creation and the annihilation operators. So, we now know how to write down a state psi in terms of a dagger, etcetera the next thing is talking about one body operators.

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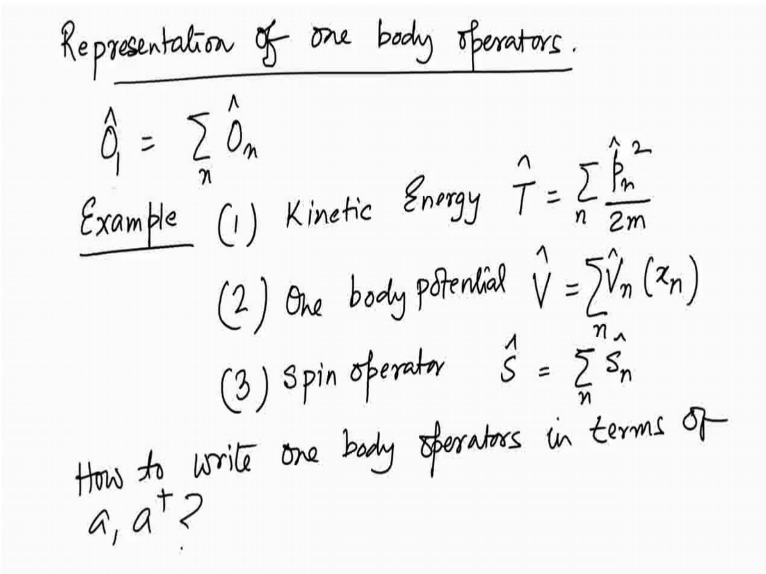

So, this is the next thing. So, representation of one body operators and there are many examples of one body operators and they would in principle be written as this and then there is a sum and then there is a n. So, we always put a cap when we particularly want to denote operators and. So, this single particle operator this sub one or the subscript one actually talk about that it is a 1 body operator. So, it is a summation over such operators for n particle where n is any number in principle can go from 0 to infinity and so, I am writing down a 1 body operator as a sum of the one body operators of a system where n refers to the number of particles or any other quantum number that is relevant for the problem and similarly we can have an example for this is. So, one example is the kinetic energy operator.

So, this kinetic energy operator talks about or this quantifies the rather it is it gives you the observable for the kinetic energy for a given system and we can write this as t which is equal to p n square over 2 m where m is the mass of the particle ok. So, this is the total energy of a system which consists of the individual energies of the particles which are represented like this, then we can have one body potential which is written like V of.

So, this will be like V n x n and sum over n here p is also an operator which can have a form which is my minus I H cross del which is the differential operator and similarly we can also have the spin operator. So, S which is a sum over n and a S n and so on. So, there are many examples of that. So, the question is that how to write one body operators in terms of the creation and the annihilation operators. So, we will write then as a dagger. So, that is the question that we are going to handle now.

So, now let us look at this problem and let us define occupation number operator, operator which is n lambda which is equal to a lambda dagger a lambda.

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Occupation number operator $\hat{n}_\lambda = a_\lambda^\dagger a_\lambda$ (1)

$$\hat{n}_{\lambda_j} |n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle = n_{\lambda_j} |n_{\lambda_1}, n_{\lambda_2} \cdots\rangle \quad (2)$$

Counts the number of particles in state λ.

$\hat{O}_1$ is assumed to be diagonal in λ basis.

$$\hat{O}_1 = \sum O_{\lambda_i} |\lambda_i\rangle\langle\lambda_i| \; ; \; O_{\lambda_i} = \langle\lambda_i|\hat{O}|\lambda_i\rangle$$

Matrix elements of $\hat{O}_1$

$$\langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots | \hat{O}_1 | n_{\lambda_1}, n_{\lambda_2} \cdots\rangle = \sum O_{\lambda_i} n_{\lambda_i} \langle n'_{\lambda_1}, n'_{\lambda_2} \cdots | n_{\lambda_1}, n_{\lambda_2} \cdots\rangle \quad (3)$$

So, this operator operates on a particle state say lambda j which. So, this is the; so, this is the operator and it is acting on a many particle state and gives me a n lambda j and then returns me back the state n lambda 1 n lambda 2, etcetera. So, it basically counts the number of particles in the state lambda. So, I will write this because this is important counts the number of particles in the state particular state lambda.

