Lectures on Quantum Mechanics

Wave Mechanics of a Particle With Spin

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Note This document contains gray boxes. These boxes record a short account of discussion that took place in the summer course with the students.

1 Introduction

Today I am going to describe how you do wave mechanics of particle with spin half. I have decided to pull this topic early in the course for several reasons. Normally in a regular course and in most text books this topic comes. I wish to introduce it as early as possible.

There are several reasons for this. For one thing it is an important topic. When we want to compute some predictions of quantum mechanics and compare it with experimental data, we have to bring in spin at some stage.So let me ask what is spin?

Secondly, to describe, as we will see, spin is very easy.

The third reason is that the way I have organised this course is to emphasize how postulates are applied to solve problems. I wish to illustrate how postulates are applied to solving problems. The postulates give you starting point to solve the problem. For most problems you want to solve you will need to go back to the postulates.

Time dependent Schrodinger equation (TDSE) has been my starting for free particle and rigid box problems, If we know the wave function at initial time, solving TDSE gives you wave function at any time. This can be used to compute any measurable quantity and compare with experiments. How do you do computations is contained in the third postulate (Measurement postulate).

What all we wish to compute? Average values, probabilities, wave fucntion at a later time etc.

We have seen how all this is computed for free particle and for particle in a box. I am going to repeat story for a particle with spin. So that you can understand postulates. You will that calculation part, *i.e.* the algebra, is very simple as compared to other situations.

What all we need to start? You will need to recall the postulates. I have finished typing postulates for you and print copies and give you a copy each. Once you have a it copy, you must bring this print out in every lecture.

So let us start. The questions that we need to answer are :

- **Q1: What is spin?**
- **Q2: How do we describe a particle with spin in quantum mechanics?**
- **Q3: How do we compute various properties and observables quantities?**

2 What is spin?

You have already learned how to do wave mechanics of a particle without spin. We have to start with it wave function. What is wave function of a spin one particle? for spin one particle? and so on.

Before we take up question number two, let me ask you what do you understand by spin. An earlier lecture "Rise of Wave Mechanics" has a brief description of why spin was needed? when it was introduced? and by whom?

Spin is a new concept, whenever you come across a new concept like this do not accept until you have understood very precisely.

Let us discuss

So let me ask what is spin?

`Ans 3:    Spin is a measurable quantity.`

Priyanka's answer is very good answer and will be starting point for my discussion.

We understand what is position, momentum, acceleration etc. from our school days. This answer does not give me any understanding of spin. But answer does not give me any understanding in the same sense. The above statement does not tell me what is spin all about?

Let us discuss

So give me some more answers.

Ans: `Spin is a angular momentum of a point particle at rest. It is a measurable quantity.`

Que: *So if it is angular momentum of the particle at rest, how is it different from* $\vec{r} \times \vec{p}$*?*

Ans: `For a point particle the angular momentum` $\vec{r} \times \vec{p}$ `is zero.`

Que: *Why is it zero?*

Ans: `Because the particle is at rest.`

I will explain Chetan's answer. Suppose we have a point particle. In classical theory its state is described by position and momentum. For a particle at rest the momentum is zero. Therefore $\vec{L} = \vec{r} \times \vec{p}$ is zero. When we say that electron has spin half, it means it has angular momentum $\frac{\hbar}{2}$ in addition to orbital angular momentum that particle $\vec{L} = \vec{r} \times \vec{p}$.

Note that a **point particle** cannot have angular momentum other than $\vec{L}$; a rigid body can. So for example a ball or this duster can rotate and have angular momentum even if its center of mass is at rest.

Thus spin of a point particle is an extra angular momentum on top of orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$. This is an new thing that is coming from experiments. You have to keep asking questions. Why does one need it? and so on. You have to keep asking questions like lawyers will ask twenty questions in a court?

So let us recall where (which experiment?) spin came from. Why was it introduced? It was first introduced for electron. Remember that an electron is a charged particle, angular momentum for a charged particle comes with magnetic moment. So does spin angular momentum for an electron. Thus an electron has magnetic moment associated with orbital angular momentum and and an extra magnetic moment associated with spin angular momentum.

The extra magnetic moment is sometimes called intrinsic magnetic moment. This gives rise to observable effects in Zeeman effect and spectral lines. A 'part' of Zeeman effect, *normal Zeeman effect* could be explained as coming from orbital motion. A 'part' could not be explained that way and required introduction of spin and associated magnetic moment.

You know that the sodium yellow line has a fine structure and actually consists of two line of wave lengths 5890 A and 5896 A. All atomic spectra exhibit a fine structure. This is now explained in terms of intrinsic magnetic moment.

Let us discuss

Q: `If a particle is moving in a straight line, it has angular momentum?`

Ans: *Yes it has angular momentum. If a particle is moving in a circle it has angular momentum. In general use* $\vec{r} \times \vec{p}$.

