

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

**Lecture - 15**  
**Relativistic Quantum Mechanics of the Hydrogen Atom**

Greetings, we will continue our discussion on the Dirac equation, we saw that the Dirac equation has got 4 components. So, today we will see that we really need 2 components to deal with the electron spin, and we will see there is a mechanism to reduce a 4 component formalism to a 2 component formalism and that is the foldy equation that we are lead to. But then there is a more systematic way of doing it which it was a foldy wouthuysen transformations, so I will introduce you to that as well.

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$E^2 = m^2c^4 + \vec{p}\vec{p}c^2$

4-component wavefunction      $E = \pm\sqrt{m^2c^4 + \vec{p}\vec{p}c^2}$


Multicomponent wavefunction : non-zero spin

Electron spin requires two components,  
- but Dirac equation admits  
4-component wavefunction

**Dirac equation – admits 'negative energy' solutions**

[1] Reduction to 2-component 'Pauli' relation.

[2] Foldy Wouthuysen Transformation:  
"..... as far as it goes....." – *Trigg's QM*

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Now, when you have a multi component wave function that is a signature of a spin, and now we really need 2 components if there is electron is concern. But, then the Dirac equation which is setup based on this quadratic scalar of the 4 momentum, since it admits negative energy solutions it allows for the antiparticles. And then the procedure to go over to the 2 component wave equation is what I will discuss today, and I will also begin a discussion on the foldy wouthuysen transformations as we go along which is a very rigorous way of doing it.

It is a much more rigorous way of doing it, which is a correct way of doing it nevertheless it is also approximate and it goes as far as it goes as trick tells us in his book.

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$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\varphi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} = \left( c \vec{\alpha} \cdot \vec{\pi} + \beta mc^2 + e\phi \right)_{4 \times 4} \begin{pmatrix} \tilde{\varphi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix}$$

$$\vec{\alpha}_{4 \times 4} = \begin{bmatrix} 0_{2 \times 2} & \vec{\sigma}_{2 \times 2} \\ \vec{\sigma}_{2 \times 2} & 0_{2 \times 2} \end{bmatrix} \quad \beta_{4 \times 4} = \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & -1_{2 \times 2} \end{bmatrix} \quad \psi_{4 \times 1} = \begin{pmatrix} \tilde{\varphi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix}$$

$$\text{r.h.s.} = \left( c \begin{bmatrix} 0_{2 \times 2} & \vec{\sigma}_{2 \times 2} \\ \vec{\sigma}_{2 \times 2} & 0_{2 \times 2} \end{bmatrix} \cdot \vec{\pi} + \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & -1_{2 \times 2} \end{bmatrix} mc^2 + \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & 1_{2 \times 2} \end{bmatrix} e\phi \right)_{4 \times 4} \begin{pmatrix} \tilde{\varphi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix}$$

Vector algebra!  
Matrix algebra  
QM, operator algebra

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So, this is the 4 component Dirac equation, now and you have got a 4 component wave functions. So, these 4 components I have written as phi delta and chi delta, phi delta is has 2 components and chi delta also has 2 components, so together it is a 4 component wave function. And then alpha and beta are the Dirac matrixes, now you can see the 4 by 4 structure by explicitly writing the Dirac matrixes alpha and beta, and you have to admit that you are going to have to use the vector algebra, matrix algebra, quantum mechanics, operator algebra everything will go together.

Because, you know the terms that you see in this expression sigma for example, it is not just a vector, it is a vector operator it itself has a matrix structure sigma are 2 by 2 matrixes. So, whatever mathematics you do is very simple there is nothing beyond you know matrix algebra or vector algebra and a little bit of calculus because you also have the differential operators. So, the mathematics is very simple, but you have to be very careful that you have to use all of it together, so the first thing I will do is to demonstrate the reduction to the 2 component foldy relation.

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$$i\hbar \frac{\partial}{\partial t} \psi_{4 \times 1} = \left( c \vec{\alpha} \cdot \vec{\pi} + \beta mc^2 + e\phi \right)_{4 \times 4} \psi_{4 \times 1} \quad \psi_{4 \times 1} = \begin{pmatrix} \tilde{\phi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix}$$


[1] Reduction to 2-component 'Pauli' relation.

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\phi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} = \left( c \vec{\sigma} \cdot \vec{\pi} \begin{bmatrix} 0_{2 \times 2} & 1_{2 \times 2} \\ 1_{2 \times 2} & 0_{2 \times 2} \end{bmatrix} + \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & -1_{2 \times 2} \end{bmatrix} mc^2 + \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & 1_{2 \times 2} \end{bmatrix} e\phi \right)_{4 \times 4} \begin{pmatrix} \tilde{\phi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix}$$

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\phi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} = c \vec{\sigma}_{2 \times 2} \cdot \vec{\pi} \begin{pmatrix} \tilde{\chi}_{2 \times 1} \\ \tilde{\phi}_{2 \times 1} \end{pmatrix} + mc^2 \begin{pmatrix} \tilde{\phi}_{2 \times 1} \\ -\tilde{\chi}_{2 \times 1} \end{pmatrix} + e\phi \begin{pmatrix} \tilde{\phi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix}$$

[1]  $i\hbar \frac{\partial}{\partial t} \tilde{\phi} = c \vec{\sigma} \cdot \vec{\pi} \tilde{\chi} + mc^2 \tilde{\phi} + e\phi \tilde{\phi}$

[2]  $i\hbar \frac{\partial}{\partial t} \tilde{\chi} = c \vec{\sigma} \cdot \vec{\pi} \tilde{\phi} - mc^2 \tilde{\chi} + e\phi \tilde{\chi}$



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Now, this is the 4 component form and you have the sigma dot pi extracted from this alpha dot pi, and then you have got the 2 by 2 matrixes 0 1 1 0. And that essentially gives 2 equations because the 0 1 1 0 when this operator operates on this, you will get chi goes to the top and phi comes over here. Because, this is not a diagonal unit matrix, it has got 0 elements along the diagonal, and it has 0 1 1 0 structure which is what gives you the chi phi over here. And in the second term m c square you get phi minus chi, so that is what you get.

Now, this is really because of the block diagonal structure you can look at this as really 2 sets of equations, one is an equation for the time derivative of phi delta, and the other is a time derivative of chi delta. But, on the right hand side you find not just phi delta, but also chi delta, and in the second equation you find not just chi delta, but also phi delta. So, these are coupled equations for phi delta and chi delta, and we will examine if these can be decoupled. So, you have 2 sets of equation there is no approximation as yet, it is just a Dirac equation that we are looking at in a different form.

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$$i\hbar \frac{\partial}{\partial t} \tilde{\phi} = c \vec{\sigma} \cdot \vec{\pi} \tilde{\chi} + mc^2 \tilde{\phi} + e\phi \tilde{\phi}$$


$$i\hbar \frac{\partial}{\partial t} \tilde{\chi} = c \vec{\sigma} \cdot \vec{\pi} \tilde{\phi} - mc^2 \tilde{\chi} + e\phi \tilde{\chi}$$

Stationary state solution  $\begin{bmatrix} \tilde{\phi} \\ \tilde{\chi} \end{bmatrix} = e^{-\frac{E_0}{\hbar} t} \begin{bmatrix} \phi \\ \chi \end{bmatrix}$  where  $E_0 = mc^2$

$\phi, \chi$  : slowly varying functions of time

$$E_0 \begin{bmatrix} \phi \\ \chi \end{bmatrix} + i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \phi \\ \chi \end{bmatrix} = c \vec{\sigma} \cdot \vec{\pi} \begin{bmatrix} \chi \\ \phi \end{bmatrix} + mc^2 \begin{bmatrix} \phi \\ -\chi \end{bmatrix} + e\phi \begin{bmatrix} \phi \\ \chi \end{bmatrix}$$

**Recall!** Stationary state solution to the time-dependent Schrodinger equation results in time-independent equation.

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And these are the 2 sets of equations that we get, what we now do is to extract the major time dependence in  $\phi$  and  $\chi$ , in this harmonic term  $e^{-i E_0 t / \hbar}$ , where  $E_0$  is the rest energy of the particle. Now, notice that this is a huge energy this is like half a million electron volts, and in atomic physics you are dealing with rather low energy phenomenon. If you look at atomic spectra, atomic transitions, the visible light for example, or might go beyond the visible get into the violet, the ultraviolet, you might get into the x rays right.

And even then in atomic spectroscopy deep inertial transitions are also involved, you are still involved with transitions of the order of few tens of thousands of electron volts nothing more. So, in atomic processes you are not dealing with very high energies and therefore, compared to the processes that we are interested in, the rest energy is a huge amount of energy compared to any energy that we are going to be concerned with. And therefore, since most of the time dependence is already contained over here, these terms  $\phi$  and  $\chi$  you have only factored out this  $e^{-i E_0 t / \hbar}$  from  $\phi$ .

