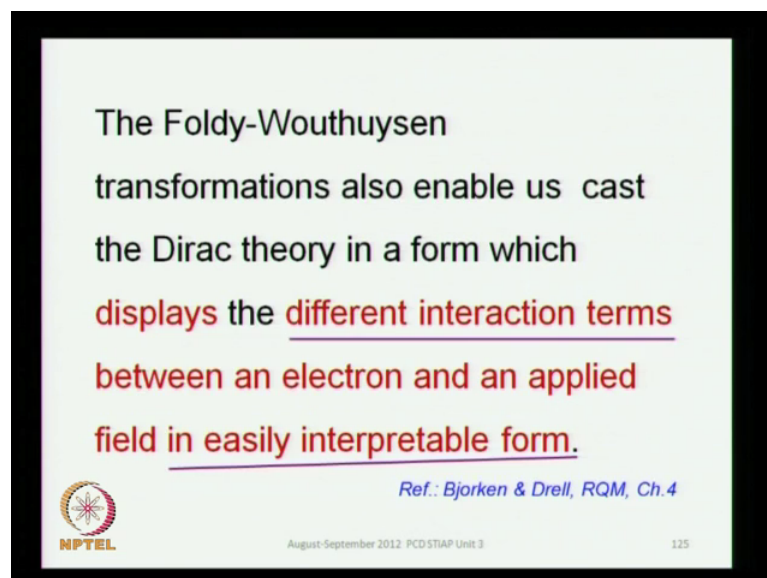


Select/Special Topics in Atomic Physics
P. C. Deshmukh
Department of Physics
Indian Institute of Technology, Madras

Lecture - 17
Relativistic Quantum Mechanics of the Hydrogen Atom

Greetings, so we begun to get some feel about the Foldy Wouthuysen transformations, and essentially the Foldy Wouthuysen transformations achieve quite a large, but one thing that I want to draw your attention to is this remark from Berok and Drels book.

(Refer Slide Time: 00:38)




That they help us to see different interactions of an electron with the electronic field in a form that we can really recognize, we can interpret easily that is a kind of form that we see in various books, if you read Banson and Jhosan books physics atoms and molecules, you will see various terms. You know which are referred to relativistic terms, spin orbit interaction and so on, but those the terms are not directly manifested in the Dirac equation. They involve the Foldy Wouthuysen transformations help us achieve is to display them, in a form that can be very easily interpreted.

(Refer Slide Time: 01:21)

$$\begin{aligned}
 H &= \beta mc^2 + c\vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) + e\phi \\
 &= \beta mc^2 + 0 + \varepsilon \\
 H' &= e^{+iS_1} H e^{-iS_1} + e^{+iS_1} \left(-i\hbar \frac{\partial}{\partial t} \right) e^{-iS_1} \\
 H' &= \beta mc^2 + \varepsilon' + \theta' \\
 \text{where} \\
 \varepsilon' &= \varepsilon + \frac{\beta\theta^2}{2mc^2} - \frac{\beta\theta^4}{8m^3c^6} - \frac{1}{8m^2c^4} [\theta, [\theta, \varepsilon]] - \frac{i}{8m^2c^4} [\theta, \dot{\theta}] \\
 \theta' &= \frac{\beta}{2mc^2} [\theta, \varepsilon] - \frac{\theta^3}{3m^2c^4} + \frac{i\beta\dot{\theta}}{2mc^2}
 \end{aligned}$$

The leading 'odd' term is now of order $\mathcal{O}\left(\frac{1}{m}\right)$



August-September 2012 PCD STAP Unit 3 126

So, our basic problem is right here, that you have the Hamiltonian, which contains the odd operators, and you want to transfer it to different representation using this transformation relation that we have discussed. And our objective is to make the transform Hamiltonian, relatively free from the odd operator, we cannot make it completely free from the odd operators, but as much as we can. So, we discussed the first Foldy Wouthuysen transformation, and then you have the leading odd term, which is of the order $1/m$.

(Refer Slide Time: 02:15)


To reduce the importance of the 'odd' terms further:

II FWT: $S_2 = \frac{-i\beta\theta'}{2mc^2}$

$$H'' = e^{+iS_2} H' e^{-iS_2} + e^{+iS_2} \left(-i\hbar \frac{\partial}{\partial t} \right) e^{-iS_2}$$

$H'' = \beta mc^2 + \varepsilon'' + \theta''$ III FWT: $S_3 = \frac{-i\beta\theta''}{2mc^2}$

$$H''' = e^{+iS_3} \left(H'' - i\hbar \frac{\partial}{\partial t} \right) e^{-iS_3} = \beta mc^2 + \varepsilon'$$

$$H''' = \beta mc^2 + \varepsilon + \frac{\beta\theta^2}{2mc^2} - \frac{\beta\theta^4}{8m^3c^6} - \frac{1}{8m^2c^4} [\theta, [\theta, \varepsilon]] - \frac{i}{8m^2c^4} [\theta, \dot{\theta}]$$


August-September 2012 PCD STAP Unit 3 127

And then what we are going to do is to have another Foldy Wouthuysen transformation, and now you subject the first transform hamiltonian to the second Foldy Wouthuysen transformation which is s 2, which is through this operator. And now, you get a transform Hamiltonian which is h double prime, and now you do it one more time following the same procedure.

So, we have seen how to work out this algebra, it is little laborious it is fun to do, and when you do it third time you get a transform Hamiltonian, which is free from the odd operators to a very satisfactory extent. And this is the form you get, for the Hamiltonian in the Dirac Hamiltonian, in the representation after subjecting the original Hamiltonian to three successive Foldy Wouthuysen transformations. Now, you know what these operators α and β are, these are the short forms for the various terms that we introduced earlier.

(Refer Slide Time: 03:39)

$$H'' = \beta mc^2 + \epsilon + \frac{\beta \theta^2}{2mc^2} - \frac{\beta \theta^4}{8m^3 c^6} - \frac{1}{8m^2 c^4} [\theta, [\theta, \epsilon]] - \frac{i}{8m^2 c^4} [\theta, \dot{\theta}]$$

$$\frac{\theta^2}{2mc^2} = \frac{\left(c\vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) \right)^2}{2mc^2} = \frac{1}{2m} \left\{ \vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) \right\} \left\{ \vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) \right\}$$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m} \left\{ \begin{pmatrix} \vec{0} & \vec{\sigma} \\ \vec{\sigma} & \vec{0} \end{pmatrix} \cdot \vec{\pi} \right\} \left\{ \begin{pmatrix} \vec{0} & \vec{\sigma} \\ \vec{\sigma} & \vec{0} \end{pmatrix} \cdot \vec{\pi} \right\}$$

$$= \frac{1}{2m} \begin{pmatrix} \vec{0} & \vec{\sigma} \cdot \vec{\pi} \\ \vec{\sigma} \cdot \vec{\pi} & \vec{0} \end{pmatrix} \begin{pmatrix} \vec{0} & \vec{\sigma} \cdot \vec{\pi} \\ \vec{\sigma} \cdot \vec{\pi} & \vec{0} \end{pmatrix}$$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m} \begin{pmatrix} \vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi} & 0 \\ 0 & \vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi} \end{pmatrix}$$

$$= \frac{1}{2m} \vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi} \mathbf{1}_{\text{tot}}$$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m} \{ \vec{\pi}^2 + i\vec{\sigma} \cdot \vec{\pi} \times \vec{\pi} \} \mathbf{1}_{\text{tot}}$$

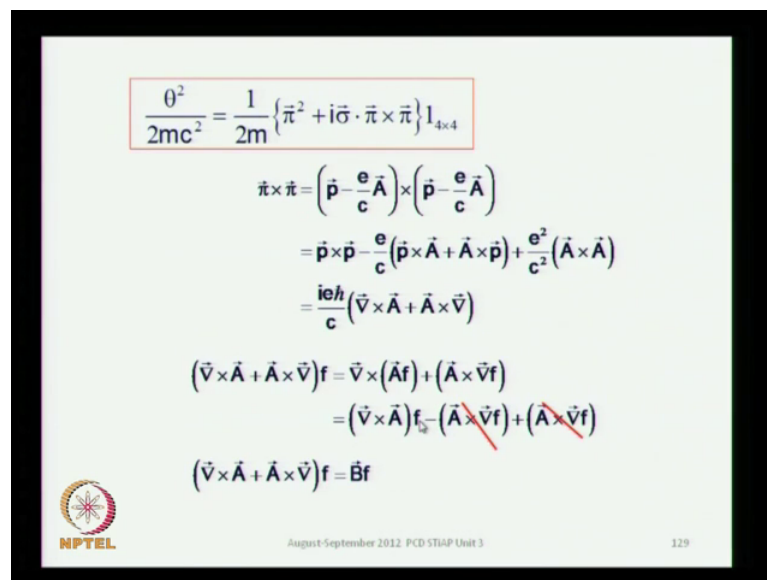
August-September 2012 PCD ST&P Unit 3
128

And if you look at it you still need to evaluate all this commutator, and their number of terms to work with, and we will suggest you how these terms are analyzed, or at least you know the general trend in that analysis of this, so that you can work out the details. So, look at this term this is theta square by twice m c square, which is appearing here, so let us see its explosive form theta is the c alpha dot p minus c over c by a. So, now, I am using the Gaussian units, which is what I need to use, and some of the earlier relations, I

think very natural units, where I have put c equal to 1, and you know it cross was also z equal to 1.

So, here we have placed them, and now you have this α dot, this generalized momentum, and then you have the square of it, so now, if you plug in the expression for α which is this matrix operators $0 \sigma \sigma 0$. Then you get σ dot π and σ dot π from these terms, and you can write this a σ dot π σ dot π times the unit 4 by 4 matrix. And for σ dot π σ dot π , you can use the poly identity which we have used a number of times as a matter of fact, we are going to use it quite often it is something, which gets very extensively used.

