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ADVANCED QUANTUM MECHANICS AND  
INTRODUCTION TO GROUP THEORY  
(PHYS5000) LECTURE NOTES

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LECTURE NOTES BASED ON A COURSE GIVEN BY ROMAN KONIUK.  
THE COURSE BEGINS WITH A DISCUSSION ON ADVANCED QUANTUM MECHANICS AND THEN  
MOVES TO GROUP THEORY, HYDROGEN, AND THE DIRAC EQUATION

YORK UNIVERSITY, 2012

PRESENTED BY: ROMAN KONIUK

L<sup>A</sup>T<sub>E</sub>X NOTES BY: JEFF ASAF DROR

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## I. FOUNDATIONS OF QUANTUM MECHANICS

## A. Vector Spaces, Dual Spaces, and Scalar Products

## 1. Vector Spaces

In this class we will use the Bra and Ket spaces. Ket vector spaces obey the following:

$$|a\rangle + |b\rangle \in V \quad (\text{I.1})$$

$$|a\rangle + |0\rangle = |a\rangle \quad (\text{I.2})$$

$$|a\rangle + |-a\rangle = |0\rangle \quad (\text{I.3})$$

$$|a\rangle + (|b\rangle + |c\rangle) = (|a\rangle + |b\rangle) + |c\rangle \quad (\text{I.4})$$

$$|a\rangle + |b\rangle = |b\rangle + |a\rangle \quad (\text{I.5})$$

$$\alpha |a\rangle \in V \quad (\text{I.6})$$

$$\alpha (\beta |a\rangle) = (\alpha\beta) |a\rangle \quad (\text{I.7})$$

Vectors in this space are linearly independent. In other words

$$\sum_{i=1}^n a_i |i\rangle = 0 \quad (\text{I.8})$$

$$\Rightarrow a_i = 0 \quad \forall i \quad (\text{I.9})$$

## 2. Dual Spaces

The adjoint of a vector  $|a\rangle$  in the vector space defines a “bra”  $\langle a|$ . Such that if

$$|c\rangle = \alpha |a\rangle + \beta |b\rangle \quad (\text{I.10})$$

then

$$\langle c| = \alpha^* \langle a| + \beta^* \langle b| \quad (\text{I.11})$$

## 3. Scalar Products

For any vectors  $|a\rangle, |b\rangle \in V$  we denote  $\langle a|b\rangle$  is the scalar product “bra-ket”. The inner product is in general a complex number. i.e.

$$\langle a|b\rangle \in \mathbb{C} \quad (\text{I.12})$$

Inner products obey the relation

$$\langle a|b\rangle = (\langle b|a\rangle)^* \quad (\text{I.13})$$

The inner product of a vector with itself is a positive definite quantity:

$$\langle a|a\rangle \geq 0 \quad (\text{I.14})$$

Further

$$\langle a|a\rangle = 0 \Rightarrow |a\rangle = |0\rangle \quad (\text{I.15})$$

The Schwartz inequality says that

$$|\langle a|b\rangle|^2 \leq \langle a|a\rangle \langle b|b\rangle \quad (\text{I.16})$$

The space of ket vectors and the dual space of bra vectors form a hilbert space. Hilbert space is a complete space. We define the norm of a vector as

$$|a| = \sqrt{\langle a|a\rangle} \quad (\text{I.17})$$

The set of vectors

$$|1\rangle, |2\rangle, \dots, |n\rangle \quad (\text{I.18})$$

Form an orthonormal basis.

## B. Tensor Product(Outer Product)

Let  $|a^1\rangle$  represent the state of particle 1 and let  $|a^2\rangle$  represent the state of particle 2. Then the two-particle system is represented by the tensor product

$$|a^1\rangle \otimes |a^2\rangle = |a^1\rangle |a^2\rangle = |a^1 a^2\rangle \quad (\text{I.19})$$

Any operator  $\Omega^1$  only operates on  $|a^1\rangle$  and any operator  $\Omega^2$  only operates on  $|a^2\rangle$ . The commutator of operators that act on different particles must be zero:

$$[\Omega^1, \Omega^2] = 0 \quad (\text{I.20})$$

### C. Operators

Let

$$\Omega |a\rangle = |a'\rangle \quad (\text{I.21})$$

If  $\Omega$  is a linear operator then

$$\Omega \alpha |a\rangle = \alpha \Omega |a\rangle \quad (\text{I.22})$$

where  $\alpha \in \mathbb{C}$  and

$$\Omega (\alpha |a\rangle + \beta |b\rangle) = \alpha \Omega |a\rangle + \beta \Omega |b\rangle \quad (\text{I.23})$$