And the residual factor is  $\phi$  without the  $\delta$ , so the residual factor will also have a little bit of time dependence. But, it will be marginal time dependence, it will depend weakly on time not very strongly because most of the strongest dependence on time is already factored out in this big term. So, now the functions  $\phi$  and  $\chi$  which appear without the tilde these are slowly varying functions of time.

So, let us now take the time derivative of phi delta and chi delta, so you will of course, get the e to the minus this is the simple exponential function, you can take it is differentia with respect to time. And then you will have this e to the minus i e 0 over h cross extracted, when you take the derivative with respect to time, this will cancel the corresponding term on the right hand side. And you get now an equation of this form right good. So, now phi and chi both have a time dependence, it is not the time dependence is totally eliminated. But, these are weakly time dependent and we will now examine the solution of these 2 equations, so let us do that now.

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$\phi, \chi$ : slowly varying functions of time

$$E_0 \begin{bmatrix} \phi \\ \chi \end{bmatrix} + i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \phi \\ \chi \end{bmatrix} = c\vec{\sigma} \cdot \vec{\pi} \begin{bmatrix} \chi \\ \phi \end{bmatrix} + mc^2 \begin{bmatrix} \phi \\ -\chi \end{bmatrix} + e\phi \begin{bmatrix} \phi \\ \chi \end{bmatrix}$$

$$E_0 \begin{bmatrix} \phi \\ \chi \end{bmatrix} + i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \phi \\ \chi \end{bmatrix} = c\vec{\sigma} \cdot \vec{\pi} \begin{bmatrix} \chi \\ \phi \end{bmatrix} + E_0 \begin{bmatrix} \phi \\ -\chi \end{bmatrix} + e\phi \begin{bmatrix} \phi \\ \chi \end{bmatrix}$$

$$+i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \phi \\ \chi \end{bmatrix} = c\vec{\sigma} \cdot \vec{\pi} \begin{bmatrix} \chi \\ \phi \end{bmatrix} + e\phi \begin{bmatrix} \phi \\ \chi \end{bmatrix} - 2E_0 \begin{bmatrix} 0 \\ \chi \end{bmatrix}$$

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So, these are slowly varying functions of time, and you have m c square over here, which i have written as E 0. You can you have a term in E 0 phi chi over here, which you can bring to the right hand side, and then on the left hand side you get just i h cross del by del t of this phi chi, this E 0 together with this E 0 and this minus sign will give you a minus 2 e 0, but this term will cancel this one. So, you get minus 2 E 0 0 chi over here right, so now, let us analyze this relationship all have done is to move one term to the right hand side.

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$$+i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \phi \\ \chi \end{bmatrix} = c\vec{\sigma} \cdot \vec{\pi} \begin{bmatrix} \chi \\ \phi \end{bmatrix} + e\phi \begin{bmatrix} \phi \\ \chi \end{bmatrix} - 2mc^2 \begin{bmatrix} 0 \\ \chi \end{bmatrix}$$


2<sup>nd</sup> Eq.  $+i\hbar \frac{\partial}{\partial t} \chi = c\vec{\sigma} \cdot \vec{\pi} \phi + \underbrace{e\phi \chi - 2mc^2 \chi}_{\text{since } e\phi \ll 2mc^2}$

$\phi, \chi$ : slowly varying functions of time

$0 \approx c\vec{\sigma} \cdot \vec{\pi} \phi - 2mc^2 \chi$  since  $e\phi \ll 2mc^2$

$\vec{\sigma} \cdot \vec{\pi} \phi \approx 2mc \chi \Rightarrow \frac{\vec{\sigma} \cdot \vec{\pi}}{2mc} \phi \approx \chi \Rightarrow \begin{matrix} \chi: \text{small} \\ \phi: \text{large} \end{matrix}$

1<sup>st</sup> Eq.  $+i\hbar \frac{\partial}{\partial t} \phi \approx c\vec{\sigma} \cdot \vec{\pi} \frac{\vec{\sigma} \cdot \vec{\pi}}{2mc} \phi + e\phi \phi$



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Now, this is again 2 equations look at this lower one, which is the derivative of chi and this is c sigma dot pi operating on phi plus e phi operating on chi minus twice m c square operating on chi, there is always a unit operator which is setting over there. Now, if you look at these terms, these 2 terms have got chi, so if you compare the coefficients e phi and twice m c square, this is huge energy e phi is also energy right. This is much larger and therefore, you can ignore e phi compared to twice m c square, so between these 2 terms the only significant term is twice m c square.

So, that is what I have written over I have ignored this term, and now I have begun to make approximations. And it looks like reasonable approximation to do because the energies we are talking about are m c square or twice m c square which is even more, so you can throw off e phi compared to this. And now you have got on the left hand side the time derivative of chi, but chi is only mildly time dependent, which is to say that it is mostly time independent.

And therefore, it is derivative can be considered to be very nearly 0, so here is an approximation no doubt, but not a bad one. So, the left hand side becomes nearly 0 because chi is mostly independent of time being only mildly dependent on time, so the left hand side is very nearly 0 and the right hand side between these terms I have taken the significant term, which is minus twice m c square chi. And because this is not quite

exact I write this as nearly equal to or rather than exactly equal to, but having understood this difference we can use the equivalent.

Now, what does this tell us that these 2 terms whose difference goes to 0 must be equal, the difference of 2 terms goes to 0. And therefore,  $\chi$  is  $\sigma \cdot \pi$  operating on  $\phi$  divided by twice  $m c$  more or less, within the scheme of approximation that we have made. And it is nearly given by this relationship which includes, so  $\chi$  and  $\phi$  are linearly related, but the proportionality has got a denominator which is twice  $m c$ , which is a product of two large terms,  $m$  is huge it is half a million electron volts,  $c$  is huge it is the highest speed that you can think of.

So, there are two large terms in the denominator and that tells us that  $\chi$  is much smaller than  $\phi$ , which is why this  $\chi$  is sometimes called as the small component of the wave function, and this  $\phi$  is called as the large component, there is a good reason for it. So, this is the small and these are the small and the large components, and now we can express this relationship, in the first equation which is for  $\phi$  which is for the large component.

And in the large component equation which is  $i \hbar \text{grad} \phi = \frac{1}{2m} (\sigma \cdot \pi)^2 \phi$  operating on  $\chi$  and this  $\chi$  can be now replaced by  $\frac{\sigma \cdot \pi}{2m c} \phi$ , which is what we have done over here. And now you have got a relationship which does not have  $\chi$  at all, so we have sort of decoupled the relations approximately, but quite fruitful.


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$$+i\hbar \frac{\partial}{\partial t} \psi = \left[ \frac{\vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi}}{2m} + e\phi \right] \psi$$

$$\boxed{\vec{\sigma} \cdot \vec{a} \vec{\sigma} \cdot \vec{b} = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot \vec{a} \times \vec{b}}$$

$$\vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi} = \vec{\pi} \cdot \vec{\pi} + i\vec{\sigma} \cdot \vec{\pi} \times \vec{\pi}$$

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

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


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So, you can cancel the  $c$  and what you have is this relationship for the large component, and now there is a little bit of you know very well known mathematics that you can do. Because, you are well aware of this identity involving the foldy operator  $\sigma$  right, this is well known identity that you would have used in the large number of examples, in your first course in quantum mechanics. So, here you have  $\sigma \cdot a$  time  $\sigma \cdot b$ , but our interest is in  $\sigma \cdot \pi$  and  $\sigma \cdot \pi$ , so both  $a$  and  $b$  are the same and this is what we have got.

So, let us simplify this relationship further  $\pi \times \pi$  is what appears over here, which is of course, not 0 these are operators these are quantum operators. And you find exactly what they turn out to be, so you first have a look at this term  $\pi \times \pi$ , which is the generalized momentum, which includes the magnetic vector potential as well. And if you throw the quadratic term in  $A$  square over  $c$  square, again the denominator  $c$  is large, the vector potential is weak in most of the situations that you talk about, so you can throw the quadratic term in  $A$  square over  $c$  square. And then what you are left with is only the linear terms in which you have got  $p \times A$  plus  $A \times p$ , so this is the term that we will examine further.