(Refer Slide Time: 05:36)



$$\frac{\theta^2}{2mc^2} = \frac{1}{2m} \left\{ \vec{\pi}^2 + i \vec{\sigma} \cdot \vec{\pi} \times \vec{\pi} \right\} 1_{4 \times 4}$$

$$\vec{\pi} \times \vec{\pi} = \left(\vec{p} - \frac{e}{c} \vec{A} \right) \times \left(\vec{p} - \frac{e}{c} \vec{A} \right)$$

$$= \vec{p} \times \vec{p} - \frac{e}{c} (\vec{p} \times \vec{A} + \vec{A} \times \vec{p}) + \frac{e^2}{c^2} (\vec{A} \times \vec{A})$$

$$= \frac{ie\hbar}{c} (\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla})$$

$$(\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla}) f = \vec{\nabla} \times (\vec{A} f) + (\vec{A} \times \vec{\nabla} f)$$

$$= (\vec{\nabla} \times \vec{A}) f - \cancel{(\vec{A} \times \vec{\nabla} f)} + \cancel{(\vec{A} \times \vec{\nabla} f)}$$

$$(\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla}) f = \vec{B} f$$

NPTEL
August-September 2012 PCD STAP Unit 3
129

So, this is our explicit expression for this term, and we have to analyze this further, so this is what we get for one of the terms in the transform Hamiltonian. Now, you need the π cross π over here, which will involve this thrall of a operator and a dot del operator, but then we have studied this. That this is operator and this will operate on an operand and we have done this analysis earlier, we should always be very careful whenever we have the gradient operator.

So, this is not just the magnetic field B , but it is the del cross a operator, which should operate on an operands, so you will end up taking the curl of a product of A and f . So, when you do that then these two terms cancel, and you get the magnetic field coming from this, so that is what will go here.

(Refer Slide Time: 06:34)

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m} \left\{ \vec{\pi}^2 + i\vec{\sigma} \cdot \vec{\pi} \times \vec{\pi} \right\} 1_{4 \times 4}$$

$$\vec{\pi} \times \vec{\pi} = \frac{ie\hbar}{c} (\vec{v} \times \vec{A} + \vec{A} \times \vec{v})$$

$$\vec{v} \times \vec{A} = (\vec{v} \times \vec{A}) - \vec{A} \times \vec{v} \equiv \vec{B} - \vec{A} \times \vec{v}$$

Note the difference!

$$(\vec{v} \times \vec{A} + \vec{A} \times \vec{v}) \mathbf{f} = \vec{B} \mathbf{f}$$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m} \left\{ \vec{\pi}^2 - \frac{e\hbar}{c} \vec{\sigma} \cdot \vec{B} \right\} 1_{4 \times 4}$$

contributes to $\frac{\beta \theta^2}{2mc^2}$ in H^m

NPTEL August-September 2012 PCD STIAP Unit 3 130

And now, you have the magnetic field and that tells you that this theta square twice m c square operator is this pi square over 2 m, and then with this i sigma dot pi cross pi term, for which we use this relation, we get e h crossover c times sigma dot B. So, this is a term, which will contribute to the beta theta square over twice m c square, in the transform Hamiltonian.

(Refer Slide Time: 07:09)

$$H^m = \beta \left(mc^2 + \frac{\theta^2}{2mc^2} - \frac{\theta^4}{8m^3c^6} \right) + \varepsilon - \frac{1}{8m^2c^4} [0, [\theta, \varepsilon]] - \frac{i}{8m^2c^4} [\theta, \dot{\theta}]$$

$$H^m = \beta \left(mc^2 + \frac{\theta^2}{2mc^2} - \frac{\theta^4}{8m^3c^6} \right) + \varepsilon - \frac{1}{8m^2c^4} \left\{ [0, [\theta, \varepsilon] + i\dot{\theta}] \right\}$$

$$[0, \varepsilon] + i\dot{\theta} = c [\vec{\alpha} \cdot (\vec{p} - e\vec{A}), e\phi] + ic \frac{d}{dt} (\vec{\alpha} \cdot \vec{\pi})$$

$$= c [\vec{\alpha} \cdot \vec{p}, e\phi] - ce [\vec{\alpha} \cdot \vec{A}, e\phi] + ic \left\{ \left(\frac{d\vec{\alpha}}{dt} \right) \cdot \vec{\pi} + \left(\vec{\alpha} \cdot \frac{d\vec{\pi}}{dt} \right) \right\}$$

$$[0, \varepsilon] + i\dot{\theta} = -i\hbar ec [\vec{\alpha} \cdot \vec{V}, \phi] + ic \left\{ \left(\frac{d\vec{\alpha}}{dt} \right) \cdot \vec{\pi} + \left(\vec{\alpha} \cdot \frac{d\vec{\pi}}{dt} \right) \right\}$$

$$[\vec{\alpha} \cdot \vec{V}, \phi] \mathbf{f} = (\vec{\alpha} \cdot \vec{V} \phi - \phi \vec{\alpha} \cdot \vec{V}) \mathbf{f}$$

$$= \vec{\alpha} \cdot \vec{V} \phi \mathbf{f} - \phi \vec{\alpha} \cdot \vec{V} \mathbf{f} = (\vec{\alpha} \cdot \vec{V} \phi) \mathbf{f} + (\vec{\alpha} \cdot \vec{V} \mathbf{f}) \phi - \phi \vec{\alpha} \cdot \vec{V} \mathbf{f} = (\vec{\alpha} \cdot \vec{V} \phi) \mathbf{f}$$

NPTEL August-September 2012 PCD STIAP Unit 3 131

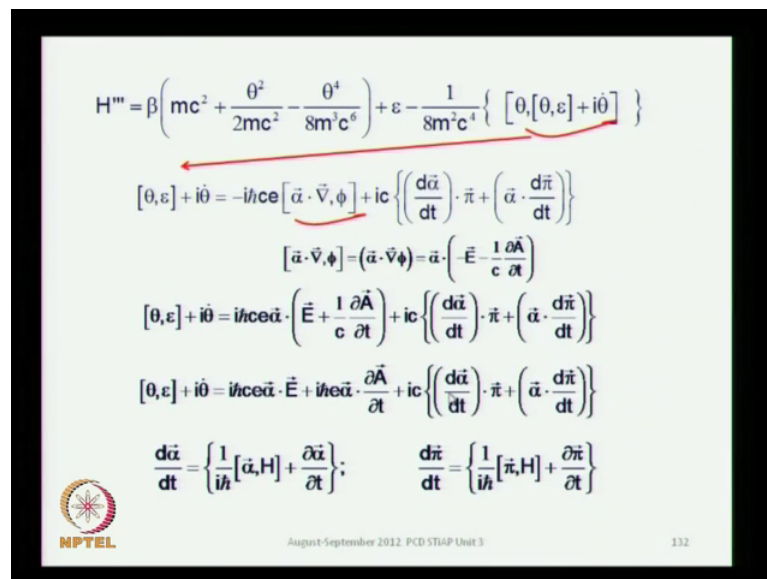
But, there are the other terms there is this beta theta square over twice m c square, there are plenty of other terms you work with. So, let us have a look at this one, this is theta

comma e plus i theta dot, and we have some indications of all these terms to be used, so substitute the terms explicitly. So, theta is c times alpha dot the generalized momentum which is phi minus e A, then this epsilon is e phi, so all I have done is to substitute these terms, and I have a time derivative of this scalar product of these 2 operators.

So, I get d alpha by d t dot p plus alpha dot d pi by d t, but the rate of change of any operator d omega by d t you get it from the Heisenberg equation of motion, so you can use that and insert it. So, first of all this term would go away, this is not going to contribute anything, this commutator would go to 0, then we have this a dot alpha dot gradient term. And again we have to remind ourselves that whenever we see the gradient term, you have to be careful with that operator because this is a commutator of alpha dot del with phi.

So, this commutator is alpha dot del phi minus phi alpha dot del, operating on f and if you follow the same reasoning as we did in earlier. You see that these two terms cancel, and you are left with only alpha dot del phi, so that is what you have got from this commutator. So, from this commutator that two terms, which reduced to a single equivalent operator, which is alpha dot del phi, and we will use this over here, and then simplify this relation for combination of these two terms.

(Refer Slide Time: 09:18)



$$H^m = \beta \left(mc^2 + \frac{\theta^2}{2mc^2} - \frac{\theta^4}{8m^3c^6} \right) + \epsilon - \frac{1}{8m^2c^4} \{ [\theta, [\theta, \epsilon] + i\dot{\theta}] \}$$

$$[\theta, \epsilon] + i\dot{\theta} = -i\hbar c e [\vec{\alpha} \cdot \vec{\nabla}, \phi] + i c \left\{ \left(\frac{d\vec{\alpha}}{dt} \right) \cdot \vec{\pi} + \left(\vec{\alpha} \cdot \frac{d\vec{\pi}}{dt} \right) \right\}$$

$$[\vec{\alpha} \cdot \vec{\nabla}, \phi] = (\vec{\alpha} \cdot \vec{\nabla} \phi) = \vec{\alpha} \cdot \left(-\vec{E} - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \right)$$

$$[\theta, \epsilon] + i\dot{\theta} = i\hbar c e \vec{\alpha} \cdot \left(\vec{E} + \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \right) + i c \left\{ \left(\frac{d\vec{\alpha}}{dt} \right) \cdot \vec{\pi} + \left(\vec{\alpha} \cdot \frac{d\vec{\pi}}{dt} \right) \right\}$$

$$[\theta, \epsilon] + i\dot{\theta} = i\hbar c e \vec{\alpha} \cdot \vec{E} + i\hbar e \vec{\alpha} \cdot \frac{\partial \vec{A}}{\partial t} + i c \left\{ \left(\frac{d\vec{\alpha}}{dt} \right) \cdot \vec{\pi} + \left(\vec{\alpha} \cdot \frac{d\vec{\pi}}{dt} \right) \right\}$$

$$\frac{d\vec{\alpha}}{dt} = \left\{ \frac{1}{i\hbar} [\vec{\alpha}, H] + \frac{\partial \vec{\alpha}}{\partial t} \right\}; \quad \frac{d\vec{\pi}}{dt} = \left\{ \frac{1}{i\hbar} [\vec{\pi}, H] + \frac{\partial \vec{\pi}}{\partial t} \right\}$$

NPTEL
August-September 2012 PCD STIAP Unit 3
132

So, this is the term which we are looking at this alpha dot del comma phi commutator, we have simplified and this del phi you know is related to the electric intensity, but there

will in the expression for the electric intensity. There will also be the rate of change of the vector potential, so there is a minus 1 over c del a by del t, and now you can put in this term in place of this commutator. Now, these are known things, these things you know from the electrodynamics, you know them from elementary vector calculus, you know them from quantum mechanics and what you do here is put it all together.

So, that what makes it really interesting, so put it all together, and now you have these terms systematically written as e plus 1 over say del a by del t. You see where it is coming from, and then you have the d alpha by d t and t phi by d t for the these two terms, and here you can use the Heisenberg equation of motion, and use these to represent these derivatives. So, do not forget that this is an operator, so which is why you have to use the equation of motion for the operator.