The product of two operators simply means to carry out the operators in sequence:

$$\Omega \Lambda |a\rangle = \Omega (\Lambda |a\rangle) \quad (\text{I.24})$$

The inverse of an operator  $\Omega$  is denoted by  $\Omega^{-1}$ :

$$\Omega^{-1} \Omega = I = \Omega \Omega^{-1} \quad (\text{I.25})$$

### D. Matrix Representations

Consider  $|a\rangle$  and the operator  $\Omega$  such that

$$\Omega |a\rangle = |b\rangle \quad (\text{I.26})$$

the matrix form of  $\Omega$  has the elements  $\Omega_{ij} = \langle i | \Omega | j \rangle$ . If we consider the expansions

$$|a\rangle = \sum_i a_i |i\rangle \quad (\text{I.27})$$

$$|b\rangle = \sum_j b_j |j\rangle \quad (\text{I.28})$$

If  $|a\rangle$  is given then you can find  $a_i$  since

$$\langle i | a \rangle = \langle i | \sum_n |n\rangle \quad (\text{I.29})$$

$$= a_i \quad (\text{I.30})$$

$$b_j = \sum_i a_i \Omega_{j,i} \quad (\text{I.31})$$

The matrix elements of the identity operator are

$$I = \langle i | I | j \rangle = \delta_{i,j} \quad (\text{I.32})$$

### E. Projection Operators

Consider the set of basis vectors  $|1\rangle, |2\rangle, \dots, |n\rangle$ . The projection operator of any vector onto the  $i^{\text{th}}$  basis vector is given by

$$\mathcal{P}_i = |i\rangle \langle i| \quad (\text{I.33})$$

This is clear since

$$\mathcal{P}_i |a\rangle = \langle i | a \rangle |i\rangle \quad (\text{I.34})$$

$$= a_i |i\rangle \quad (\text{I.35})$$

Now consider the following

$$|a\rangle = \sum_i a_i |i\rangle \quad (\text{I.36})$$

$$= \sum_i \langle i|a\rangle |i\rangle \quad (\text{I.37})$$

$$= \sum_i |i\rangle \langle i|a\rangle \quad (\text{I.38})$$

$$= \sum_i P_i |a\rangle \quad (\text{I.39})$$

Hence

$$\sum_i P_i = I = \sum_i |i\rangle \langle i| \quad (\text{I.40})$$

The projection operator squared is simply the projection operator since

$$\mathcal{P}^2 = |i\rangle \langle i| (|i\rangle \langle i|) \quad (\text{I.41})$$

$$= |i\rangle \langle i| \quad (\text{I.42})$$

$$= \mathcal{P} \quad (\text{I.43})$$

The matrix representation of  $P_i$  is:

$$\langle j|P_i|k\rangle = \langle j|i\rangle \langle i|k\rangle \quad (\text{I.44})$$

$$= \delta_{j,i} \delta_{i,k} \quad (\text{I.45})$$

$$(\text{I.46})$$

This looks like

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{I.47})$$

The identity is given by

$$\mathcal{I} = \sum_i P_i \quad (\text{I.48})$$

## F. Hermitian and Unitary Operators

Hermitian operators obey

$$\Omega = \Delta^\dagger \quad (\text{I.49})$$

In other words operators for which the operator is equal to the hermitian conjugate. Unitary operators are operators for which

$$U^\dagger = U^{-1} \quad (\text{I.50})$$

In quantum mechanics observables are associated with Hermitian operators. For examples

$$x \rightarrow x \quad (\text{I.51})$$

$$p_x \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x} \quad (\text{I.52})$$

The eigenvalues of Hermitian operators are all real (since they correspond to observables). The states corresponding to distinct eigenvalues are orthogonal.

Unitary operators are used to transform to another basis (called unitary since they preserve the scalar product). Proof:

$$\langle b|a \rangle = \langle Ub'|Ua' \rangle \quad (\text{I.53})$$

$$= \langle b'|U^\dagger U|a' \rangle \quad (\text{I.54})$$

$$= \langle b'|a' \rangle \quad (\text{I.55})$$

Hence the scalar product is conserved. Other things that are preserved by unitary transformations are trace, determinant, and algebraic equations involving matrices and vectors.

Any operator in quantum mechanics doesn't take you out of the Hilbert space.

Let

$$A|a \rangle = |a' \rangle \quad (\text{I.56})$$

Then

$$U^\dagger A|a \rangle = U^\dagger |a' \rangle \quad (\text{I.57})$$

$$U^\dagger A U U^\dagger |a \rangle = U^\dagger |a' \rangle \quad (\text{I.58})$$

$$A' U^\dagger |a \rangle = U^\dagger |a' \rangle \quad (\text{I.59})$$

$$(\text{I.60})$$

where  $A' = UAU^\dagger$  is called a unitary-similarity transformation.

Typically use a unitary-similarity transformation to diagonalize an operator. We most typically diagonalize the Hamiltonian (then we can just read off the eigenvalues).

$$U \Omega U^\dagger = U_D \quad (\text{The subscript D means diagonal}) \quad (\text{I.61})$$

] The way we solve for  $U$  is by solving the characteristic equation (also called the secular equation).