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$$\begin{aligned}\vec{\pi} \times \vec{\pi} &= -\frac{e}{c}(\vec{p} \times \vec{A} + \vec{A} \times \vec{p}) & (\vec{p} \times \vec{A} + \vec{A} \times \vec{p}) &=? \\ (\vec{p} \times \vec{A} + \vec{A} \times \vec{p})f(\vec{r}) &= -i\hbar(\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla})f(\vec{r}) \\ (\vec{p} \times \vec{A} + \vec{A} \times \vec{p})f(\vec{r}) &= -i\hbar[\vec{\nabla} \times \vec{A}f(\vec{r}) + \vec{A} \times \vec{\nabla}f(\vec{r})] \\ (\vec{p} \times \vec{A} + \vec{A} \times \vec{p})f(\vec{r}) &= -i\hbar[(\vec{\nabla} \times \vec{A})f(\vec{r}) - \vec{A} \times \vec{\nabla}f(\vec{r}) + \vec{A} \times \vec{\nabla}f(\vec{r})] \\ (\vec{p} \times \vec{A} + \vec{A} \times \vec{p})f(\vec{r}) &= -i\hbar(\vec{\nabla} \times \vec{A})f(\vec{r}) = (\vec{p} \times \vec{A})f(\vec{r}) \\ (\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla}) &= (\vec{\nabla} \times \vec{A}) & (\vec{p} \times \vec{A} + \vec{A} \times \vec{p}) &= (\vec{p} \times \vec{A}) \\ \vec{\pi} \times \vec{\pi} &= -\frac{e}{c}(\vec{p} \times \vec{A}) = -\frac{e}{c}(-i\hbar \vec{\nabla} \times \vec{A}) = \frac{ie\hbar}{c} \vec{B}\end{aligned}$$

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And we ask what this is, and to find out what it is, it is of course, an operator what we do is to operate on an arbitrary function  $f$  of space, and analyze the result. The momentum operator of course, the gradient operator it is minus  $\hbar$  cross  $\nabla$ , and there are 2 terms on the right side, this is the first term  $\nabla$  cross  $A$  operating on  $f$ . But, this is the curl of a product of 2 functions, this is a curl of a product of 2 functions  $A$  itself is a function of  $r$ .

The curl is going to involve the space derivative operators as we know, and you must take the space derivative operators operate on everything it is going to operate upon. And the derivative operators in the sitting in the gradient operator, will operate on the product of these functions, one of which is a vector which is the vector potential. The other is a scalar, which is an arbitrary function of space it does not matter what function it is.

So, this is the curl of a product of 2 functions and the curl of a product of a vector and a scalar is the curl of the vector times the scalar minus  $A$  cross the gradient of the scalar function. This is the vector identity I make use of which you would have studied in your vector calculus course, so this is the curl of product of this, and now having exploited this I find that when I look at consider the last term over here, these two terms are actually the same, because both involve the cross product of  $A$ , with the gradient of  $f$  one with a plus sign and the other with a minus sign. So, they will cancel each other, and now what you are left with is an identity, which is valid for an arbitrary function of  $f$  it does not matter what function it is, we did not choose any particular form of the function  $f$ .

And therefore, we have an operator equivalence in the context in which we are using this right, which means that in our context we can replace this del cross A plus A cross del operator by the magnetic field which is a curl of A.

So, we do that we replace the curl of A by the magnetic field and keep track of this minus i h cross over here and a minus e over c over here, keep track of the sign or everything. And we get this pi cross pi to be equal to i e h cross over c times the magnetic field, now this pi cross pi term, we know where it appears.

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$$+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{\vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi}}{2m} + e\phi \right] \varphi$$

$$\vec{\sigma} \cdot \vec{a} \vec{\sigma} \cdot \vec{b} = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot \vec{a} \times \vec{b}$$

$$\vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi} = \vec{\pi} \cdot \vec{\pi} + i\vec{\sigma} \cdot \vec{\pi} \times \vec{\pi}$$


$$\vec{\pi} \times \vec{\pi} = \frac{ie\hbar}{c} \vec{\nabla} \times \vec{A} = \frac{ie\hbar}{c} \vec{B}$$

$$\vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi} = \vec{\pi} \cdot \vec{\pi} + i\vec{\sigma} \cdot \left( \frac{ie\hbar}{c} \vec{B} \right)$$

$$\frac{1}{2m} (\vec{\sigma} \cdot \vec{\pi} \vec{\sigma} \cdot \vec{\pi}) = \frac{1}{2m} \left( \vec{\pi} \cdot \vec{\pi} - \frac{e\hbar}{c} \vec{\sigma} \cdot \vec{B} \right)$$

$$+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{\pi^2}{2m} - \frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B} + e\phi \right] \varphi$$

Pauli eq. for the 'large' component

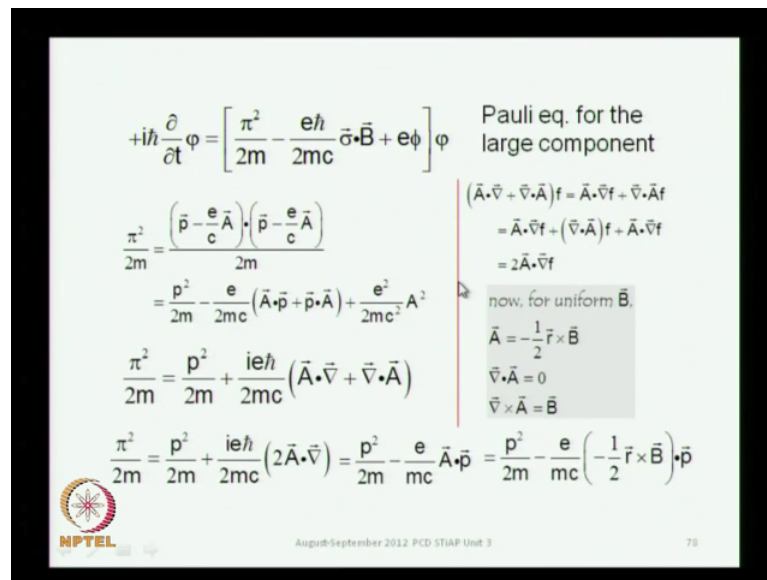
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We need it over here, and here instead of pi cross pi we can plug in i e h cross over c times the magnetic field. So, we do that and now we have to look at what is it that we really need, we have actually sigma dot pi times operating on sigma dot pi divided by 2 m. So, let us not forget this 1 over 2 m factor and you also have this pi dot pi term, so you have the pi square over 2 m minus e h cross over twice m c this 2 m together with c sigma dot B. And then you have this electric potential energy which is e phi, and this equation is known as the Pauli equation for the large component.

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$$+i\hbar \frac{\partial}{\partial t} \psi = \left[ \frac{\pi^2}{2m} - \frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B} + e\phi \right] \psi \quad \text{Pauli eq. for the large component}$$

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

$$= \frac{p^2}{2m} - \frac{e}{2mc} (\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) + \frac{e^2}{2mc^2} A^2$$

$$\frac{\pi^2}{2m} = \frac{p^2}{2m} + \frac{ie\hbar}{2mc} (\vec{A} \cdot \vec{\nabla} + \vec{\nabla} \cdot \vec{A})$$

$$\frac{\pi^2}{2m} = \frac{p^2}{2m} + \frac{ie\hbar}{2mc} (2\vec{A} \cdot \vec{\nabla}) = \frac{p^2}{2m} - \frac{e}{mc} \vec{A} \cdot \vec{p} = \frac{p^2}{2m} - \frac{e}{mc} \left( -\frac{1}{2} \vec{r} \times \vec{B} \right) \cdot \vec{p}$$

$$\begin{aligned} (\vec{A} \cdot \vec{\nabla} + \vec{\nabla} \cdot \vec{A}) f &= \vec{A} \cdot \vec{\nabla} f + \vec{\nabla} \cdot \vec{A} f \\ &= \vec{A} \cdot \vec{\nabla} f + (\vec{\nabla} \cdot \vec{A}) f + \vec{A} \cdot \vec{\nabla} f \\ &= 2\vec{A} \cdot \vec{\nabla} f \end{aligned}$$

now, for uniform  $\vec{B}$ ,

$$\vec{A} = -\frac{1}{2} \vec{r} \times \vec{B}$$

$$\vec{\nabla} \cdot \vec{A} = 0$$

$$\vec{\nabla} \times \vec{A} = \vec{B}$$

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Now, let us examine this a little bit further this is the Pauli equation, we also have to look at this operator pi square, which is the inner product of these 2 operators. This pi is the generalized momentum it includes the vector potential, once again you can throw the A square over c square term, and then you are left with p square over 2 m and this term in which the momentum is the minus i h cross gradient. So, you get a sum of A dot del plus del dot A term, and just the way you handle them corresponding terms involving the cross, you do the same with the dot.

And you let it operate on an arbitrary function of f, and find that this is nothing, but twice A dot del operator, it is exactly the same reasoning right. So, this operator is now replaced by twice A dot del, which is what comes here, so now, you have got this operator, and you can express you can put these 2 terms for this, which is written in terms of the momentum operator. And now let us think of a uniform magnetic field, for which the vector potential is minus half r cross B, you can see this very easily that this generates a uniform magnetic field.


It is divergent and curl both would vanish curl would of course, give you the magnetic field, but divergence will vanish it is uniform. And this vector potential is then replaced by minus half r cross B, so this is rather straight forward electrodynamics, now let us put these 2 terms in place pi square over 2 m in the Pauli equation.