(Refer Slide Time: 10:50)

$$H^m = \beta \left(mc^2 + \frac{\theta^2}{2mc^2} - \frac{\theta^4}{8m^3c^6} \right) + c - \frac{1}{8m^2c^4} \left\{ [\theta, [\theta, \epsilon] + i\dot{\theta}] \right\}$$

$$[\theta, \epsilon] + i\dot{\theta} = i\hbar c e \vec{\alpha} \cdot \vec{E} + i\hbar e \vec{\alpha} \cdot \frac{\partial \vec{A}}{\partial t} + i c \left\{ \left[\frac{1}{i\hbar} [\vec{\alpha}, H] + \frac{\partial \vec{\alpha}}{\partial t} \right] \cdot \vec{\pi} + \left[\vec{\alpha} \cdot \left[\frac{1}{i\hbar} [\vec{\pi}, H] - e \frac{\partial \vec{A}}{\partial t} \right] \right] \right\}$$

$$= i\hbar c e \vec{\alpha} \cdot \vec{E} + i\hbar e \vec{\alpha} \cdot \frac{\partial \vec{A}}{\partial t} + c \left\{ \frac{1}{\hbar} [\vec{\alpha}, H] \cdot \vec{\pi} + \frac{1}{\hbar} \vec{\alpha} \cdot [\vec{\pi}, H] \right\} - i e c \vec{\alpha} \cdot \frac{\partial \vec{A}}{\partial t}$$

$$[\theta, \epsilon] + i\dot{\theta} = i\hbar c e \vec{\alpha} \cdot \vec{E}$$

$$\frac{1}{8m^2c^4} \left\{ [\theta, [\theta, \epsilon] + i\dot{\theta}] \right\} = \frac{i\hbar c e}{8m^2c^4} [\vec{\alpha} \cdot \vec{E}] = \frac{i\hbar c}{8m^2c^4} \left[c \vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) \cdot \vec{\alpha} \cdot \vec{E} \right]$$

$$= \frac{i\hbar}{8m^2c^3} [\vec{\alpha} \cdot \vec{p} \cdot \vec{\alpha} \cdot \vec{E}] = \frac{i\hbar}{8m^2c^3} (\vec{\alpha} \cdot \vec{p} \cdot \vec{\alpha} \cdot \vec{E} - \vec{\alpha} \cdot \vec{E} \cdot \vec{\alpha} \cdot \vec{p})$$

NPTEL
August-September 2012 PCD STIAP Unit 3
133

And now, you have got from the equation motion these terms, you have collected all of them, and since we have them written on this screen. It says me that time to write all these terms on the board, but this entire file is uploaded at the course page, so you can go through it carefully. And make sure that you follow the derivation term by term, but here I want to show, you in the class, and this way we can go much faster than we would, if I would to write this on the black board, but if you have any difficulty you should stop me.

So, this entire file has been uploaded, and you have these terms coming from the equation of motion, so what we have got, all the terms have been spelled out explicitly.

Now, these commutators again if you make use of the matrix structure, and look at the commutation properties, you will be able to see that they cancel each other. So, that you have to work out the matrix operation, and there is also a vector algebra, which is evolve you have to respect the vector algebra, the matrix algebra, the operator algebra everything come together.

And by using that these terms will make no contribution, these two terms cancel each other, they are the same with opposite sign, this one with the plus sign, and this one with the minus sign. So, these two terms cancel each other, and you are left you are left to lot of simplifications, and this is what gives you one part of this commutator and; that means, that you have to get commutation of theta with alpha dot e. So, here you had, so many terms now all of them are replace by just one commutator is now, what you have to determine. So, your task is much easier now, and when you do that again do a term by term it simplifies a lot, because you get.

(Refer Slide Time: 13:27)

$$H^m = \beta \left(mc^2 + \frac{0^2}{2mc^2} - \frac{0^4}{8m^3c^6} \right) + \varepsilon - \frac{1}{8m^2c^4} \{ [0, [0, \varepsilon] + i\hbar] \}$$

$$\frac{1}{8m^2c^4} \{ [0, [0, \varepsilon] + i\hbar] \} = \frac{ie\hbar}{8m^2c^4} (\vec{\alpha} \cdot \vec{p} \vec{\alpha} \cdot \vec{E} - \vec{\alpha} \cdot \vec{E} \vec{\alpha} \cdot \vec{p})$$

$$\frac{1}{8m^2c^4} \{ [0, [0, \varepsilon] + i\hbar] \} = \frac{ie\hbar}{8m^2c^4} \left\{ \begin{pmatrix} \vec{0} & \vec{\sigma} \cdot \vec{p} \\ \vec{\sigma} \cdot \vec{p} & \vec{0} \end{pmatrix} \begin{pmatrix} \vec{0} & \vec{\sigma} \cdot \vec{E} \\ \vec{\sigma} \cdot \vec{E} & \vec{0} \end{pmatrix} - \begin{pmatrix} \vec{0} & \vec{\sigma} \cdot \vec{E} \\ \vec{\sigma} \cdot \vec{E} & \vec{0} \end{pmatrix} \begin{pmatrix} \vec{0} & \vec{\sigma} \cdot \vec{p} \\ \vec{\sigma} \cdot \vec{p} & \vec{0} \end{pmatrix} \right\}$$

$$\frac{1}{8m^2c^4} \{ [0, [0, \varepsilon] + i\hbar] \} = \frac{ie}{8m^2c^4} \left\{ \begin{pmatrix} \vec{\sigma} \cdot \vec{p} \vec{\sigma} \cdot \vec{E} & 0 \\ 0 & \vec{\sigma} \cdot \vec{p} \vec{\sigma} \cdot \vec{E} \end{pmatrix} - \begin{pmatrix} \vec{\sigma} \cdot \vec{E} \vec{\sigma} \cdot \vec{p} & 0 \\ 0 & \vec{\sigma} \cdot \vec{E} \vec{\sigma} \cdot \vec{p} \end{pmatrix} \right\}$$

$$\frac{1}{8m^2c^4} \{ [0, [0, \varepsilon] + i\hbar] \} = \frac{ie\hbar}{8m^2c^4} (\vec{\sigma} \cdot \vec{p} \vec{\sigma} \cdot \vec{E} - \vec{\sigma} \cdot \vec{E} \vec{\sigma} \cdot \vec{p}) I_{4 \times 4}$$

$$\frac{1}{8m^2c^4} \{ [0, [0, \varepsilon] + i\hbar] \} = \frac{ie\hbar}{8m^2c^4} (\vec{p} \cdot \vec{E} + i\vec{\sigma} \cdot \vec{p} \times \vec{E} - \vec{E} \cdot \vec{p} - i\vec{\sigma} \cdot \vec{E} \times \vec{p}) I_{4 \times 4}$$

Rather familiar expressions over here, this alpha dot p alpha dot e this will suggest to you what kind of relation you can use, because whenever you see term of this kind you know that you will be able to use the poly identity. So, it is not to have remember, what I am going to do next those suggestions are built into the structure of the equations, and if you just used them you will be automatically led to do the right thing that is the idea. So, here you see the poly identity emerging out of this matrix structure and you get the sigma dot

$\mathbf{p} \cdot \boldsymbol{\sigma} \cdot \mathbf{e}$, from this matrix multiplication of these two operators, these are matrix operators.

So, you have the term over here in the first row, and first column will be this $\boldsymbol{\sigma} \cdot \mathbf{p} \cdot \boldsymbol{\sigma} \cdot \mathbf{e}$ over here, and also in the 2 2 positions, but each $\boldsymbol{\sigma}$ is 2 by 2 matrix of course, so you are really working with 4 by 4 matrices, which is what you always do in the Dirac formalism. So, you got the $\boldsymbol{\sigma} \cdot \mathbf{p} \cdot \boldsymbol{\sigma} \cdot \mathbf{e}$, and now you can use the Pauli identity, which is which will give you $\mathbf{p} \cdot \mathbf{E}$ plus $i \boldsymbol{\sigma} \cdot \mathbf{p} \times \mathbf{E}$, and you have a similar expression over here, but this time you have got the $\mathbf{e} \times \mathbf{p}$.

(Refer Slide Time: 15:15)

$$H = \beta \left(mc^2 + \frac{p^2}{2m} \right) + e \left\{ \left[0, \left[0, E \right] + i0 \right] \right\}$$

$$\frac{1}{8m^2c^2} \left\{ \left[0, \left[0, E \right] + i0 \right] \right\} = \frac{ie\hbar}{8m^2c^2} \left(\mathbf{p} \cdot \mathbf{E} + i\boldsymbol{\sigma} \cdot \mathbf{p} \times \mathbf{E} - \mathbf{E} \cdot \mathbf{p} - i\boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{p} \right) I_{4 \times 4}$$

$$\mathbf{p} \cdot \mathbf{E} = -i\hbar \nabla \cdot \mathbf{E} = -i\hbar (\nabla \cdot \mathbf{E}) f = -i\hbar (\mathbf{E} \cdot \nabla) f$$

$$- \left[(-i\hbar \nabla \cdot \mathbf{E}) + (\mathbf{E} \cdot (-i\hbar \nabla)) \right] f = - \left[(\mathbf{p} \cdot \mathbf{E}) + (\mathbf{E} \cdot \mathbf{p}) \right] f$$

$\mathbf{p} \cdot \mathbf{E} = (\mathbf{p} \cdot \mathbf{E}) + (\mathbf{E} \cdot \mathbf{p})$ The range of applicability of the gradient does not go beyond the bracket in the first term on the rhs

$$\frac{1}{8m^2c^2} \left\{ \left[0, \left[0, E \right] + i0 \right] \right\} =$$

$$= \frac{ie\hbar}{8m^2c^2} (\mathbf{p} \cdot \mathbf{E}) + \frac{ie\hbar}{8m^2c^2} (\mathbf{E} \cdot \mathbf{p}) - \frac{e\hbar}{8m^2c^2} \boldsymbol{\sigma} \cdot \mathbf{p} \times \mathbf{E} - \frac{ie\hbar}{8m^2c^2} \mathbf{E} \cdot \mathbf{p} + \frac{e\hbar}{8m^2c^2} \boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{p}$$

NPTEL August-September 2012 PCD STAP Unit 3 135

So, these are the two terms, now let us have a look at this $\mathbf{p} \cdot \mathbf{E}$ term \mathbf{p} again has a gradient operator, so you have to be careful with it. And what you find from a careful handling of this gradient operator, which now which we have done a number of times, you see that this $\mathbf{p} \cdot \mathbf{E}$ will give you this scalar $\mathbf{p} \cdot \mathbf{E}$ plus $\mathbf{E} \cdot \mathbf{p}$. So, this is not the same as this, this is an operator this is the result of all the operation carried out.