In this case we have taken lambda j as one of the representative states of this many particle system. So, if we have such a definition for an occupation number operator then we can write down any one particle operator say let us call it as o 1 as we have written earlier which considered is assumed to be diagonal in lambda basis what it means is that a o one operator equal to o lambda i and there is a. So, this is equal to a lambda i and a lambda i. So, this is the meaning that is diagonal in the lambda basis and where my o lambda i equal to a lambda i o and a lambda i.

The lambda is a particular state as we have shown that. So, now, with this nomenclature let us calculate the matrix elements of o one. So, the matrix elements of o one is written as n lambda 1 prime n lambda 2 prime there is no prime here. So, these are just the state and then I have this and n lambda 1 n lambda 2 I am sure that you know that the matrix elements of an operator is computed in this fashion. So, you squeeze it between 2 states which are from the Hilbert space.

So, n lambda prime and n lambda form the Hilbert space of the problem and then you have a, this is equal to a o lambda I n lambda I and now I will have this n lambda 1 prime n lambda 2 prime and so on and then n lambda 1 n lambda 2 and so on. So, that is my matrix elements of the one body operator which I am trying to write in terms of the creation and the annihilation operators.

So, this equality actually holds for any set of states. So, one can write down for o 1 the second quantized representation as in the following.

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$$\hat{O}_1 = \sum_{\lambda=0}^{\infty} O_\lambda n_\lambda = \sum_{\lambda=0}^{\infty} \langle \lambda | \hat{O}_1 | \lambda \rangle a_\lambda^\dagger a_\lambda \quad (4)$$

One can generalize,

$$\hat{O}_1 = \sum_{\mu\nu} \langle \mu | \hat{O}_1 | \nu \rangle a_\mu^\dagger a_\nu \quad (5)$$

Spin operator

$$(S_i)_{\alpha\alpha'} = \text{Components of the spin} = \frac{1}{2}(\sigma_i)_{\alpha\alpha'}$$

Pauli Spin matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\hat{S} = \sum a_{\lambda\alpha'}^\dagger S_{\alpha\alpha'} a_{\lambda\alpha}$$

So, your o 1 is this and so, this is a lambda equal to 0 to infinity and then there is a o lambda n lambda which is equal to a lambda equal to 0 to infinity and a lambda o 1 lambda and a lambda dagger a lambda. So, because we have said if you look at equation let us call this as equation 1 and let us call this as equation 2 this as equation 3. So, if you look at equation one then my operator o 1 is represented as the matrix element of that operator in the lambda basis as you can see and then there is a lambda dagger a lambda which is nothing, but the occupation number n lambda that is written here and let us call this as equation 4.

So, the interpretation is straight forward that single a 1 body operator enrages a single particle state at a time and then the others other states are simply just the spectators and in a diagonal representation one simply counts the number of particles in a state lambda which is given by n lambda and multiplied it corresponding to the Eigen value of the one particle operator between its Eigen states lambda and now one can generalize it to a non diagonal basis and can write this as this operator now in terms of a general basis where the operator is not diagonal in the lambda basis you can still write it as. So, this is the representation of a general representation of a 1 body operator in terms of the creation and the annihilation operators.

So, this is called as the second quantization or the second quantized notation for a 1 body operator let us take an example let us call this is equation five and now let us write down for a spin operator. So, we are giving examples and this I will write this S I operator and write the matrix elements of the S I operators between 2 states which is given by alpha and alpha prime. So, this is basically nothing, but the components of the spin in ordinary quantum mechanics you have studied spins even in a non-relativistic mechanics quantum mechanics we add spin by hand where as in the Dirac theory the realistic theory the spin comes naturally.

So, the. So, in for a spin half object the spin operator is a 2 by 2 operator and for spin one, it is 3 by 3 operator for spin half it has a special name called as a Pauli spin matrices. So, the components of the spin, this is equal to half of a sigma i and alpha alpha prime there is a H cross here in place of one, but we have taken it as this H cross has been taken as one here.