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$$\frac{\pi^2}{2m} = \frac{p^2}{2m} - \frac{e}{mc} \left( -\frac{1}{2} \vec{r} \times \vec{B} \right) \cdot \vec{p}$$

$$\frac{\pi^2}{2m} = \frac{p^2}{2m} + \frac{1}{2} \frac{e}{mc} \vec{r} \times \vec{B} \cdot \vec{p} \quad \frac{\pi^2}{2m} = \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} \vec{B} \times \vec{r} \cdot \vec{p}$$

$$\frac{\pi^2}{2m} = \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} \vec{B} \cdot \vec{r} \times \vec{p} = \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} \vec{B} \cdot \vec{\ell}$$

$$\frac{\pi^2}{2m} = \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} \vec{\ell} \cdot \vec{B}$$


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So, these are the 2 terms which will take place of pi square over 2 m in the Pauli equation, but when we do that you have got minus sign here and a minus sign here. So, that gives you a plus sign, and then you have got r cross B which you can write as B cross r with a minus sign. And then you have a triple product, scalar triple product B cross r dot p, you can interchange the dot and the cross and look at this as B dot r cross p.

Because, that is what gives you the orbital angular momentum operator, so you get the B dot r cross p which is the B dot l operator. Now, that is good that places the pi square over 2 m in a form that I think we are going to like much more because now you get the l dot B term keep track of this e over twice m c, it is an important factor.

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$$+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B} + e\phi \right] \varphi \quad \text{Pauli eq. for the large component}$$

$$\frac{p^2}{2m} = \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} \vec{\ell} \cdot \vec{B} \quad \text{and} \quad \vec{s} = \frac{\hbar}{2} \vec{\sigma}$$

$$\Rightarrow$$

$$+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} \vec{\ell} \cdot \vec{B} - \frac{e}{mc} \vec{s} \cdot \vec{B} + e\phi \right] \varphi$$

$$+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{e}{2mc} (\vec{\ell} + 2\vec{s}) \cdot \vec{B} + e\phi \right] \varphi$$

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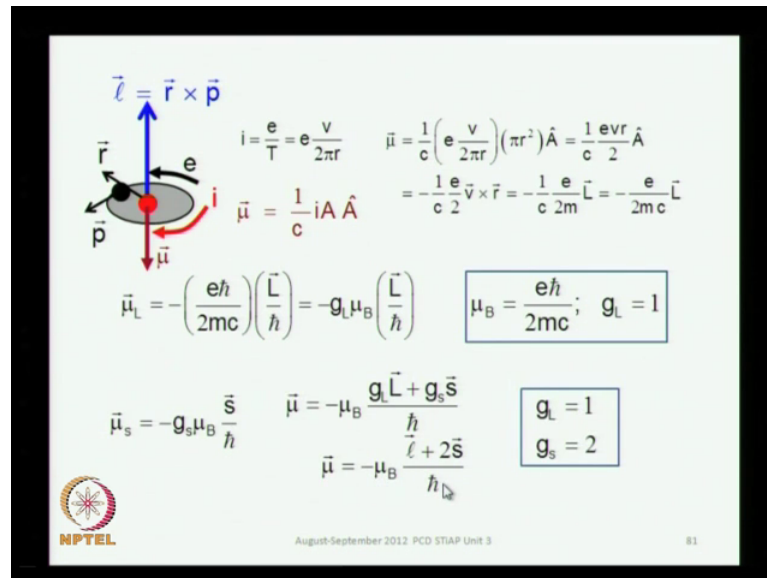
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This is the Pauli equation for the large component, this is the  $e$  over twice  $m c$  and now I will like to remind you that the spin angular momentum is  $\hbar$  cross over 2 times the Pauli spin vector  $\sigma$  right. So, you can write this as minus  $e$  over  $m c$   $s$  dot  $B$  because you have got  $\hbar$  cross by 2  $\sigma$  over here, this is  $\hbar$  cross  $\sigma$  by 2, so that is replaced by the operator  $s$  this term is nothing, but  $e \hbar$  cross over twice  $m c$  twice  $s$  over  $\hbar$  cross now  $\hbar$  cross cancel the 2 cancels, and then you are left with minus  $e$  over  $m c$   $s$  dot  $B$ .

What do you have, you combine these 2 terms both involved the dot product with the magnetic field. So, you can see that it is the magnetic field energy interaction energy with a magnetic dipole type of term, so you see your beginning to see something like a  $\mu$  dot  $B$  term that you expect to find when you have a magnetic moment placed in a magnetic field. So, you are beginning to see that term, so you need to recognize it fully this is the expression that you now get  $1$  plus  $2 s$  dot  $b$  minus  $e$  over  $2 m c$ .

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So, just remind yourself of this picture which comes from old quantum theory, which you must take with a pinch of salt. And much more than a pinch of salt, but use it nevertheless, and if have an electron in a bohr orbit then it has got an angular momentum  $\vec{r} \times \vec{p}$ , which is orthogonal to the plane of the orbit. The conventional current is in the opposite direction just because the electron is a negative charge that is how it was defined historically.

So, the conventional current is in the opposite direction and this current loosely speaking although we are using this old quantum theory, and orbits which we know do not really exist. So, this is rated which the charge goes that is a current, which is  $e$  over the time it takes to go through this orbit right, and that will be the ratio of the velocity to the circumference far enough. So, that is the  $1$  over  $t$  and you also know that if you have a current loop, it generates a magnetic field.

And this magnetic field can be represented by a magnetic moment, which is given by the cross product of  $i$  and the area enclosed by the loop the  $i$  cross  $A$  is the term that you typically look at in  $SI$  system of units right. The equivalent magnetic moment of a current carrying loop is  $i$  cross  $A$   $i$  is not quite a vector, but of course, you are looking at the magnitude of the current multiplied by the direction, in which the current is moving. So, that is the interpretation of  $i$  cross  $A$ , now we are using gaussian in  $cgs$ , so there is not just  $iA$ , but  $1$  over  $c$  times  $iA$  in the system of units that we are using.

So, that is the difference with the  $\sin \theta$  and  $\sin \theta$  it would be just  $i A$  because this were orthogonal, so the  $\sin \theta$  is 1, but in our system of units this is  $1$  over  $c$  times  $i A$ . So, this is the magnetic moment effective magnetic moment of the bohr orbit, and this effective moment which is  $1$  over  $c$  times  $i$ ,  $i$  is  $e v$  over twice  $\pi r$  the area enclosed is  $\pi r^2$   $r$  being the radius of the bohr orbit. So, you simplify this and you find that this is here you find the angular momentum popping up.

Because, you have got the  $v r$  times the direction of the angular momentum right, so you get essentially the angular momentum, but  $v \times r$  is not really the angular momentum, you have got the  $r \times p$ . So, there is over  $1$  over  $m$  which should show up right  $r \times p$  is the angular momentum, you have minus of  $r \times b$ , so you have  $A$   $1$  over  $m$  coming up, and this is what you get  $e$  over twice  $m c$  times angular momentum.

So,  $e$  over twice  $m c$  times the angular momentum  $I$  multiply and divide by  $\hbar$ , so I have an  $\hbar$  cross in the numerator here, and an  $\hbar$  cross in the denominator here, which preserves the balance. And that allows me to factor out this term  $e \hbar$  cross over twice  $m c$ , which is called as the bohr magneton this is  $e \hbar$  cross over twice  $m c$ , and the reason you have a see there is because of the twice of units that we are using.

But, if you used some other choice of units you would not see that, which is ironical that you do not see the  $c$ . Now, let us look at this, this is the magnetic moment for orbital motion, you can always define a corresponding magnetic moment for spin angular momentum. Essentially what you find is that, for an angular momentum you have a corresponding magnetic moment, and you expect a similar situation for the spin angular momentum that there is a corresponding magnetic moment.

But, then the proportionality something that we really do not know, what it would be like and we cannot really demand that it must be the same. So, to provide for a variance you insert a factor  $g$  which is equal to unity for the orbital angular momentum case, and you ask what the corresponding  $g$  for the spin should be like. So, this is our expression and it turns out that  $g$   $s$  must be equal to  $2$ , according to this particular formalism it is a fairly accurate answer it is not strictly speaking accurate.