So, now you can put all of these terms back in the expression for $1/8m^2c^2$ to the 4, and you write all of these terms coming from here. And you find that this $\mathbf{E} \cdot \mathbf{p}$ term cancels this $\mathbf{E} \cdot \mathbf{p}$, this $\mathbf{E} \cdot \mathbf{p}$ is a descendent of this term here, this is a point $\mathbf{E} \cdot \mathbf{p}$. So, that is a one which is coming here, and these two cancel each other, now you have these three terms, 1 2 and 3.

(Refer Slide Time: 16:38)

$$\begin{aligned}
 H''' &= \beta \left(mc^2 + \frac{p^2}{2mc^2} - \frac{p^4}{8m^3c^6} \right) + \epsilon - \frac{1}{8m^2c^4} \left\{ [0, [\theta, \epsilon] + i\dot{\theta}] \right\} \\
 &= \frac{1}{8m^2c^4} \left\{ [0, [\theta, \epsilon] + i\dot{\theta}] \right\} = \\
 &= \frac{ie\hbar}{8m^2c^2} (\vec{p} \cdot \vec{E}) - \frac{e\hbar}{8m^2c^2} \vec{\sigma} \cdot \vec{p} \times \vec{E} + \frac{e\hbar}{8m^2c^2} \vec{\sigma} \cdot \vec{E} \times \vec{p} \\
 &\quad \boxed{\vec{p} \times \vec{E} = (\vec{p} \times \vec{E}) - \vec{E} \times \vec{p}} \\
 &= \frac{ie\hbar}{8m^2c^2} (\vec{p} \cdot \vec{E}) - \frac{e\hbar}{8m^2c^2} \vec{\sigma} \cdot \vec{p} \times \vec{E} + \frac{e\hbar}{8m^2c^2} \vec{\sigma} \cdot \vec{E} \times \vec{p} + \frac{e\hbar}{8m^2c^2} \vec{\sigma} \cdot \vec{E} \times \vec{p} \\
 &= \frac{e\hbar^2}{8m^2c^2} (\text{div } \vec{E}) + \frac{ie\hbar^2}{8m^2c^2} \vec{\sigma} \cdot \text{curl } \vec{E} + \frac{e\hbar}{4m^2c^2} \vec{\sigma} \cdot \vec{E} \times \vec{p}
 \end{aligned}$$

NPTEL
August-September 2012 PCD STIAP Unit 3
136

And three of which $\vec{p} \times \vec{E}$ again with a careful handling of the gradient sitting in the \vec{p} , will give you these two terms $\vec{p} \times \vec{E}$ minus $\vec{E} \times \vec{p}$, we have done this, so there is a gradient sitting over here, so using this these two terms. So, instead of $\vec{p} \times \vec{E}$ term, now you have the this $\vec{p} \times \vec{E}$ is coming from here, and then here you have a term in minus of $\vec{E} \times \vec{p}$, but then together with this minus sign is become a plus, so you get a term in this plus $\vec{E} \times \vec{p}$.

And then you can combine this term and this term, which is coming from these two, and now you notice that the last two terms these two terms are exactly the same. This is $e\hbar$ cross over $8m^2c^2$ $\vec{\sigma} \cdot \vec{E} \times \vec{p}$, so these are the same terms. So, instead of the 1 over 8 factor here you will have the 1 over 4 , because you can combine those two terms, so that is what you have got you get the 1 over 4 here coming from these two terms, and then from here you get this $\vec{\sigma} \cdot \text{curl } \vec{E}$. And now, you have perhaps to beginning to see some formality with some of the terms, you may have seen in perturbation theory, but they will become even more explicitly manifest after just a few more steps.

(Refer Slide Time: 18:37)

$$H''' = \beta \left(mc^2 + \frac{p^2}{2mc^2} - \frac{p^4}{8m^3 c^6} \right) + \varepsilon - \frac{1}{8m^2 c^4} \{ [0, [0, \varepsilon] + i\dot{0}] \}$$

$$\frac{p^2}{2mc^2} = \frac{1}{2m} \left\{ \vec{\pi}^2 - \frac{e\hbar}{c} \vec{\sigma} \cdot \vec{B} \right\} \quad \theta = c\vec{\alpha} \cdot \vec{\pi} = c\vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right)$$

$$\frac{1}{8m^2 c^4} \{ [0, [0, \varepsilon] + i\dot{0}] \} = \frac{e\hbar^2}{8m^2 c^2} (\text{div } \vec{E}) + \frac{ie\hbar^2}{8m^2 c^2} \vec{\sigma} \cdot \text{curl } \vec{E} + \frac{e\hbar}{4m^2 c^2} \vec{\sigma} \cdot \vec{E} \times \vec{p}$$

$$H''' = \beta \left(mc^2 + \frac{\left(\vec{p} - \frac{e}{c} \vec{A} \right)^2}{2m} - \frac{\vec{p}^4}{8m^3 c^6} \right) - \beta \frac{1}{2mc} e\hbar \vec{\sigma} \cdot \vec{B} +$$

$$+ e\hbar \frac{e\hbar^2}{8m^2 c^2} (\text{div } \vec{E}) - \frac{ie\hbar^2}{8m^2 c^2} \vec{\sigma} \cdot \text{curl } \vec{E} - \frac{e\hbar}{4m^2 c^2} \vec{\sigma} \cdot \vec{E} \times \vec{p}$$

Relativistic K.E. correction

$$\vec{E} = -\frac{\partial V}{\partial \vec{r}} \hat{e}_r = -\frac{1}{r} \frac{\partial V}{\partial r} \vec{r}$$

NPTEL August-September 2012 PCD STAP Unit 3 137

So, this is what we have got these are the three terms, so you get the diversion of \vec{p} you get the sigma dot curl of \vec{p} and sigma dot \vec{E} cross \vec{p} , so let us write insert them in the transform Hamiltonian. Now, when you take care of all the terms and put them back into the transform Hamiltonian, which is the transform Hamiltonian arrive at after three Foldy Wouthuysen transformations.

The transform Hamiltonian, then has got, so many terms 1 2 3, and then you have got another 1 over here, and all of these terms are now amenable to easy interpretation rather easy interpretation. This was not a form which we could see them in the Dirac Hamiltonian, they were there it is not anything that we have added Ad-hoc this is comes straight out of Dirac Hamiltonian by subjecting it to a property transformations.

You immediately see that this electric intensity is nothing but the gradient of the potential and this e/r is this position vector divided by r , so you see the form minus 1 over r del v by del r . And now, you have got this r , which will come here, so you will get sigma dot r cross \vec{p} , which is the sigma dot \vec{l} , which is the spin orbit term that you have seen in perturbation theory it comes. So, nicely out of the Foldy Wouthuysen transformation, it was there in the Dirac equation, but it was not visible.

When you subject the Foldy Wouthuysen transformation to one to three transformations, then in the third result which is the h triple prime you see this form appearing. So, this is the $e\hbar$ cross over $4m^2 c^2$ 1 over r del v by del r sigma dot r cross \vec{p} , then

you have got a term in p to the 4 this happens to be the relativistic kinetic energy directional, discuss this in just a few minutes.

(Refer Slide Time: 21:05)

$$\begin{aligned}
 T_{KE}^{Rel} &= E - mc^2 \\
 &= (p^2 c^2 + m^2 c^4)^{\frac{1}{2}} - mc^2 \\
 &= \left(m^2 c^4 \left(\frac{p^2 c^2}{m^2 c^4} + 1 \right) \right)^{\frac{1}{2}} - mc^2 \\
 T_{KE}^{Rel} &= mc^2 \left[\left(\frac{p^2}{m^2 c^2} + 1 \right)^{\frac{1}{2}} - 1 \right] \\
 &= mc^2 \left[1 + \frac{1}{2} \left(\frac{p}{mc} \right)^2 - \frac{1}{8} \left(\frac{p}{mc} \right)^4 + \dots - 1 \right] \\
 &= \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2} + \dots
 \end{aligned}$$

NPTEL
August-September 2012 PCD STIAP Unit 3
138

Now, this is the relativistic kinetic energy which is E minus mc^2 , and you remember we defined the energy mass equivalence very carefully, at the very beginning without which we would not have this connections. So, there was a strong reason to spend some time discussing that, and you will see that it is important. So, the relativistic kinetic energy is this difference, which is the energy minus the rest mass energy, what you take away after removing the rest energy is a kinetic part, so this is a relativistic kinetic energy.

And now, all you do is to expand this term to the power half, and when you do that you get a power series, and you have got c in the denominator whose powers keep increasing. So, you can truncate it at some level of the approximation wherever you want, and if you keep the leading term the most important contribution comes from the p to the 4 term. So, this is the relativistic kinetic energy, term this is precisely the term that we saw in the Foldy Wouthuysen transform Hamiltonian.

So, there was a term in p to the 4, and we see its origin in the fact the relativistic kinetic energy is different from the Galilean kinetic energy they two are different, so its origin can be traced to the origin of the p to the 4 term, which is here this can be traced to relativistic kinetic energy part.

(Refer Slide Time: 22:43)

The slide displays the relativistic Hamiltonian H^m and its non-relativistic limit $H^m = \beta$. The terms are as follows:

- Relativistic K.E. correction:** Indicated by a red arrow pointing to the $-\frac{\vec{p}^2}{8m^2c^2}$ term in the first equation.
- Magnetic dipole term:** Indicated by a blue arrow pointing to the $\beta \frac{1}{2mc} e\hbar \vec{\sigma} \cdot \vec{B}$ term in the second equation.
- Darwin correction (zitterbewegung):** Indicated by a blue arrow pointing to the $+e\hbar \frac{e\hbar^2}{8m^2c^2} (\text{div } \vec{E})$ term in the second equation.
- Spin-orbit interaction (Thomas):** Indicated by a red arrow pointing to the $-\frac{ie\hbar^2}{8m^2c^2} \vec{\sigma} \cdot \text{curl } \vec{E}$ term in the second equation.

The slide also includes the MPTEL logo and the text "August-September 2012 PCD STAP Unit 3" and "139".

This is what we just saw, this sigma dot b is a magnetic dipole moment as is easily recognizable, then you have got a term in the divergence of p, and this was introduced in the pre Foldy Wouthuysen days as a perturbation. And it was referred to as a Darwin connection, so in some books on perturbation theory, they will begin with a non relativistic Hamiltonian, and at perturbations.