Q: `Then, what will be the total angular momentum for such a particle (`*i.e.*` for a particle with spin)?`

Ans: *The total angular momentum will be a sum of orbital and spin angular momenta. In QM addition of angular momenta is different and has to be taken up separately.*

If I have a new particle discovered today, how will the spin be measured? One can, for example, do a Stern Gerlach kind of experiment? This will work for a particle which has sufficiently long life time. Electron is stable and does not decay so one can use Stern Gerlach experiment. How do you fix spin of a particle having extremely short life time, for example $10^{-24}s$? There are several indirect methods that can be used. For example, one could use conservation of law of angular momentum to determine spin experimentally.

This is about all I want to say in answer to Q1 posed in the beginning.We now move on to the second question:

Q2: How do we describe a particle with spin in quantum mechanics?

3 Quantum mechanics of a particle with spin

So we have a particle with some extra angular momentum. This extra angular momentum is in addition to the orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$. The angular momentum $\vec{L}$ will be called *orbital angular momentum*, and the extra angular momentum will be called *spin angular momentum* or spin.

Now we want to do quantum mechanics of particle with spin. We want to do quantum mechanics because electrons protons cannot be described by classical theory and also because spin is a quantum effect.

How do we describe a a particle with spin in quantum mechanics? We get back to postulates. This where the answer Ans 3, (given above on page 3), becomes important. Spin is a measurable quantity, it is a dynamical variable. The postulates of quantum mechanics tell us that the spin is represented by hermitian operator(s).

Remember Me: Spin will be represented by some hermitian Operator(s)

But this statement "...some operator(s).." is very vague and we cannot hope to do any calculations making use of this statement. This gives us only a starting point and it does not point to you any scheme of calculations.

Now we have said that spin is angular momentum at rest. So spin should have all the properties of angular momentum.Let us see how far we can go. Angular momentum is a vector quantity so we should have *three hermitian operators* S_x, S_y, S_z, one operator will not do.

We have made some progress. But still we cannot do any calculations. We have only said that there should be three operators for spin. It is like saying that position and momentum become operators in quantum mechanics;just saying this does not give any scheme of calculation. We need commutators. Remember what I said about canonical quantization. For position and momentum operators the canonical quantization postulate gives commutators and that's a powerful tool for doing calculations. In fact it contains all quantum mechanics.

So we need to make a guess for commutators of spin operators. Can we guess what should assume for commutators of spin operator.

Let us discuss

Que: *What is your guess?*

Ans: `Spin operators commute with themselves.`

Rem: *Why? Do the angular momentum operators commute? NO!*

Remember Me:

So we should assume that the spin commutators to be same as that for angular momentum. So my next statement is that we know the commutation relations for angular momentum. So we write the same thing for spin. Thus we assume

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y. \tag{1}$$

With these equations, the quantum mechanics of spin is over. We do not need any more information. What we ever want to know, or we want to compute, will come out of the commutation relations.

You might want to know what kind of wave function an electron will have or a spin one particle will have. All this can be inferred from the commutation relations. Heisenberg did not have wave functions. All quantum could be done using commutators. Pauli could derive Hydrogen atom energy levels using commutation relations. Heisenberg did not have wave function; wave function came later.

Wave functions are useful. All the information about wave functions will come out of commutators. Only thing that is required is that you must know your mathematics well and you must know how to use postulates.

So we add some more information that for a point particle, each spin operator commutes with position and momentum operators. The basis for assuming this is that there is no evidence that there is uncertainty relation between spin and position (or momentum).

OK, there, you have some question? Tell me.
Go ahead and ask your question.

Let us discuss

Q: `If a particle is moving in a straight line, does it have angular momentum?`

Ans: *Yes it has angular momentum. If a particle is moving in a circle it has angular momentum. In general use* $\vec{r} \times \vec{p}$.

Q: `Then, what will be its total angular momentum?`

Ans: *The total angular momentum will be a sum of orbital and spin angular momenta. In QM addition of angular momenta is different and has to be taken up separately.*

Remember Me:

So will also assume that

$$[\vec{S}, x_k] = 0, \qquad [\vec{S}, p_k] = 0. \qquad k = 1, 2, 3. \tag{2}$$

Another justification for assuming the above commutators is that whatever we predict, using the above commutation rules, this agrees with experiments. There is no contradiction with experiments. So these assumptions are fine.