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$$+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{e}{2mc} (\vec{\ell} + 2\vec{s}) \cdot \vec{B} + e\phi \right] \varphi$$

$$\vec{\mu} = -\mu_B \frac{\vec{\ell} + 2\vec{s}}{\hbar}$$

$$\mu_B = \frac{e\hbar}{2mc}$$

$$\vec{\mu} = -\frac{e\hbar}{2mc} \frac{\vec{\ell} + 2\vec{s}}{\hbar} = -\frac{e}{2mc} (\vec{\ell} + 2\vec{s})$$

Gyromagnetic ratio;  $g=2$   
 g value: measure of MAGNETIC MOMENT  
 - Dimensionless magnetic moment



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But, that is what you get from here it is not bad, and in terms of the bohrmagneton magnetic moment is then  $\hbar$  plus  $2s$  by  $\hbar$  cross you can put this back in the Pauli equation, and you find that you have got a  $\vec{\mu} \cdot \vec{B}$  term as you expect. So, this is this  $g$  is almost equal to 2 very nearly equal to 2, you can make quarter fill theoretical corrections to that. And that is a problem of considerable challenge, and I will comment on this a little later in this course.

But, it is also related to the fine structure constant, and how accurately you know the fine structure constant, and these are really the problems of interest. And experimentalist are working extremely hard to get the accurate value of  $g$  it is not exactly 2, but that is what you get from this formalism, you will also get the same value from the Dirac equation as from the more complete analysis of the Dirac equation, this has also come out of the Dirac equation from the Pauli reduction. So, this is the gyro magnetic ratio it is called because it is involved in the proportionality between the angular momentum, between the mechanical angular momentum and the magnetic moment.



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**Dirac equation in 'standard representation'**


$$i\hbar \frac{\partial \psi_{4 \times 1}}{\partial t} = \left( c \vec{\alpha} \cdot \left( \vec{p} - \frac{e}{c} \vec{A} \right) + \beta mc^2 + e\phi \right) \psi_{4 \times 1}$$

$$\psi_{4 \times 1} = \begin{pmatrix} \tilde{\varphi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} \quad \begin{bmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{bmatrix} = e^{-\frac{E_0 t}{\hbar}} \begin{bmatrix} \varphi \\ \chi \end{bmatrix} \quad \text{where } E_0 = mc^2$$

**Pauli 2-component**  $+i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} (\vec{\ell} + 2\vec{s}) \cdot \vec{B} + e\phi \right] \varphi$

**2-components: required for the two spin degrees of freedom for the electron with  $j=\frac{1}{2}$**

To determine expectation values to order  $\frac{v^2}{c^2}$ , one has to employ all the four components



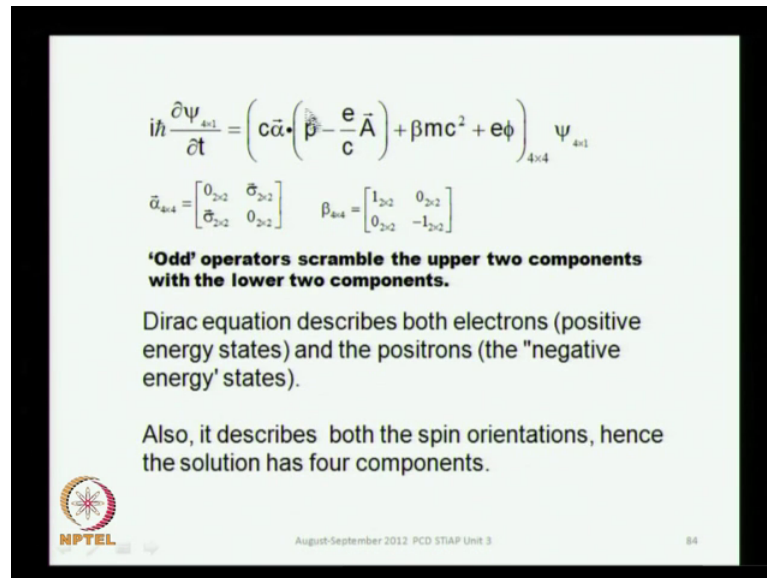
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So, this is the reduction to the 2 component Pauli equation, so you get the  $p^2$  over  $2m$  plus  $\frac{1}{2} \frac{e}{mc} (\vec{\ell} + 2\vec{s}) \cdot \vec{B}$ . And this would work well for an electron because for the electron you expect the formalism to have two components there is a provision for that, and you are with it you can go ahead and do a lot of quantum mechanics with this including the spin.

Now, this is not really very satisfactory because if you have to do quantum mechanics, you have to not just look at the Dirac equation or the Pauli equation, but you have to do some physics with these equation like with Dirac equation wave function, you ought to look at the probability densities, the charge densities expectation values of operators and so on. So, there is a lot of other things that you do and when you begin to do that it turns out that you end up mixing the large component with the small component, you cannot avoid it.

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$$i\hbar \frac{\partial \psi_{4 \times 1}}{\partial t} = \left( c \vec{\alpha} \cdot \left( \vec{p} - \frac{e}{c} \vec{A} \right) + \beta m c^2 + e \phi \right) \psi_{4 \times 1}$$

$$\vec{\alpha}_{4 \times 4} = \begin{bmatrix} 0_{2 \times 2} & \vec{\sigma}_{2 \times 2} \\ \vec{\sigma}_{2 \times 2} & 0_{2 \times 2} \end{bmatrix} \quad \beta_{4 \times 4} = \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & -1_{2 \times 2} \end{bmatrix}$$

**'Odd' operators scramble the upper two components with the lower two components.**

Dirac equation describes both electrons (positive energy states) and the positrons (the "negative energy" states).

Also, it describes both the spin orientations, hence the solution has four components.

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And you therefore, look for a more systematic way of decoupling the large component from the small component. Because, what is happening in the four component theory, which you approximately separate it into an equation for the small component, and an equation for the large component. The large component equation being the Pauli equation it seemed alright, but then what is happening here is that if you look at these two operators, the beta operator which is a Dirac operator it is not going to mix the large and the small part.


Because, it has got 0 in the all diagonal positions, but the operator alpha will because it has got 0 along the diagonal and sigma's over here. So, the operators of this kind these are called as odd operator, the other are called even operators, so the odd operators will scramble the large component and the small component, and you really do not have a decoupling of the large component from the small component in Dirac theory. The coupling is intrinsic to the Dirac equation, it is intrinsic to the nature of the Dirac matrixes.

Because, the Dirac matrixes the alpha is an odd operator, it is something that you cannot really get rid of you cannot just wish it away. And there is this coupling that you really cannot wish away, there are these negative energy solutions that you cannot wish away.


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$E^2 = \vec{p} \cdot \vec{p} c^2 + m^2 c^4$        $E = +\sqrt{\vec{p} \cdot \vec{p} c^2 + m^2 c^4}$   
 $E = -\sqrt{\vec{p} \cdot \vec{p} c^2 + m^2 c^4}$


  $E \geq 0$  : empty  
*in vacuum*

  $E \leq 0$  : occupied

Fully occupied and fully unoccupied states are not observable



Singly occupied particle,  
 or anti-particle state is observable.  
 Particle-AntiParticle annihilation

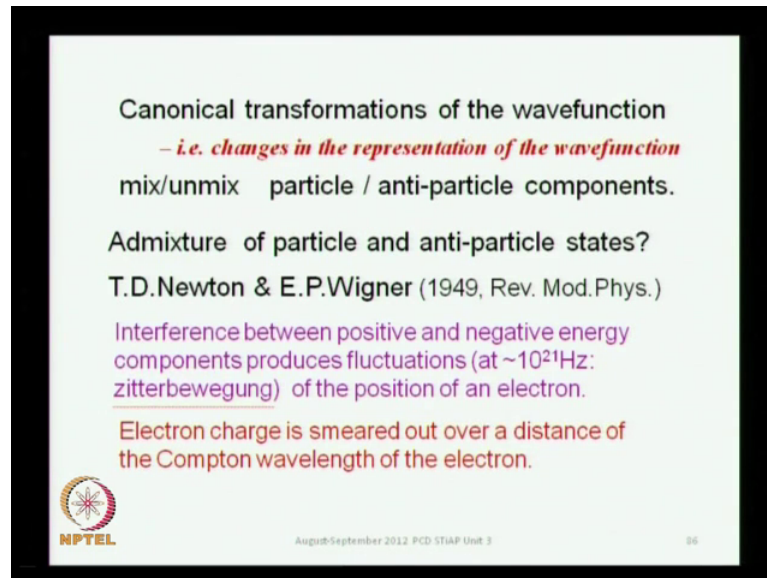


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And then you know the original you know before one developed a very thorough and rigorous understanding of it, there were these proposals that all the negative energy solutions are fully occupied, and you do not therefore, see anything if it is fully occupied in vacuum there is nothing. So, you do not see anything right, but if you have a hole in this sea, and if you have a particle in this sea then of course, these particles and anti particles would be visible, they could inhale it each other and emit energy.

So, these were some of the proposals which came up with and they are very fruitful, their origin comes from the fact that the Lorentz's and variant scalar coming from the full momentum, gives you the  $E$  square term whose solutions allow both for positive energy as well as negative energy that is the origin of these negative energy since.

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Canonical transformations of the wavefunction  
– i.e. *changes in the representation of the wavefunction*  
mix/unmix particle / anti-particle components.