That this is the perturbation due to the relativistic kinetic energy, because your original Hamiltonian is not really relativistic let us take into the account some of the relativistic features. And let us do it perturbatively because after all the non relativistic theory is not accept, it gives the good starting point it certainly does, and the reason of course, is that the speed of light is extremely high, even if it finite it is a extremely high.

So, the non relativistic Schrodinger equation non relativistic quantum mechanics is not accept that not quite accurate, and we are now looking at those effects, which are really important, because an atomic spectroscopy and in the atomic processes. It does become important to take into account relativistic effects, and not just for heavy atoms, but even for very small atoms even for the hydrogen atom. It is absolutely important to take these effects into the account, and these could be introduced perturbatively in non relativistic mechanics.

So, you can add the kinetic energy correction as a perturbation, you can add this is a correction you can add the spin orbit correction, actually these two terms together

contribute to the spin orbit term, rather than just the last one. The last one is more famous because curl of \mathbf{p} for the hydrogen atom vanishes, that is the spherical symmetric potential, so you know the curl of \mathbf{p} vanishes. So, this one is not a important, but if you are dealing with a potential, which is not strictly you know central field then you are going to have to take this into the account and you cannot throw it away.

So, relativistic quantum mechanics will give you not just the $\sigma \cdot \mathbf{l}$ term, not just the $\mathbf{l} \cdot \mathbf{l}$ term, but an additional term which must be taken into the account as an integral part of the spin orbit interaction. That is the relativistic effect, for a central field it is just a $\sigma \cdot \mathbf{l}$ square and of course, there is this $d\mathbf{v}$ by $d\mathbf{r}$ and so on.

(Refer Slide Time: 25:44)

$$\left\langle -\frac{\hat{\mathbf{p}}^4}{8m^3c^2} \right\rangle = \left\langle -\left(\frac{\hat{\mathbf{p}}^2}{2m}\right)^2 \frac{1}{2mc^2} \right\rangle = \frac{-1}{2mc^2} \left\langle \left(\frac{\hat{\mathbf{p}}^2}{2m}\right)^2 \right\rangle$$

$$= \frac{-1}{2mc^2} \left\langle (E_n - V)^2 \right\rangle = \frac{-1}{2mc^2} [E_n^2 - 2E_n \langle V \rangle + \langle V^2 \rangle]$$

$$V = -\frac{Ze^2}{r} \quad \text{H.W. Show that: } \left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2 a} \quad \& \quad \left\langle \frac{1}{r^2} \right\rangle = \frac{1}{\left(\ell + \frac{1}{2}\right) n^3 a^2}$$

$$E_n = -\frac{1}{2n^2} \frac{mZ^2 e^4}{\hbar^2} = -\frac{me^2 Z^2 e^2}{\hbar^2 2n^2}$$

$$= -\left(\frac{e^2}{\hbar c}\right)^2 \frac{mc^2 Z^2}{2n^2} = -mc^2 \frac{(Z\alpha)^2}{2n^2} \quad \alpha = \left(\frac{e^2}{\hbar c}\right)$$

$$\Delta E_{\text{rel KE}} = -E_n \left(\frac{Z\alpha}{n}\right)^2 \left[\frac{3}{4} - \frac{n}{\ell + \frac{1}{2}} \right]$$

NPTEL Prof. Bransden & Joachain – Physics of Atoms & Molecules / Ch 5
August-September 2012 PCD STIAP Unit 3 140

So, there are these terms and one can make corrections perturbatively, it is a good idea to see the correspondence, so look at the perturbative corrections due to the kinetic energy part. This is the relative relativistic kinetic energy correction, we are coming from the \mathbf{p} to the 4 term, now you see that this is the square of \mathbf{p} square, and this is E_n minus V whole square. And you really need the expectation values of the potential energy had also the square of the potential energy, so you need the average values of $1/r$ because a potential energy goes as $1/r$, and you also need the average energy of $1/r^2$ over r square.

Now, these problems you would have been done in non relativistic hydrogen atom, how to get the average expectation value of any operator. So, if you take the n th wave function

for the hydrogen atom, and determine the average values of $1/r$ and $1/r^2$. You will see that $1/r$ goes as $1/n^2$ and $1/r^2$ goes as $1/n^3$, A is the Bohr constant, and then there are other constants and other quantum numbers, which come.


So, you can use these relations, put them into the expression for the average energy for the potential energy, and the square of the potential energy. And that will give you an estimate of the perturbative correction due to the relativistic kinetic energy, and it turns out to go as α^2 , where α is a fine structure constant. This is the reason it is called as a fine structure constant, because it changes this non relativistic structure, even if, so in only a fine small detail, and it contributes some details to the atomic structure.

So, this is the fine structure constant, but this is not the only term which is coming because of relativity, and this is the most important lesson from the Foldy Wouthuysen transformations. Because, if you perturbative corrections to non relativistic Hamiltonian, then which are the corrections you want to make these. You could make the Darwin correction, you could make this correction, you could make this correction, so there are three corrections that you can talk about.

And perturbatively you might say that this is the most important one, I will do that, I could do that second term or I could do the third term or I could do the second and third, but not the first. But, whenever you are making corrections, it is extremely important that if you include one term of a given order, then you considered all terms of the same order. And you are certainly making an approximation, so it is not an exact formalism that you are developing anyway. Whether, it is the Foldy Wouthuysen scheme of the doing things or the perturbative way of doing things, you are not doing an exact analysis, you are making the approximations.

So, make sure that your approximation is sensible, because when you make an approximation and say that argue that these terms are not going to take into the account, because they are weak they are ignorable. Nothing wrong in making that argument, but you cannot ignore those terms, which are of the same order as some of these other terms you have chosen to include. So, you have to take into account all of them, and when you do not do that you will; obviously, get wrong results.

(Refer Slide Time: 29:42)



$$\begin{aligned} \langle H_{\text{spin-orbit}} \rangle &= \left\langle \frac{e\hbar}{4m^2c^2} \frac{1}{r} \frac{\partial V}{\partial r} \vec{\sigma} \cdot \vec{\ell} \right\rangle = \frac{e\hbar}{4m^2c^2} \left\langle \frac{1}{r} \frac{\partial V}{\partial r} \right\rangle_{\text{radial}} \langle \vec{\sigma} \cdot \vec{\ell} \rangle \\ &= \frac{e\hbar}{4m^2c^2} (-Ze) \left\langle \frac{1}{r^3} \right\rangle \left\langle \frac{2\vec{s} \cdot \vec{\ell}}{\hbar} \right\rangle \end{aligned}$$

$$\vec{s} = \frac{\hbar}{2} \vec{\sigma} \quad \alpha = \left(\frac{e^2}{\hbar c} \right)$$

$$\begin{aligned} \langle H_{\text{spin-orbit}} \rangle &= \frac{Ze^2}{2m^2c^2} \left\langle \frac{1}{r^3} \right\rangle \langle \vec{s} \cdot \vec{\ell} \rangle \\ &= \frac{Ze^2}{2m^2c^2} \frac{Z^3}{\ell(\ell+1/2)(\ell+1)n^3a^3} \left[\frac{\hbar^2}{2} \{j(j+1) - \ell(\ell+1) - s(s+1)\} \right] \end{aligned}$$

$$\begin{aligned} E_n &= -\frac{1}{2n^2} \frac{mZ^2e^4}{\hbar^2} \\ &= -mc^2 \frac{(Z\alpha)^2}{2n^2} \end{aligned}$$

Spin-orbit correction
- same order as 'relativistic mass' correction

August-September 2012 PCO SHAIP Unit 3

So, now this is the correction due to the relativistic kinetic energy, and now let see the correction due to the spin orbit term, which is the sigma dot l term over here. And here again you can go ahead and determine the expectation value of this operator, this is the first order perturbation theory result, which is quite familiar to you. So, you need the radial integral for 1 over r cube, because del v by del r will give, you the derivative of 1 over r which goes as 1 over r square.

So, you need the expectation value of 1 over r cube because of that reason, and then you get you need the expectation value of this operator in angular momentum states. So, when you evaluate this, h del l you know how to get it from j square, because j is l plus s, so j dot j will be l square plus twice l dot s minus s square, and you can you know do the substitutions and get this result. So, you have a twice s dot l terms, so you will get h cross square by 2 j into j plus one minus l into l plus 1 minus s into s plus 1. And then the average value a 1 over r cube, will give this term and 1 over n cube, and some of the other quantum numbers including the orbital angular quantum number.


(Refer Slide Time: 31:27)

$$\begin{aligned}
 \langle H_{\text{spin-orbit}} \rangle &= \frac{Ze^2}{4m^2c^2} \frac{\hbar^2 Z^3}{n^3 a^3 \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)} \left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\} & \alpha &= \left(\frac{e^2}{\hbar c} \right) \\
 &= \frac{Ze^2 \hbar^2}{m^2 c^2} \left(\frac{me^2}{\hbar^2} \right)^3 \frac{Z^3}{4n^3 \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)} \left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\} & a &= \frac{\hbar^2}{me^2} \\
 &= Z^4 mc^2 \left(\frac{e^2}{\hbar c} \right)^4 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{4n^3 \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)} & \vec{s} &= \frac{\hbar}{2} \vec{\sigma}
 \end{aligned}$$

$$\begin{aligned}
 E_n &= -\frac{1}{2n^2} \frac{mZ^2 e^4}{\hbar^2} \\
 &= -mc^2 \frac{(Z\alpha)^2}{2n^2}
 \end{aligned}$$

Spin-orbit correction

- same order as 'relativistic mass' correction

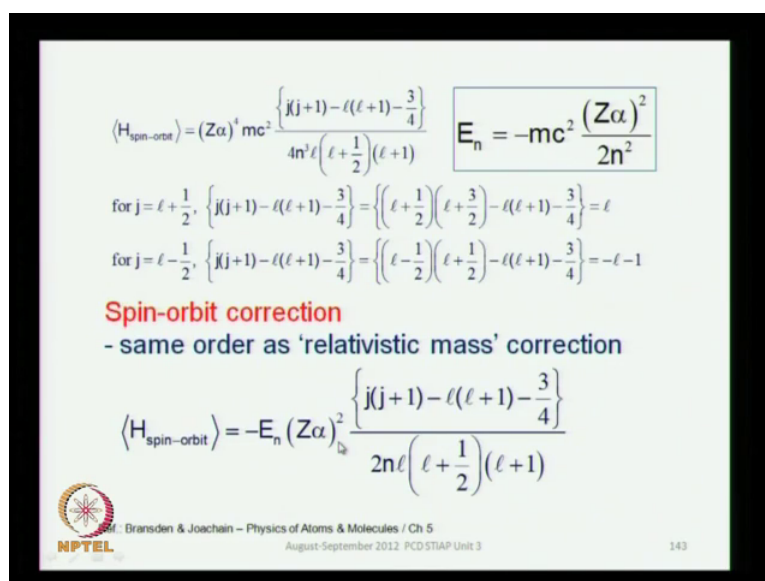


Prof. L. Brando & Kachin – Physics of Atoms & Molecules / Ch 5
August-September 2012 PCO SHAP Unit 3

So, this is the correction to the energy, because of the spin orbit term, and it is as important as the relativistic kinetic energy term, which is sometimes referred to as relativistic vast term. But, more appropriately it should be called as relativistic kinetic energy term, because we do not make a distinguish distinction between mass and energy, that is something that we have already taken care of.