So, this is the representation of rather of a spin operator and this spin operator is going to be now written in terms of the creation and the annihilation operators. So, just before that. So, just for completeness let me introduce the Pauli spin matrices as. So, I have a sigma x which is 0 1 1 0 a sigma y corresponding to the special direction y and there is a sigma z which is 1 0 0 minus 1 the important thing about them is that the trace of all these is 0 identity sigma x and sigma y are of diagonal matrices where sigma z is diagonal. In fact, because its diagonal it is chosen as a preferred variable or the z axis is chosen as the proffered direction in most of the problems that we do in physics and. So, what I mean by trace equal to 0 is that the sum of diagonal elements is equal to 0 you can see that check that here.

So, now I can write down a spin operator as simply equal to a lambda alpha prime dagger S alpha alpha prime a lambda alpha where lambda actually denotes some other quantum number and here it is basically the space variable. So, lambda denotes a space variable such as x and y. So, this is the representation of the spin operator in the second quantized notation where we have written as. So, this is the matrix element S alpha alpha prime is the matrix element as we have shown in above and then a lambda dagger and a lambda alpha etcetera they are creation and annihilation operators let us do an another example which is of used to us let us do it for the kinetic energy and. So, we can also do it for.

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Kinetic energy and a one body potential

$$\hat{H} = \int d^d r\, a^{\dagger}(\vec{r})\left[\frac{\hat{p}^2}{2m} + V(\vec{r})\right] a(\vec{r})\,;\quad \hat{p} = -i\hbar\vec{\nabla}$$

A local density operator

$$\rho(\vec{r}) = a^{\dagger}(\vec{r})\, a(\vec{r})$$

Kinetic energy and a 1 body potential and this will specifically write in the real space basis.

So, a Hamiltonian consisting of the kinetic energy and a 1 body potential is written as d d r a dagger r and there is a p square over 2 m plus a V of r and. So, these rs are so, these are vectors and written as this and. So, this is the Hamiltonian which consists of a kinetic energy and a 1 body potential the kinetic energy is given by p square over 2 m and. So, and this V of r is just a potential at a given site r and a p is written as minus i H cross del where del is a operator it is a differential operator that acts on space.

And similarly, a local density operator can be written as rho of r equal to a dagger r a r and in the above example, you see that we have written it because r is a space variable in continuum in the continuum representation we have written it as an integral instead of a sum and this integral is taken in d dimensional. So, it is a d d r. So, where as in 3 dimension we would write it as d cube r or you can write it as a volume integral d V the same thing.

So, now having done the one body operator, let us talk about the 2 body operator representation of 2 body.

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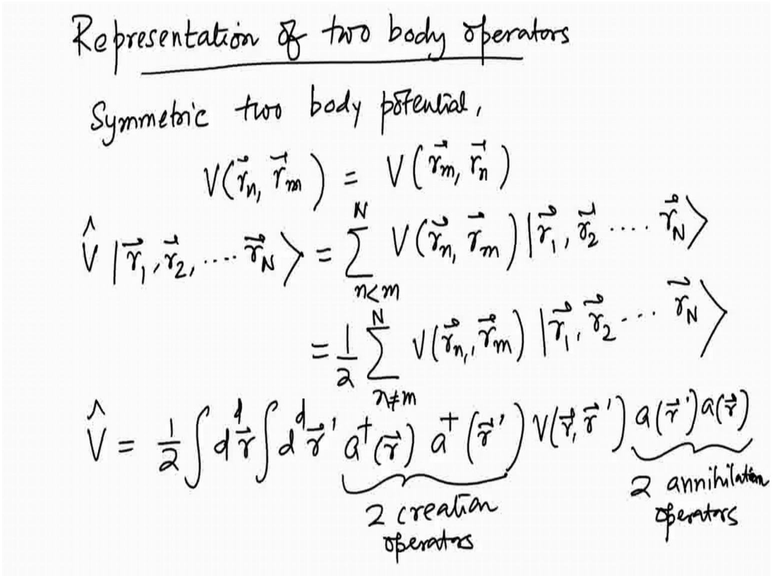

So, these 2 body operators are used to denote pair wise interaction between particles. So, whenever 2 particles are interacting with each other by a potential which could be of any form which could have form such as one over r which is called as a Coolum interaction or for that matter any other form of interaction then this called as a 2, we need a 2 body operator to represent that and in principle, we can do it for any n body operator.