Admixture of particle and anti-particle states?  
T.D.Newton & E.P.Wigner (1949, Rev. Mod.Phys.)

Interference between positive and negative energy components produces fluctuations (at  $\sim 10^{21}$ Hz: *zitterbewegung*) of the position of an electron.

Electron charge is smeared out over a distance of the Compton wavelength of the electron.

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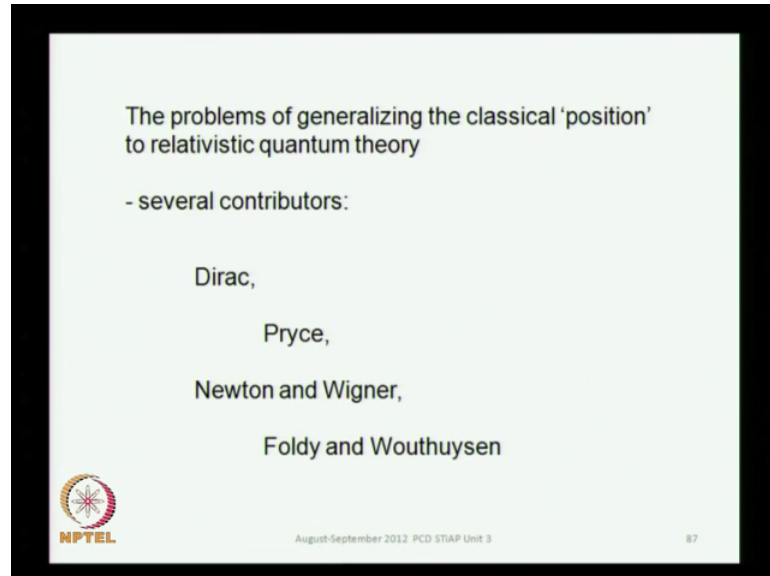
So, you have these particle and anti particle components, but these are mixed and then a systematic way of decoupling the particle, and the anti particle states is to carry out a transformation of your equation of motion. In some theatricals form, which will lead to this decoupling, but this is the question that we raise that is it possible to decouple the particle and anti particle states, which will lead to some decoupling. It is not happening to the Dirac equation as we have seen it.

But, perhaps if we subject the Dirac equation to certain transformations, will it lead to a form to a structure in which this can be decoupled, we did a chain this decoupling in the Pauli equation. But, then it was in some approximate manner, and it lead to some inconsistencies, so we want to do if we can do better than that, and this was a question which was originally raised by Newton and Wigner. And then there several other contributors who wait what happens is that when you consider the interference between positive and negative energy states.

They actually produce fluctuations in the position of an electron, and this has got a very nice name it is called as [FL] or if somebody knows better how to pronounce it any German over here, I have no idea how best to pronounce it that is a nice name that is what it is called. And what it says as that the electron charge gets some sort of a you know speared out, you cannot really come to the conclusion of you know localizing it a

point. And this is the consequence of an a mixture of you know the particle and the anti particle states.

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And these problems were studied by Dirac himself who made the original suggestion, Pryce contributed to it, Newton and Wigner's contribution is very significant I gave a reference to that work. But, the one that I am going to discuss which takes us to a foldy satisfactory understanding of this situation, was done foldy and wouthuysen and these are known as the foldy wouthuysen transformation of the Dirac equation, to a new form to economical form. In which you are able to achieve some decoupling between the large part and the small part, so you get some sort of a decoupling between matter and anti matter states.

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The Zitterbewegung is caused by interference between the positive and negative energy components of the wave packet.

- It vanishes if the wave packet is a superposition of only positive or only negative energy solutions.

"Zitterbewegung" is eliminated when you take expectation values for wave-packets made up completely positive energy states (or completely negative energy states), as achieved by the Foldy - Wouthuysen transformation.



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So, this zitterbewegung is avoided in the foldy wouthuysen transformation because it is present in the Dirac representation. But, when you subject it to a transformation to new states, to a new representation which is known as the foldy wouthuysen transformation, you will find that it is not quite eliminated. But, very nearly, so much better than what it is in the Pauli approximation.

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L. L. Foldy and S. A. Wouthuysen, Phys Rev., 78, 29(1950)  
J. D. Bjorken and S. D. Drell, Relativistic Quantum Mechanics, McGraw-Hill (1964).

PHYSICAL REVIEW VOLUME 78, NUMBER 1 APRIL 1, 1950


On the Dirac Theory of Spin 1/2 Particles and Its Non-Relativistic Limit\*

LESLIE L. FOLDY  
Case Institute of Technology, Cleveland, Ohio

AND

SIGMUND A. WOUTHUYSEN†  
University of Rochester, Rochester, New York  
(Received November 25, 1949)

By a canonical transformation on the Dirac Hamiltonian for a free particle, a representation of the Dirac theory is obtained in which positive and negative energy states are separately represented by two-component wave functions. Playing an important role in the new representation are new operators for position and spin of the particle which are physically distinct from those operators in the conventional representation. The components of the time derivative of the new position operator all commute and have for eigenvalues all values between  $-c$  and  $c$ . The new spin operator is a constant of the motion unlike the spin operator in the conventional representation. By a comparison of the new Hamiltonian with the non-relativistic Pauli-Hamiltonian for particles of spin  $\frac{1}{2}$ , one finds that it is these new operators rather than the conventional ones which pass over into the position and spin operators in the Pauli theory in the non-relativistic limit. The transformation of the new representation is also made in the case of interaction of the particle with an external electromagnetic field. In this way the proper non-relativistic Hamiltonian (essentially the Pauli-Hamiltonian) is obtained in the non-relativistic limit. The same methods may be applied to a Dirac particle interacting with any type of external field (various meson fields, for example) and this allows one to find the proper non-relativistic Hamiltonian in each such case. Some light is cast on the question of why a Dirac electron shows some properties characteristic of a particle of finite extension by an examination of the relationship between the new and the conventional position operators.

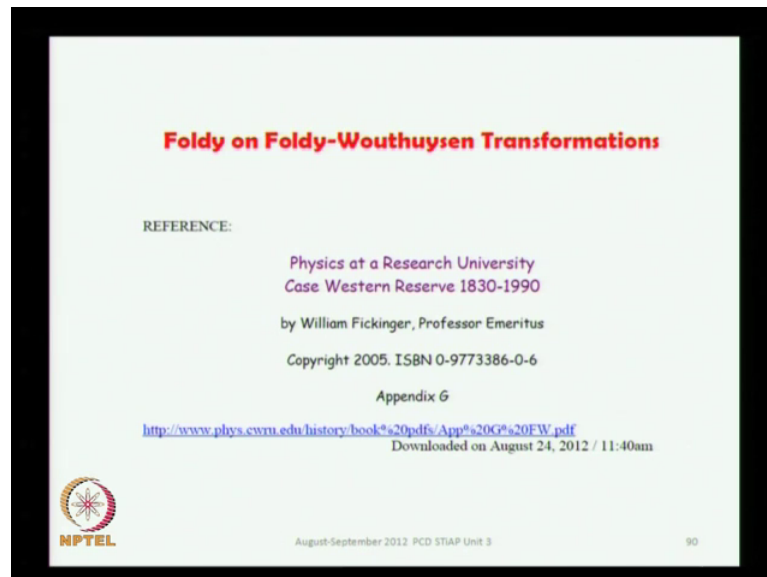


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Now, this is a classic paper of by foldy and wouthuysen I strongly recommend that you read it, and I do not know if it is already uploaded at work course website, and if it not I

think we will do it by the evening. It is a classic paper very readable, very enjoyable and you will love reading it you will also develop the confidence that yes you can read original papers by contributors, and you can do physics the way they would have done.

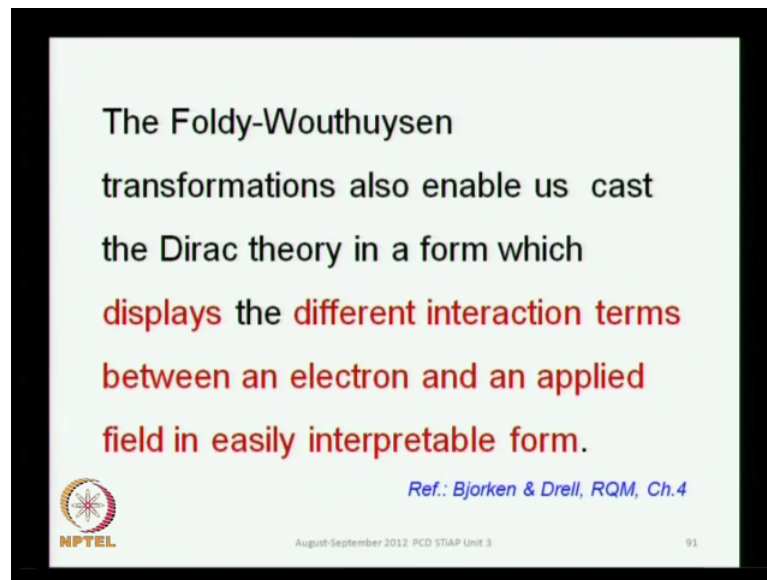
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Now, I will also draw your attention to memoir written by foldy on his work, this is a very nice paper which I have already uploaded at work course website. And I will strongly encourage you to read it because it tells us how foldy went about this problem, what were his experiences, how did he work with his colleagues and others, and this is a nice historical you know kind of story that you should be acquainted with, which is why it has be uploaded. Because, foldy of course, is a great scientist extremely important contribution.