So, you can simplify this expression for the average value of the spin orbit interaction, these are the constants that you make use of the bore radius and fine structure constants. And you find that this is the same as what is some books called as it is relativistic mass correction, but it is a relativistic kinetic energy correction, as I prefer to call.

(Refer Slide Time: 32:15)



$$\langle H_{\text{spin-orbit}} \rangle = (Z\alpha)^4 mc^2 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{4n^3 \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)}$$

$$E_n = -mc^2 \frac{(Z\alpha)^2}{2n^2}$$

for $j = \ell + \frac{1}{2}$, $\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\} = \left\{ \left(\ell + \frac{1}{2} \right) \left(\ell + \frac{3}{2} \right) - \ell(\ell+1) - \frac{3}{4} \right\} = \ell$

for $j = \ell - \frac{1}{2}$, $\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\} = \left\{ \left(\ell - \frac{1}{2} \right) \left(\ell + \frac{1}{2} \right) - \ell(\ell+1) - \frac{3}{4} \right\} = -\ell - 1$

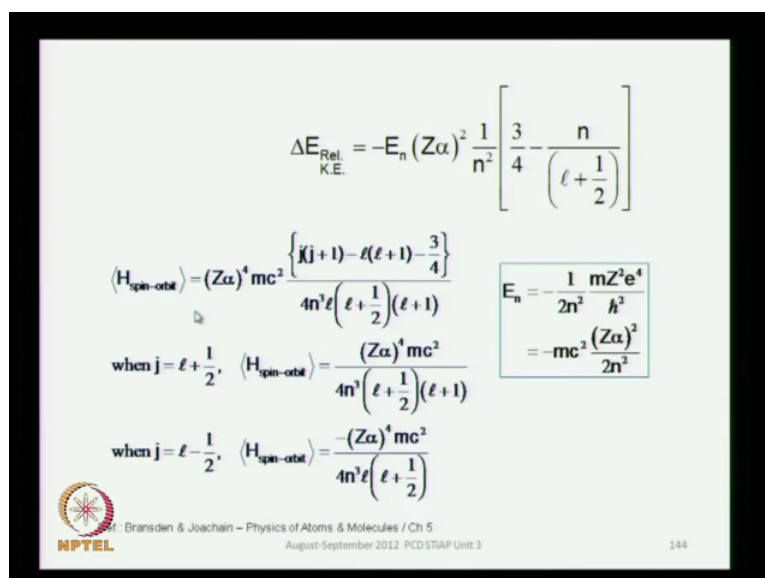
Spin-orbit correction
- same order as 'relativistic mass' correction

$$\langle H_{\text{spin-orbit}} \rangle = -E_n (Z\alpha)^2 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{2n \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)}$$

NPTEL | Bransden & Joachain – Physics of Atoms & Molecules / Ch 5
August-September 2012 PCD STAP Unit 3 | 143

So, this is what you get the spin orbit correction again goes as z alpha square.

(Refer Slide Time: 32:26)



$$\Delta E_{\text{Rel. K.E.}} = -E_n (Z\alpha)^2 \frac{1}{n^2} \left[\frac{3}{4} - \frac{n}{\left(\ell + \frac{1}{2} \right)} \right]$$

$$\langle H_{\text{spin-orbit}} \rangle = (Z\alpha)^4 mc^2 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{4n^3 \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)}$$

$$E_n = -\frac{1}{2n^2} \frac{mZ^2 e^4}{h^2} = -mc^2 \frac{(Z\alpha)^2}{2n^2}$$

when $j = \ell + \frac{1}{2}$, $\langle H_{\text{spin-orbit}} \rangle = \frac{(Z\alpha)^4 mc^2}{4n^3 \left(\ell + \frac{1}{2} \right) (\ell + 1)}$

when $j = \ell - \frac{1}{2}$, $\langle H_{\text{spin-orbit}} \rangle = \frac{-(Z\alpha)^4 mc^2}{4n^3 \ell \left(\ell + \frac{1}{2} \right)}$

NPTEL | Bransden & Joachain – Physics of Atoms & Molecules / Ch 5
August-September 2012 PCD STAP Unit 3 | 144

Now, this is the correction for from relativistic kinetic energy, which goes as z alpha square and now you are left with one more term.

(Refer Slide Time: 32:39)

$$\langle H_{\text{spin-orbit}} \rangle = (Z\alpha)^4 mc^2 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{4n^3 \ell \left(\ell + \frac{1}{2} \right) (\ell + 1)} \quad \ell \neq 0$$

$$\langle H_{\text{spin-orbit}} \rangle_{j=\ell+\frac{1}{2}} = \frac{(Z\alpha)^4 mc^2}{4n^3 \left(\ell + \frac{1}{2} \right) (\ell + 1)}; \quad \langle H_{\text{spin-orbit}} \rangle_{j=\ell-\frac{1}{2}} = \frac{-(Z\alpha)^4 mc^2}{4n^3 \ell \left(\ell + \frac{1}{2} \right)}$$

$$\Delta_{\text{spin-orbit splitting}} = \frac{(Z\alpha)^4 mc^2}{4n^3} \left[\frac{1}{(\ell+1)} - \frac{1}{\ell} \right] \frac{1}{\left(\ell + \frac{1}{2} \right)}$$

$$E_n = -\frac{1}{2n^2} \frac{mZ^2 e^4}{\hbar^2}$$

$$= -mc^2 \frac{(Z\alpha)^2}{2n^2}$$

$$= \frac{(Z\alpha)^4 mc^2}{4n^3} \left[\frac{-1}{\ell \left(\ell + \frac{1}{2} \right) (\ell + 1)} \right]$$

Bransden & Joachain – Physics of Atoms & Molecules / Ch 5
MPTEL August-September 2012 PCD STIAP Unit 3 145

Because, here is a simplification of this further, the spin orbit interaction of course, is important only for ℓ not equal to 0 states, for ℓ equal to 0, the $\ell + \frac{1}{2}$ and $\ell - \frac{1}{2}$ will give you the same thing. So, this is when ℓ is not equal to 0, you can explicitly put in the values, and find these simplified expressions for the spin orbit spreading.

(Refer Slide Time: 33:11)

$$\begin{aligned} \hat{h}_{\text{Darwin}} &= -\frac{e\hbar^2}{8m^2c^2} (\text{div } \vec{E}) = -\frac{e\hbar^2}{8m^2c^2} \left(\vec{\nabla} \cdot \frac{-Ze^2}{r^2} \hat{e}_r \right) \\ &= \frac{\hbar^2 Ze^2}{8m^2c^2} \left(\vec{\nabla} \cdot \frac{\hat{e}_r}{r^2} \right) = \frac{\hbar^2 Ze^2}{8m^2c^2} (4\pi\delta^3(\vec{r})) \\ &= \frac{\pi\hbar^2 Ze^2}{2m^2c^2} \delta^3(\vec{r}) \end{aligned}$$

$$E_n = -\frac{1}{2n^2} \frac{mZ^2 e^4}{\hbar^2}$$

$$= -mc^2 \frac{(Z\alpha)^2}{2n^2}$$

$$\langle \hat{h}_{\text{Darwin}} \rangle = \frac{\pi\hbar^2 Ze^2}{2m^2c^2} \langle \psi_{n,\ell=0,m=0} | \delta^3(\vec{r}) | \psi_{n,\ell=0,m=0} \rangle$$

$$\ell = 0 \Rightarrow \frac{\pi\hbar^2 Ze^2}{2m^2c^2} |\psi_{n,\ell=0,m=0}(r=0)|^2 = -E_n \frac{(Z\alpha)^2}{n}$$

Bransden & Joachain – Physics of Atoms & Molecules / Ch 5
MPTEL August-September 2012 PCD STIAP Unit 3 146

What are the diversion terms, this is the Darwin correction, now the Darwin correction requires you take the diversions $\nabla \cdot \frac{1}{r^2}$ which is the diversions of $1/r^2$, which gives the δ function. The diversions of $1/r^2$ gives you the Dirac delta, and you

will, therefore need the average value or the expectation value involving this delta function.


So, when you revolve, when you determine the expectation value of the operators, you must use the delta function integration expectation value is an integral; obviously, so this is let say you take the expectation value for some n s state. This is the important for l equal to 0, so this is let us say for some non relativistic wave functions ψ_n with l equal to 0 and m equal to 0. And you determine this integral, and this will give you minus $e n z$ alpha square over n , so again you find that the Darwin correction is also of the same order of magnitude as the other two.

So, it is important to take into account, all the 3 if you want to make relativistic corrections at all or none at all, if you do only one or the other then it is not enough. And that is the difficulty with perturbative approach to quantum mechanics, because whenever you try to make improvisation. And add terms, which you even if they are in the right direction, they can still give completely wrong answer, because you may have two contributors of same order magnitude.

They could come with opposite signs and they could just kill each other, or they could come with the same sign they can they could add to each other, so these are various factors that you have to consider when you do the perturbation theory. So, this of course, it is important only if n equal to 0, because it requires a finite amplitude of wave function at the nucleus at r equal to 0. And you know if that all the radial functions of the hydrogen atom, they goes as r to the power l , as r goes to 0.

So, as r goes to 0 the wave function goes at the r to the power l , and for l equal to 0 this will be finite at the origin at r equal to 0, but for l equal to 1 2 3 and everything else this would go to 0. And it would go to 0 faster for higher values of l which is a centrifugal barrier effect, which I had discussed in unit 1 I believe, but this is of importance for the n s states, so this is for the l equal to 0 state that this is important.