However, interaction potential is beyond the 2 body term is not something that we encounter in physical problems or we see in physical problems and that is why we shall restrict ourselves to a 2 body operator and that could be good enough for writing a Hamiltonian for a system for a many particle system. So, let us see how we can do that and for doing that we know that in classical problems there is no sort of it can be written straight forwardly because of the distinguishability of particles; however, in quantum many body theory or quantum mechanics the indistinguishability makes it somewhat harder to write.

So, let us take a symmetric potential symmetric 2 body potential by symmetric what I mean is that V r n r m where m n and m, they refer to 2 sides may be and this is equal to V r m r n. So, the potential or the interaction potential that one body exerts one body at n exerts on another body at m is the same as the interaction potential that is exerted by the body at m and on n. So, this is we have now. So, we will write this as. So, we will take a real space representation and these are vectors and we have say we are going from initially we have started with a coordinate representation or a position representation for a many particle state and then we had gone to a occupation number or the number operator formalism and now, in this particular case, we are coming back to the real space representations, but ultimately you will have to write down a Hamiltonian in the same basis or rather if you have to solve it, you have to do it on the same basis; however, here we prefer to do it in the real space basis and we write it as this V r n r m, we can put vectors here as well and this is equal r 1, r 2 and there is a r n.

So, this is where we have to restrict the sum to all n values which are less than m otherwise we would be double counting because V r n r m is same as V r m r n if we do not have this constraint then we would be double counting this interaction term; however, it is difficult to keep track of these indices one being less than the other. So, it is easier to introduce a factor of half and write this as n equal to or n not equal to m and it goes like this.

So, this is my representation of the 2 body operator written. So, as it acts on a basis state that is given by this. Now we can take a a 2 body interaction term in vacuum as this is equal to a half and again written as a d d r and a d d r prime and e dagger r a dagger r prime and V r r prime a r prime a r. So, that is the that is the form of the potential or a 2 body potential this see that it contains 2 creation operators and 2 annihilation operators as opposed to the one body term which contain one creation operator and one annihilation operator.

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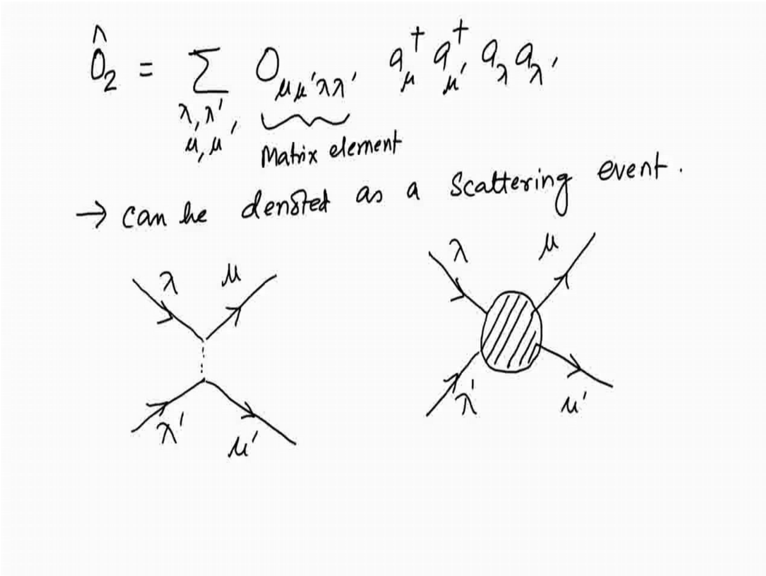

Now, this can be written as in the general sense and in any basis just like what we have done it for the one body operator we will write the 2 body operator as. So, this is written in terms of scattering events I will describe how and this is equal to lambda lambda prime and a mu prime and then this is o mu, mu prime lambda lambda prime and there is a mu dagger a mu prime dagger a lambda a lambda prime.