But, sure enough he is not somebody like maybe Einstein or Wigner or nesjbo alright which you will never might want to put him in the same class Pauli was very close, but maybe not there. And if you would like to raise yourself at least to this class, and of some of you already belong to the class of Einstein and nesjbo do not waste time in this classroom. But, if you would like to get at least not to the top class, but at least to the next bracket, then try to read this paper. And them see how these minds work, how they do physics the way they did, and you will really learn something from this paper. So, I strongly encourage you it is a completely historical memoir, but it is wonderful to read.

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The Foldy-Wouthuysen transformations also enable us to cast the Dirac theory in a form which displays the different interaction terms between an electron and an applied field in easily interpretable form.

Ref.: Bjorken & Drell, RQM, Ch.4

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So, this has been uploaded at the course webpage please go through it, and we will be using bjorken and drell's book to a large part and also a greiner's relativistic quantum mechanics a combination of greiner and bjorken and drell. And as bjorken and drell point out that these transformations, they help us cast the Dirac theory in a form, which other than the advantages that I already mentioned. They also display the physical interactions in a form that we are really able to see and recognize.

I mentioned at the very beginning of this unit on relativistic quantum mechanics, that you often see the spin orbit interaction written as, you know  $\frac{1}{r} \frac{dV}{dr} \mathbf{L} \cdot \mathbf{S}$ . And one needs to ask where does this term come from, and we certainly did not see that in the Dirac equation either. But, it is there it is sitting over there, and it will get manifest when you subject the Dirac equation to the foldy wouthuysen transformation.

So, foldy wouthuysen transformations they achieve not only this decoupling of the particle and anti particle states, at least in the approximation which is far better than the Pauli approximation. Not that it is exact that is why says, that these work it goes as far as it does, but then in addition to that they also display the physical interaction in a form, which we can easily interpret, which is why the foldy wouthuysen transformations are really fantastic to learn.




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Non-Relativistic limit of the Dirac equation for an electron in an external potential is not reached simply by  $c \rightarrow \infty$

The limiting process is attained by carrying out a unitary transformation which **block diagonalizes** the Dirac Hamiltonian and **separates the positive and negative energy** part of its spectrum.

This unitary transformation, is the Foldy–Wouthuysen transformation, and it is equivalent to a change of picture.



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And you will see that you can think of the non relativistic limit, and what you exploit is the diagonal structure over here, of the Dirac matrixes. And essentially, you carry out a unitary transformation which is known as the foldy wouthuysen transformation, and then it leads to a different representation of the Dirac equation, which is sometimes called as a different picture because you see things in a different way.

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$$(\beta mc^2 + c\vec{\alpha} \cdot \vec{\pi} + e\phi)_{4 \times 4} \begin{pmatrix} \tilde{\psi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\psi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} \quad H\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$H_{\text{Dirac}} = (\beta mc^2 + c\vec{\alpha} \cdot \vec{\pi} + e\phi)_{4 \times 4}$$

**Foldy-Wouthuysen transformations:**

- Systematic procedure to go from 4-component Dirac theory to a 2-component theory.
- Transform the relativistic equations in such a way that the odd operators play an ignorable role in the transformed representation.

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \xrightarrow{\text{FW}} H'\psi' = i\hbar \frac{\partial \psi'}{\partial t} \xrightarrow{\text{FW}} H''\psi'' = i\hbar \frac{\partial \psi''}{\partial t}$$

$$H'''\psi''' = i\hbar \frac{\partial \psi'''}{\partial t}$$


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So, this is actually a systematic way of going from a 4 component theory to a 2 component theory it does a lot, this is the Dirac equation. And what you want to achieve

in these transformations, is to get to a representation in which the odd operators will not play a very major role. The role of the odd operator, if you can find some mechanism to scale by a factor of  $1/m$ , where  $m$  is a large mass right that is the rest mass energy.

So, you reduce the importance of the odd operators by a factor of  $m$ , and if that is not good enough it leads you to a new form, in which the odd operators have got an importance, which is weaker by a factor of  $m$  you do it again. So, subject it to a Foldy-Wouthuysen transformation, so that  $H\psi$  would go over to  $H'\psi'$ , and this whole equation transforms from  $H\psi = i\hbar \frac{\partial \psi}{\partial t}$  to  $H'\psi' = i\hbar \frac{\partial \psi'}{\partial t}$ , which is the Dirac equation you begin with the Dirac equation.

Subjected to Foldy-Wouthuysen transformation to a new representation, which I use primes for  $i$  and  $\hbar$  cross are scalars. And if this is not good enough subject it to another Foldy-Wouthuysen transformation, do it one more time why not, and if you do it once twice and thrice it is good enough for most of the application in relativistic quantum mechanics at least in atomic physics.

(Refer Slide Time: 45:49)

$$\begin{aligned}
 &(\beta mc^2 + c\vec{\alpha} \cdot \vec{\pi} + e\phi)_{4 \times 4} \begin{pmatrix} \tilde{\psi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\psi}_{2 \times 1} \\ \tilde{\chi}_{2 \times 1} \end{pmatrix} \\
 &H\psi = i\hbar \frac{\partial \psi}{\partial t} \quad \psi \rightarrow \psi' = e^{iS}\psi \\
 &H(e^{-iS}\psi') = i\hbar \frac{\partial}{\partial t} (e^{-iS}\psi') \quad \Omega_{op} \rightarrow \Omega'_{op} = e^{iS}\Omega_{op}e^{-iS} \\
 &H(e^{-iS}\psi') = i\hbar \left[ \left( \frac{\partial e^{-iS}}{\partial t} \right) \psi' + e^{-iS} \left( \frac{\partial \psi'}{\partial t} \right) \right] \\
 &e^{+iS} H(e^{-iS}\psi') = i\hbar \left[ e^{+iS} \left( \frac{\partial e^{-iS}}{\partial t} \right) \psi' + e^{+iS} e^{-iS} \left( \frac{\partial \psi'}{\partial t} \right) \right] \\
 &\Rightarrow i\hbar \frac{\partial \psi'}{\partial t} = e^{+iS} H(e^{-iS}\psi') - i\hbar e^{+iS} \left( \frac{\partial e^{-iS}}{\partial t} \right) \psi' = \left[ e^{+iS} \left( H - i\hbar \frac{\partial}{\partial t} \right) e^{-iS} \right] \psi'
 \end{aligned}$$

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So, that is what we are going to do, now let us see how we do it, so this is the Dirac equation you are looking for a transformation  $\psi$  going to  $\psi'$ , through a transformation operator which we do not know what it is, we are going to have to discover what this operator  $U$  should be like. So, we look for a transformation of this kind, and operators would then go over from  $\Omega$  any operator  $\Omega$  would go to

$\omega'$  as  $e^{i\omega t}$   $\omega' e^{-i\omega t}$ , this is the standard prescription for transformations right.

So, now, you put  $\psi$  in terms of  $\psi'$  over here, so this becomes  $e^{-i\omega t}$  operating on  $\psi'$ , and this becomes the partial derivative of  $\psi'$  instead of  $\psi$ . Now, this is a partial derivative of  $e^{i\omega t}$   $\omega'$  operating on  $\psi'$ , but let us not assume that  $\psi$  is that  $\omega'$  is independent of time, so this will be the time derivative of the operator  $e^{-i\omega t}$   $\omega'$  operating on  $\psi'$  plus  $e^{-i\omega t}$   $\omega'$  operating on the time derivative of  $\psi'$ .

So, there are 2 terms let us do it very carefully term by term, we have no reason to assume that  $\omega'$  is independent of time it is an operator whose form we have to explore. So, now you have this relationship, you operate on this entire set of equations by  $e^{i\omega t}$ , so you have got  $e^{i\omega t}$  operating on the left side, and also on the 2 terms on the right. You get the unit operator from this  $e^{i\omega t}$   $e^{-i\omega t}$ , and now if you right use this relationship because the second term is  $i\hbar \nabla \psi'$  by  $\partial t$  that would be the term you are looking for.