(Refer Slide Time: 36:19)



$$\Delta E_{\text{Rel. K.E.}} = -E_n (Z\alpha)^2 \frac{1}{n^2} \left[\frac{3}{4} - \frac{n}{\ell + \frac{1}{2}} \right]$$


$$\langle H_{\text{spin-orbit}} \rangle = -E_n (Z\alpha)^2 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{2n\ell \left(\ell + \frac{1}{2} \right) (\ell + 1)} \quad \ell \neq 0$$

$$\begin{aligned} \langle h_{\text{Darwin}} \rangle &= \frac{\pi \hbar^2 Z e^2}{2m^2 c^2} \langle \psi_{n,\ell=0,m=0} | \delta^3(\vec{r}) | \psi_{n,\ell=0,m=0} \rangle \quad \ell = 0 \\ &= \frac{\pi \hbar^2 Z e^2}{2m^2 c^2} |\psi_{n,\ell=0,m=0}(r=0)|^2 = -\frac{E_n}{n} (Z\alpha)^2 \end{aligned}$$

August-September 2012 PCD STAP Unit 3 147

And then you have these three corrections the relativistic kinetic energy, the spin orbit correction the Darwin correction, they are all of the same order z alpha square.

(Refer Slide Time: 36:28)



$$\langle H_{\text{rel K.E.}} \rangle = -E_n (Z\alpha)^2 \frac{1}{n^2} \left[\frac{3}{4} - \frac{n}{\ell + \frac{1}{2}} \right] \quad \langle h_{\text{Darwin}} \rangle = -\frac{E_n}{n} (Z\alpha)^2$$

$$\langle H_{\text{spin-orbit}} \rangle = -E_n (Z\alpha)^2 \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{2n\ell \left(\ell + \frac{1}{2} \right) (\ell + 1)}$$

$$\Delta E_{\text{relativistic}} = \Delta E_{\text{relativistic}} = -E_n \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right)$$

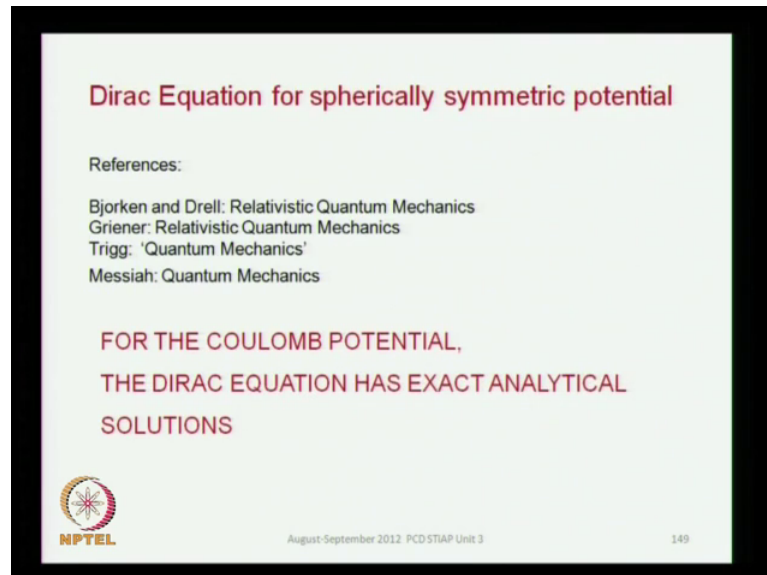
$$E_n^{\text{relativistic}} = E_n \left[1 + \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right]$$

August-September 2012 PCD STAP Unit 3 148

And you therefore, put them all together, and add the net effect of these three terms though the correction, and these three terms when you add together you get a net relativistic correction for all orbital angular momentum quantum numbers. And this is the result that you get from relativistic quantum mechanics, but if you did not use all the three, but only one or this, this is not what you going to get. So, please make a very

major note of this point, that all perturbation of the same importance must be included together.

(Refer Slide Time: 37:15)




Dirac Equation for spherically symmetric potential

References:

- Bjorken and Drell: Relativistic Quantum Mechanics
- Griener: Relativistic Quantum Mechanics
- Trigg: 'Quantum Mechanics'
- Messiah: Quantum Mechanics

**FOR THE COULOMB POTENTIAL,
THE DIRAC EQUATION HAS EXACT ANALYTICAL
SOLUTIONS**

 NPTEL

August-September 2012 PCD STIAP Unit 3 149

So, now our primary intention in doing this exercise was to solve the Dirac equation for the hydrogen atom, now we have seen what some other terms mean. And these are some references that I like very much for this topic Bjorken and Drell and Griener and Drig quantum mechanics Masaya. So, these are some of the books that I have used and for the coulomb problem for the hydrogen atom, you can solve the Dirac equation exactly. In all the forms that we used until now, we had the potential v of r , but we never actually specified it to be the coulomb potential.

(Refer Slide Time: 38:12)

Strategy for the Coulomb potential:

Eliminate all features except the radial features using constants of motion.

$$H_{\text{Dirac Hamiltonian}} = \beta mc^2 + c\vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) + e\phi$$

$$H_{\text{Dirac Electrostatic field}} = \beta mc^2 + c\vec{\alpha} \cdot \vec{p} + e\phi$$

$$H_{\text{Dirac Free particle}} = \beta mc^2 + e\phi = \beta mc^2 + c\vec{\alpha} \cdot \frac{\hbar}{i} \vec{\nabla} + e\phi$$


$$\left[H_{\text{Dirac Free particle}}, \vec{\ell} \right] \neq 0 \quad \left[H_{\text{Dirac Free particle}}, \vec{s} \right] \neq 0$$

$$\left[H_{\text{Dirac Coulomb}}, \vec{\ell} \right] \neq 0 \quad \left[H_{\text{Dirac Coulomb}}, \vec{s} \right] \neq 0$$

$$H, j^2, j_z$$

$$\vec{j} = \vec{\ell} + \vec{s}$$

& 'parity'



August-September 2012 PCD STAP Unit 3 150

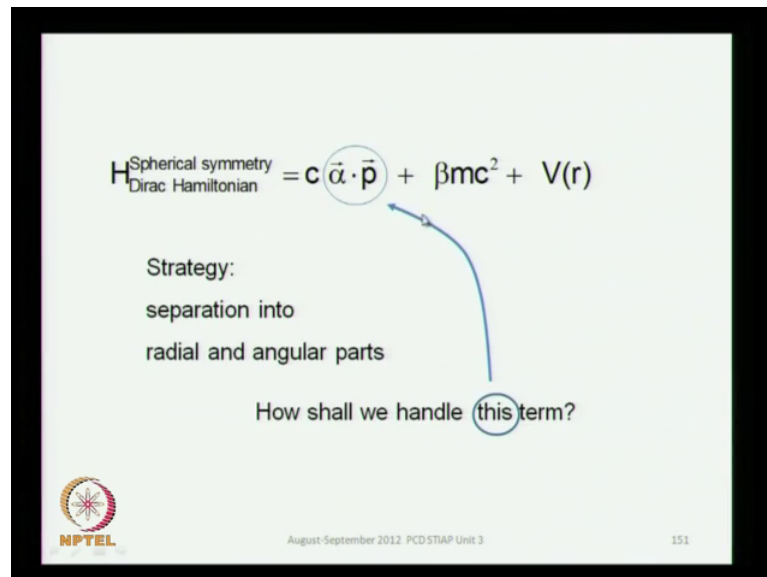
So, for the coulomb potential Dirac equation has got an exact analytical solution, so now let see how we are going to handle this, and it is not at all trivial, the reason to discuss it is because it is not a trivial extension of non relativistic methods. In non relativistic quantum mechanics, you vary in a very simple manner, you separate the radial part from the angular part right because of the 1 over r potential.

Now, that is not, so obvious for the Dirac case, because of the presence of the odd operators and if you look at the Dirac equation now. In fact, if you look at the Dirac equation even for a free particle, let alone a particle in an electromagnetic field, so even if you throw the terms in A and phi you find that the orbital angular momentum operator, and the spin angular momentum operators do not commute for the Dirac Hamiltonian even for a free particle. And then of course, they will not commute for the Dirac Hamiltonian for the coulomb problem, because these terms are also there.

So, it is not going to commute, which means that these will not give you good quantum numbers, because our whole idea of good quantum numbers is to get them, from those operators which commute to the Hamiltonian. So, that they correspond to simultaneous compatible observations, so what constitute compatible observations to give you good quantum numbers is a question, and we have to get the good quantum numbers for the Dirac Hamiltonian, and it is not going to be n l m, l cannot be a good quantum number, because l does not commute with the Hamiltonian.

So, your quantum numbers are going to be different, because of the spin orbit interaction, the spin orbit coupling. And then parity also has to be defined in a very careful manner, for the Dirac case, because of the beta operator, which is what is it one or zero minus one. So, you have to be careful with parity as well.

(Refer Slide Time: 40:46)



The slide displays the Dirac Hamiltonian for a spherically symmetric potential:

$$H_{\text{Dirac Hamiltonian}}^{\text{Spherical symmetry}} = c \vec{\alpha} \cdot \vec{p} + \beta mc^2 + V(r)$$

Below the equation, the strategy is outlined:

Strategy:
separation into
radial and angular parts

A blue arrow points from the term $\vec{\alpha} \cdot \vec{p}$ in the equation to the text "How shall we handle this term?", where "this term" is circled.

The slide includes the NPTEL logo in the bottom left corner and the text "August-September 2012 PCD STAP Unit 3" and "151" in the bottom right corner.

So, this is our statistical symmetry Dirac Hamiltonian, and now we want to explode this spherical, so somehow we want to separate the equation into a radial part and angular part. And we have to extract angular features and radial features, we have to identify them separately, and the main question is how you are going to handle this term, this alpha dot p, so let us discuss this.

(Refer Slide Time: 41:16)


$$\rho_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \quad \vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} = \vec{\sigma}^D = \vec{\sigma}^{\text{Dirac}}$$

$$\vec{S} = \frac{\hbar}{2} \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} = \frac{\hbar}{2} \vec{\sigma} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\hbar}{2} \vec{\Sigma}$$

$$\rho_1 \vec{\Sigma} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} = \vec{\alpha}$$

$$\rho_1 \vec{\alpha} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} = \vec{\Sigma}$$

$$\vec{\Sigma} \cdot \vec{p} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \cdot \vec{p} = \vec{\sigma} \cdot \vec{p} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\vec{\Sigma} \cdot \vec{p} = \frac{1}{r^2} \vec{\Sigma} \cdot \vec{r} \vec{\Sigma} \cdot \vec{r} \vec{\Sigma} \cdot \vec{p}$$


August-September 2012 PCD STAP Unit 3 152

So, these are our operators I defined 2 new operators, so this operator which got one, in off diagonal position is what I called as rho 1, I will use it, alpha we have already used which is the Dirac operators 0 sigma sigma 0. And this is sometimes called as a Dirac spin, this is made up of the poly spin, this is sigma sigma along the diagonal, along the off diagonal is a Dirac alpha, along the diagonal it is a sigma into the unit matrix operator.