So, this is the matrix element of the 2 body operator between 2 states mu, mu prime and lambda lambda prime. So, what happens is that a state form lambda and so, one particle from a state lambda and another particle from the state lambda prime they scatter on to 2 states mu and mu prime. So, these are annihilating lambda and lambda prime are annihilating and they are getting created in the state as in the mu and mu prime states. So, this is the matrix element of the 2 body operator in the mu, mu prime and lambda lambda prime states and these are the corresponding creation and annihilation operators.

So, it could happen that mu equal to mu prime or mu equal to lambda and mu prime equal to lambda prime all that can happen, but in principle this can be denoted as scattering event. So, I will draw that scattering event a pictorial representation of that scattering event can be like this and there is some interaction there and it could be going like this. So, there is a lambda coming. So, a particle from a state lambda is coming a particle from a state lambda prime is coming and they are getting created in mu and mu prime, it could also happen that the lambda goes to mu prime and lambda prime goes to mu, but that is equally a possibility for this scattering problems this.

So, this is a simplest vertex that we can think of or there could be more complicated vertices which take away you know some energy momentum which we will learn when we are doing going to do a Feynman diagrams. So, in those cases we will see that we have a vertex having a structure and that structure will depend upon the specifics of the interaction term that could actually depend upon the interaction term can actually depend upon a. So, here the interaction amplitude of the interaction term is constant, here, it could depend upon r or it could depend upon spin or it could depend upon momentum and then we have them getting recreated here. So, we have a lambda and the lambda prime and they are getting recreated as mu and a mu prime.

So, these are the basic representations of the 2 particle operators. So, now, I will summarize that; we now know how to write down a many particle state in terms of creation and annihilation operators and we also know how to write down one particle operator and 2 particle operator in the second quantized notation.

So, once again I reiterate that the name second quantization is justified as we have been able to write down both the state and the operators that represent observables in the quantized notation or what we call as second quantization where both of these quantities are represented as operators the creation and the annihilation operators and to end the discussion the proper symmetry requirements of fermions or bosons are encoded in the anti commutation and the commutation relations respectively in these problems. So, we shall wind up this discussion with an example which is for the 2 body spin-spin interaction.

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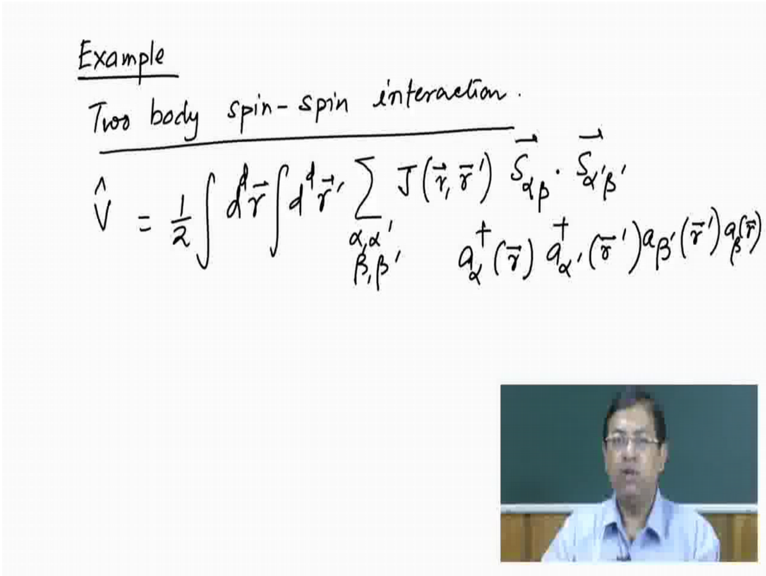

That is we are going to talk about a Hamiltonian where the only interaction that is there is a via 2 spins and they would be interacting in a particular way and this is a in a spin only model and that we would be writing it as a half factor to avoid double counting and then there is a d d r d d r prime and I have a alpha alpha prime beta, beta prime and there is a amplitude which is given by that is amplitude of the spin-spin interaction which is given by j r r prime and there is a S alpha beta dotted with S alpha prime beta prime and now I will write the.

So, r and a alpha prime dagger r prime and I also have a beta prime r prime and a beta r. So, this is a typical example of a 2 body interaction for a spinner system where 2 spins are interacting via potential which is given like this, we will get into more examples later.