Now next question is what can we do with the spin operators using commutation relations. You have already done one course. You have seen ladder operators.You have seen how eigenvalues of J^2, J_z can be computed using commutation rules only. All those results were obtained using commutation rules only and the commutators for spin are assumed to be the same. Therefore we can adopt all the results from theory of angular momentum. Thus we have the following results:

- $\vec{S}^2$, commutes with S_x, S_y, S_z.
- Sr has eigenvalues $s(s+1)\hbar^2$, where $s = 0, 1/2, 1, 3/2, \dots$.
- For a given value s of spin, the z component will have a value $m\hbar$ can be one of the $(2s+1)$ values $m = -s, -s+1, \dots, s$.
- S^2 and S_z commute so they will have simultaneous eigenvectors. Let us denote the simultaneous eigenvectors by $|s, m\rangle$. Then we have

$$S^2|s,m\rangle = s(s+1)\hbar^2|s,m\rangle, \qquad S_z|s,m\rangle = m\hbar|s,m\rangle \tag{3}$$

- If we define $S_\pm = S_x \pm S_y$, then $S_\pm$ act like ladder operators for S_z. Thus we write

$$S_\pm|s,m\rangle = \sqrt{s(s+1) - m(m\pm 1)}\,\hbar\,|s, m\pm 1\rangle \tag{4}$$

Thus if we measure total spin, S^2, the answer will be $s(s+1)\hbar^2$ and a measurement of S_z will give one of the values between $-s\hbar$ to $+s\hbar$. Remember, the total spin is like mass and charge of a particle. Just as mass and charge do not change and remain the same, the spin, value of s remains the same for particle of a particular species. A spin two particle will always remain spin two particle. But its S_z can change and have any one of the values(-2,-1,0,1,2).

For an electron spin s is always half, only S_z can change from time to time taking values $\pm 1/2$.

Let us assume that we are interested only in spin properties of a particle and we are not interested in its position and momentum. Take for example a nucleus bound inside a lattice. It motion may be neglected in certain situations. Consider a particle going through a magnetic field as in a Stern Gerlach experiment. Here we only want to know. "what pattern we see on the screen? in how many parts the beam splits?" In situations we can ignore the orbital motion and concentrate only on spin degrees of freedom.

The wave function has the information about probability amplitudes for different outcomes of a measurement.

What else do you want to know about quantum mechanics of a particle with spin? We want to know more about its wave function and how they act on wave function. . For sometime our discussion of spin wave function etc. will be carried out for electrons only.

We must list all possible values of a **commuting set** of hermitian operators. A commuting set means that operators in the set commute pair wise; each operator in the set commutes with every other operators from the same set.

We note that S^2, S_z is a commuting set. We cannot add any other spin operator, such as $S_x 0 r S_y$, because that operator will not commute with S_z.

To understand what is the wave function of a system we must ask what all can be measured simultaneously and list all possible combination of eigenvalues.

Let us list possible values for a complete set commuting set of operators, S^2, S_z, for an electron. These are just combination of eigenvalues of S^2, S_z as listed below.

Possible values of commuting observables

S^2	S_z
$\frac{3}{4}\hbar^2$	1/2
$\frac{3}{4}\hbar^2$	- 1/2

The wave function should tell us the probability amplitudes for all possible combinations of simultaneously measurable quantities. In our case about probability amplitudes for all combinations of S^2, S_z for a particle. Now S^2 for a particle, like mass and charge has a fixed, value. Thus wave function should give me one probability amplitude value of S_z and nothing less or nothing more.

The wave function is just the complete information about all such probability amplitudes. So,ignoring position and momentum, and restricting our attention to spin only the complete information about all possible probability amplitudes requires only two complex numbers α, β giving probability amplitudes for the two outcomes listed in the above table. The wave function – spin part – is just these two numbers. Thus an electron wave function can be written as a two component column vector:

$$\chi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{5}$$

Actually this is not the full wave function we have ignored the coordinates and momenta. So we will call χ as spin wave function. Thus spin wave function of a spin half particle is a two component column of complex numbers.

Any question about spin can now be answered if we know the spin wave function. For example, we can compute average value of any component of spin; we can compute the ratio of probabilities of S_y having values $\pm 1/2$, and so on.

I will summarize the situation for a spin half particle. The spin wave function of a spin half particle is a column vector of two complex numbers as in χ of (6). Then $|\alpha|^2$ gives the probability of spin being up and $|\beta|^2$ gives the probability of spin being down (along z- axis). For an electron there is nothing more to be done. All questions regarding spin alone can be answered in terms of spin wave function and spin operators. You will learn more about spin operators in the next lecture.

I am not going stop at spin 1/2 particle.Most people and text books will stop at spin half particle.I will giving you problems on spin one, spin 3/2 and spin 2.

So for example, we may want to know how does spin wave function for look for a spin one particle. The spin operators obey the same commutation rules. We can only measure $S^2 and S_z$ simultaneously. The value of S^2 for a particle is in any case is a single value $s(s+1)\hbar^2$. The possible S_z values are 1,0,-1. So list all possible out comes of simultaneous measurement of S^2 and $S_z$in a table similar to spin half given previously.

Possible values of commuting observables

S^2	S_z
$2\hbar^2$	1
$2\hbar^2$	0
$2\hbar^2$	-1

The wave function should tell us all three probability amplitudes for the above three possibilities. If we write complex numbers for each of these outcomes, we get three component wave function.

$$\chi = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \tag{6}$$

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