And this is sometime written with a as sigma with the superscript d for Dirac or sometime with this uppercase sigma, so these are the various notations that you see. Sometimes, it is written only as this sigma which is a same as a poly sigma, but from the context you know whether it is a poly sigma or the Dirac sigma, if it is the Dirac sigma it is a 4 by 4 vector operator.

Likewise, the spin angular momentum which is h cross over 2 sigma is now you extend this idea to the 4 by 4 operators, and this is h cross over 2, this uppercase sigma, so this is a notation I will be using. So, this is h cross over 2 sigma, and you have got a unit operator you can also write this as h cross over 2 sigma, or you can just not write this one operator in which case you will read it as just a usual poly h cross over 2 sigma, but from the context you should know, what you are talking about.

So, notice this rho and sigma is the same as the alpha, rho and alpha is the same as a sigma, and if you look at sigma dot p, you can extract the sigma dot p and you have a

unit operator. So, sometime you will find books, in which this sigma dot p is written only as this sigma dot p, but they have the same things, they are the same or they are different, one has got a 4 by 4 structure and the other has got a 2 by 2 structure. So, which is y 1 is poly sigma the other is the Dirac sigma, but you have to be careful while reading literature, because many books do not alert you to this, although I am sure that they would have said that somewhere, but you have read it very carefully.

So, this is sigma dot p, now I have got sigma dot p here as well so; obviously, the rest of it over here is a unit operator, which you can easily recognize, because this is a projection of sigma in some direction, because this r over r is a unit operator. I do it twice, and sigma square along any direction is equal to 1, so this is just a unit operator. Everybody comfortable, this is just a prediction of sigma on some direction, sigma dot u and what is a square of sigma dot u. It is like sigma z square is equal to 1, now everybody will agree he is right indeed it is, so it is just like sigma z square which is equal to 1.

(Refer Slide Time: 45:20)

$$\vec{\sigma} \cdot \vec{p} = \frac{1}{r^2} \vec{\sigma} \cdot \vec{r} \vec{\sigma} \cdot \vec{r} \vec{\sigma} \cdot \vec{p}$$

$$\vec{\sigma} \cdot \vec{p} = \frac{1}{r^2} \vec{\sigma} \cdot \vec{r} (\vec{r} \cdot \vec{p} + i \vec{\sigma} \cdot \vec{r} \times \vec{p}) = \frac{\vec{\sigma} \cdot \vec{e}_r}{r} (\vec{r} \cdot \vec{p} + i \vec{\sigma} \cdot \vec{L})$$

$$\vec{r} \cdot \vec{p} = r \hat{e}_r \cdot (-i\hbar \vec{\nabla}) = -i\hbar \hat{e}_r \cdot \left(\hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right)$$

$$\vec{r} \cdot \vec{p} = -i\hbar r \frac{\partial}{\partial r} = r p_r + i\hbar \quad \text{since } p_r = -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \quad \boxed{r p_r = -i\hbar r \frac{\partial}{\partial r} - i\hbar}$$

$$\vec{\sigma} \cdot \vec{p} = \vec{\sigma} \cdot \vec{e}_r \left(p_r + \frac{i}{r} (\hbar + \vec{\sigma} \cdot \vec{L}) \right)$$

$$\vec{\sigma} \cdot \vec{p} = p_r \vec{\sigma} \cdot \vec{e}_r + \frac{i}{r} \vec{\sigma} \cdot \vec{e}_r (\hbar + \vec{\sigma} \cdot \vec{L})$$

NPTEL
August-September 2012 PCD STAP Unit 3
153

So, that is what you have got, and now here you make use of the poly identity, so this is r dot p plus i sigma dot r cross p, here you would expect a 4 by 4 unit matrix sitting implicitly. So, this is sigma dot r, this is r over r square, so this is e r over r, this is a unit vector in the direction of the position vector, and this r dot p gives you if you represent the gradient operator in the spherical polar coordinate system. You will need to work with the only one component, which is this and you know that the radial momentum

operator is not just a minus $i\hbar$ cross del by del r , it is minus $i\hbar$ cross del by del r minus $i\hbar$ cross over r .

So, be careful about it, because you have to put that in the expression for $r \cdot p$, which is minus $i\hbar$ cross r del by del r plus $i\hbar$ cross, so you have the $x y$ term. So, now you write this expression for $\sigma \cdot p$, which is $\sigma \cdot E r$, and then you had $r \cdot p$ which is here, which you know is $r p r$ plus $i\hbar$ cross, so you can put that over here, you have got a $\sigma \cdot l$ coming from here.

So, you put all the terms together and you have a essentially $\sigma \cdot E r$, but then our interest is in $\alpha \cdot p$. And what is α it is $\rho_1 \sigma$, and ρ_1 is this operator is this matrix which has got 0 1 1 0 with the elements 1 in the off diagonal position. So, when pre-multiply σ by ρ_1 you get the α , so the rest of the expression is the same.

(Refer Slide Time: 47:47)

$$\vec{\alpha} \cdot \vec{p} = \rho_1 \vec{\sigma} \cdot \vec{p} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \vec{\sigma} \cdot \hat{e}_r \left(p_r + \frac{i}{r} (\hbar + \vec{\sigma} \cdot \vec{l}) \right) = \alpha_r \left(p_r + \frac{i}{r} (\hbar + \vec{\sigma} \cdot \vec{l}) \right)$$

$$\vec{\alpha} \cdot \vec{p} = \alpha_r \left(p_r + \frac{i}{r} (\hbar + \vec{\sigma} \cdot \vec{l}) \right)$$

$$\vec{\alpha} \cdot \vec{p} = \alpha_r \left(-i\hbar \frac{\partial}{\partial r} - \frac{i\hbar}{r} + \frac{i}{r} (\hbar + \vec{\sigma} \cdot \vec{l}) \right) = \alpha_r \left(-i\hbar \frac{\partial}{\partial r} + \frac{i}{r} (\vec{\sigma} \cdot \vec{l}) \right)$$

Ref. Greiner page 174

New operator: $H_{\text{Dirac}}^{\text{sph}} = c \vec{\alpha} \cdot \vec{p} + \beta m c^2 + V(r)$

$K_{4 \times 4} = \beta_{4 \times 4} (\hbar l_{4 \times 4} + \vec{\sigma}_{4 \times 4} \cdot \vec{l})$ i.e. $\beta K_{4 \times 4} = (\hbar l_{4 \times 4} + \vec{\sigma}_{4 \times 4} \cdot \vec{l})$

$$\vec{\alpha} \cdot \vec{p} = \alpha_r \left(p_r + \frac{i}{r} \beta K \right)$$

$$H_{\text{Dirac}}^{\text{sph}} = c \left(\alpha_r p_r + \frac{i}{r} \alpha_r \beta K \right) + \beta m c^2 + V(r)$$

NPTEL

August-September 2012 PCD STAP Unit 3

154

And you have $\alpha \cdot p$ which is $\alpha r \phi r i$ over r , and then you have got \hbar cross plus $\sigma \cdot l$. Now, $p r i$ have written explicitly in terms of this minus $i\hbar$ cross del over del r minus $i\hbar$ cross over r , and now this term and this term will cancel. Now, this term now you see on the right side, you have got expression involving radial character. And this is what we set out to do, because our Dirac Hamiltonian for the spherical potential is the $c \alpha \cdot p$ plus $\beta m c^2$ plus v .

And now, we have succeed in writing $\alpha \cdot \vec{p}$ with radial features, it is not completely separated into the radial and angular part. And you will see that in the next class, but you are beginning to see that you are now able to see the radial features, which is what you need to separate the radial part from the angular part. And to be able to do the analysis completely, you are going to introduce a new operator, which is defined as a k which is this $\hbar \text{ cross plus sigma dot l}$.

Why is α , so important its coming here $\hbar \text{ cross plus sigma dot l}$, this is the one which we think could create some trouble for us, this is the operator which needs to be carefully handle. So, we, in fact defined a new operator, which is βk which is equal to $\hbar \text{ cross plus sigma dot l}$, so that makes k itself go as $\beta \hbar \text{ cross plus sigma dot l}$, β square is equal to 1 you know that. So, this is a new operator that we introduce, and in terms of this new operator your $\alpha \cdot \vec{p}$ operator becomes $\alpha_r \phi_r + i \text{ over } r \beta k$, where k is this new operator that we have defined.

(Refer Slide Time: 50:10)

Slide content showing the Dirac Hamiltonian for spherical symmetry and the definition of the operator K .

$$H_{\text{Dirac}}^{\text{Spherical symmetry}} = c \vec{\alpha} \cdot \vec{p} + \beta m c^2 + V(r)$$

$$K_{\text{Dirac}} = \beta_{\text{Dirac}} (\hbar l_{\text{Dirac}} + \vec{\Sigma}_{\text{Dirac}} \cdot \vec{\ell})$$

i.e. $\beta K_{\text{Dirac}} = (\hbar l_{\text{Dirac}} + \vec{\Sigma}_{\text{Dirac}} \cdot \vec{\ell})$

$$H_{\text{Dirac}}^{\text{Sph}} = c \left(\alpha_r p_r + \frac{i}{r} \alpha_r \beta K \right) + \beta m c^2 + V(r)$$

$$H_{\text{Dirac}}^{\text{Sph}} = -i c \alpha_r \left(\hbar \frac{\partial}{\partial r} + \frac{\hbar}{r} - \frac{1}{r} \beta K \right) + \beta m c^2 + V(r)$$

References: Greiner page 174

Questions? pcd@physics.iitm.ac.in

Next: solution to the H atom

NPTEL logo

August-September 2012 PCD STAP Unit 3

155

We can rewrite the Dirac Hamiltonian in this form, in terms of this new operator, and if you collect all these terms together, you have got the Dirac Hamiltonian for the spherical potential in terms of the k operator. And this is where I will stop today and take this up from here in the next class, so we need one more class to see how you actually workout the separation between the radial and the angular part. And then see how you get the

solutions to the Dirac equation, the coulomb functions and then use them in your relativistic applications.

So thank you very much.