So, this term would go to the other side and the relation you get for  $i\hbar \nabla \psi'$  by  $\partial t$  is this term minus this. So, now your equation in the transform representation is this, this is what you get from the Dirac equation by subjecting it to the transformation, we still do not know what the transformation operator is which if you combine these two terms you recognize that this is a transformation of this operator  $\hbar \nabla$  by  $\partial t$ .

(Refer Slide Time: 48:40)


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

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

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

$$\Rightarrow H' = e^{+iS} H e^{-iS} - i\hbar e^{+iS} \frac{\partial}{\partial t} e^{-iS}$$

**OBJECTIVE:** Transform the relativistic equations in such a way that the odd operators play an ignorable role in the transformed representation.

 NPTEL

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This is what we have, and what it tells us that the new Hamiltonian in the transform representation, which is called as the foldy wouthuysen transformation. In the transform representation the new Hamiltonian is e to the i s old Hamiltonian minus i h cross del by del t e to the minus i s and we have to find what that operate is we will do the job that we want it to do. So, this is your new Hamiltonian and our criteria for choosing s is going to be this, that it must be such that in the new Hamiltonian which is H prime? Now, H prime will also have odd operators, but if the odd operators in h prime are weaker than those in the original Dirac Hamiltonian, then we have made some progress. And if that is not enough, we can do a second foldy wouthuysen transformation.

(Refer Slide Time: 50:00)

$$i\hbar \frac{\partial \psi_{4 \times 1}}{\partial t} = \left( c \vec{\alpha} \cdot \left( \vec{p} - \frac{e}{c} \vec{A} \right) + \beta mc^2 + e\phi \right) \psi_{4 \times 1}$$

$$\vec{\alpha}_{4 \times 4} = \begin{bmatrix} 0_{2 \times 2} & \vec{\sigma}_{2 \times 2} \\ \vec{\sigma}_{2 \times 2} & 0_{2 \times 2} \end{bmatrix} \quad \beta_{4 \times 4} = \begin{bmatrix} 1_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & -1_{2 \times 2} \end{bmatrix}$$


Free electron:  $i\hbar \frac{\partial \psi_{4 \times 1}}{\partial t} = (c \vec{\alpha} \cdot \vec{p} + \beta mc^2) \psi_{4 \times 1}$

$$\psi \rightarrow \psi' = e^{iS} \psi \quad H' = e^{+iS} H e^{-iS} - i\hbar e^{+iS} \frac{\partial}{\partial t} e^{-iS}$$

$$\Omega_{op} \rightarrow \Omega'_{op} = e^{iS} \Omega_{op} e^{-iS}$$

For free electron, consider time-independent

Hermitian operator:  $S = \frac{-i}{2mc} \beta \vec{\alpha} \cdot \vec{p} \alpha \left( \frac{p}{m} \right)$



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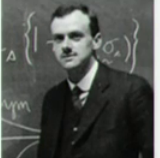
So, what we will do, I will tell you how this operator  $S$  is chosen and how this Foldy-Wouthuysen transformation is affected. So, first I will demonstrate how it is done for a free electron, so you through the terms in the magnetic vector potential, and in this and you get a simple term. So, for a free electron there is no electromagnetic potential, and you will see that this particular choice of the operator  $S$  will do the job for us, so this is something that we will see this is what Foldy-Wouthuysen discovered.

(Refer Slide Time: 50:41)

$$E^2 = m^2 c^4 + \vec{p} \cdot \vec{p} c^2$$

$$E = \pm \sqrt{m^2 c^4 + \vec{p} \cdot \vec{p} c^2}$$

Paul Adrien Maurice Dirac  
1902-1984




$$i\hbar \frac{\partial}{\partial t} \psi_{4 \times 1} = \left( c \vec{\alpha} \cdot \vec{p} + \beta mc^2 + e\phi \right) \psi_{4 \times 1}$$

$$+ i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} (\vec{\ell} + 2\vec{s}) \cdot \vec{B} + e\phi \right] \varphi$$


$g = 2$   $\vec{s} = \frac{\hbar}{2} \vec{\sigma}$

Wolfgang Pauli  
1900 - 1958



Electron spin requires two components,  
- but Dirac equation admits  
4-component wavefunction

Questions? [pcd@physics.iitm.ac.in](mailto:pcd@physics.iitm.ac.in)



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So, I will stop here for today if there are any questions I will be happy to take, and in the next class we will continue our discussion on the Foldy-Wouthuysen transformations, will first do it for the free electron. And then do it for the electron in an electromagnetic field and then of course, our interest is in the electron in the hydrogen atom. Questions.

Student: ((Refer Time: 51:14))

What I did was to you have a function which is time dependent, it is time dependence may have some very complex form, it may be harmonic, it may be some arbitrary function of time  $f$  of  $t$ . Where  $f$  of  $t$  is some polynomial function of time it may have whatever powers with whatever coefficients, so you have got a fairly complex time dependence over there. Out of that for stationary states, as you extract  $e$  to the minus  $i$   $\omega t$ , you factor out that term.

Where  $\omega$  is  $e$  over  $\hbar$  cross,  $e$  being the rest energy now  $e$  over  $\hbar$  cross this  $e$  is a very large energy, the  $e_0$  energy is a huge energy, the rest energy of the electron is like half a million electron volts 0.51 or something you can get the exact value right. And therefore, most of the time dependence that you expect in your wave function to have, is contained in this term which is dominated by the rest energy. That suggest that the residual time dependence it is like writing any function of time  $f$  of  $t$  as a product of 2 functions of time  $f_1 t$  multiplied by  $f_2 t$ .

If most of the time dependence is contained in  $f_1 t$  then  $f_2 t$  is nearly a constant that side, it comes essentially from the fact that you are dealing with an energy term which is huge, any other question?

Student: ((Refer Time: 53:28))

That is not of interest, those are the terms that correspond to the anti particles in the sea which is a full sea and you are not going to see. It now this was a original reasoning before people knew that anti matter matters as much as matter does, and then of course now one understand that these are real particles, positron exists not only positrons. But, the whole family of anti particles, but that does not take away the fact that our interest in atomic physics is in looking at the electron dynamics, and how it interacts with electronic fields.

For which you are looking for a 2 component theory number one, and second you cannot really allow for an a mixture of particle and anti particle states. If you did that you will not even be able to speak about the position of an electron, the way we have been used to. Because, this mixture of particles and anti particles states, leads to an expectation value of the position operator, which is not quite localized. In fact, it gets smeared out over a certain distance, which is of the order of content wave length that is what is called as. [FL]

Student: ((Refer Time: 55:16))

No it is not the uncertainty, it has nothing to do with uncertainty it is coming from that mixture of the particles and anti particle states, the uncertainty leads that is a different thing altogether. So, this smearing out of the electron is not the quantum uncertainty absolutely not, in addition to that there is this smearing out effect which is coming from a mixture of particle and anti particle states. But, the gap between the negative energy states and the positive energy states is already huge, twice the rest mass energy right.

So, it is already huge, so unless you supply that type of energy, you are not going to see that mixture. So, in atomic process it is not of any consequence, but what is of consequence are many of the other features which come out of the foldy wouthuysen transformation. Because, otherwise you do not even see the physical interaction in a form that you can really interpret, where is the  $\frac{d\mathbf{v}}{dt}$  by  $\frac{d\mathbf{r}}{ds}$  dot  $\mathbf{l}$  in the Dirac equation, it is sitting over there it has to be there. But, you do not see it what the foldy wouthuysen transformation will do is to display those forms, it will be visible in the transformed representation which is why it is of importance in atomic processes, any other question?

Student: ((Refer Time: 57:02))

This is for a uniform field, so we used it for a particular bond, but in our case it is not a bad approximation, because over the reason that you are talking are about over the atomic dimensions, you do not expect it to change very much.

(Refer Slide Time: 57:39)

$$E^2 = m^2 c^4 + \vec{p} \cdot \vec{p} c^2$$

$$E = \pm \sqrt{m^2 c^4 + \vec{p} \cdot \vec{p} c^2}$$


$$i\hbar \frac{\partial}{\partial t} \psi_{4 \times 1} = (c \vec{\alpha} \cdot \vec{\pi} + \beta m c^2 + e \phi)_{4 \times 4} \psi_{4 \times 1}$$

$$+ i\hbar \frac{\partial}{\partial t} \varphi = \left[ \frac{p^2}{2m} - \frac{1}{2} \frac{e}{mc} (\vec{\ell} + 2\vec{s}) \cdot \vec{B} + e\phi \right] \varphi$$


$g = 2$

$\vec{s} = \frac{\hbar}{2} \vec{\sigma}$


Electron spin requires two components,  
- but Dirac equation admits  
4-component wavefunction




Paul Adrien  
Maurice Dirac  
1902-1984



Wolfgang Pauli  
1900 - 1958

Bye!


Questions? [pcd@physics.iitm.ac.in](mailto:pcd@physics.iitm.ac.in)


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But, for now if there are any questions I will be happy to take otherwise goodbye for now.