An important unitary operator is the time-evolution operator:

$$U(t) = e^{-iHt/\hbar} = 1 - \frac{iHt}{\hbar} + \frac{1}{2} \frac{(-iHt)^2}{\hbar^2 2!} + \dots \quad (\text{I.62})$$

where  $H$  is the Hamiltonian. We use this operator to evolve states.

$$U|\alpha(0)\rangle = |\alpha(t)\rangle \quad (\text{I.63})$$

If the Hamiltonian is diagonal in some basis then

$$U = e^{-iHt/\hbar} \quad (\text{I.64})$$

$$1 - i \frac{Ht}{\hbar} + \frac{1}{2} \frac{(-iHt)^2}{\hbar^2} \quad (\text{I.65})$$

This is easy to calculate since for a diagonal matrix

$$H = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_m \end{pmatrix} \quad (\text{I.66})$$

$$H^n = \begin{pmatrix} \lambda_1^n & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_m^n \end{pmatrix} \quad (\text{I.67})$$

If we are acting on a basis vector  $\alpha = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$  then

$$U|\alpha\rangle = 1 - i\frac{\lambda_\alpha t}{\hbar} + \frac{1}{2}\left(-i\frac{\lambda_\alpha^2 t^2}{\hbar^2}\right) + \dots \quad (\text{I.68})$$

### G. Continuum Basis

So far we have dealt with the discrete basis. For a continuum basis, such as the position basis. A state of definite position is given by

$$|x'\rangle \quad (\text{I.69})$$

$$x|x'\rangle = x'|x'\rangle \quad (\text{I.70})$$

In the continuum basis we know that

$$I = \int |x\rangle\langle x| \quad (\text{I.71})$$

$$\langle x|x'\rangle = \delta(x - x') \quad (\text{I.72})$$

The scalar product of a mix of discrete and continuous states is the wavefunction:

$$\langle x|n\rangle = \psi_n(x) \quad (\text{I.73})$$

$$|\langle x|n\rangle|^2 = P(x) \quad (\text{I.74})$$

### H. Postulates of Quantum Mechanics

1. The state of a particle is represented by a “vector” in Hilbert space  $|\alpha\rangle$
2. Every observable corresponds to a Hermitian operator
3. Every measurement of the observable corresponding to the operator  $\Omega$  results only in an eigenvalue
4. The average value of an observable is calculated in quantum mechanics by

$$\langle\alpha|\Omega|\alpha\rangle \quad (\text{I.75})$$

and we call this the expectation value

5. The time evolution of a state is given by the Schrodinger equation:

$$i\hbar\frac{d}{dt}|\alpha(t)\rangle = H|\alpha(t)\rangle \quad (\text{I.76})$$

Lecture 4 - Jan. 11, 2012

In measurement  $|\alpha\rangle$  may not be in an eigenstate of  $\Omega$  but one can expand  $|\alpha\rangle = \sum_i |\omega_i\rangle \overbrace{\langle\omega_i|\alpha\rangle}^{c_i}$ . The coefficients  $\langle\omega_i|\alpha\rangle$  give the amplitude of finding the system in the eigenstate  $|\omega_i\rangle$ . The probability of being in this eigenstate is

$$P(\omega_i) = |\langle\omega_i|\alpha\rangle|^2 \quad (\text{I.77})$$

Once a measurement is made the state is in that eigenstate (until the time evolution operator acts) “collapse of the wavefunction”. We of course have

$$\sum_i P(\omega_i) = 1 \quad (\text{I.78})$$

For continuous eigenspectra. For the position spectrum:

$$\int_{\text{all } x} P(x) dx = 1 \quad (\text{I.79})$$

By dimensions we know that  $P(x)$  is a probability density.

## II. COMPATIBILITY, INCOMPATIBILITY, AND UNCERTAINTY

1. Two variables are compatible if their corresponding operators commute. For example if

$$[\Omega, \Lambda] = 0 \quad (\text{II.1})$$

then  $\Omega$  and  $\Lambda$  are compatible. In this case we can have simultaneous eigenfunctions. In other words

$$\Omega |\alpha\rangle = \omega_i |\alpha\rangle; \quad \Lambda |\alpha\rangle = \lambda_i |\alpha\rangle \quad (\text{II.2})$$

This implies exact knowledge of  $\omega_i$  and  $\lambda_i$ .

2. Two variables are incompatible if their corresponding operators don't commute. In this case you cannot have simultaneous eigenfunctions. Hence you cannot have exact knowledge of  $\omega$  and  $\lambda$  simultaneously.

The uncertainty is defined as

$$\Delta A = \left\langle \left( \langle A - \langle A \rangle \rangle \right)^2 \right\rangle^{1/2} \quad (\text{II.3})$$

$$= \langle (A - \langle A \rangle) (A - \langle A \rangle) \rangle^{1/2} \quad (\text{II.4})$$

$$= \langle A^2 - 2A \langle A \rangle + \langle A \rangle^2 \rangle^{1/2} \quad (\text{II.5})$$

$$= \left( \langle A^2 \rangle - \langle A \rangle^2 \right)^{1/2} \quad (\text{II.6})$$

This is a measure of how far on average  $A$  is away from the average. Noncommutivity is related to uncertainties by:

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [A, B] \rangle| \quad (\text{II.7})$$

As an example consider the uncertainty of  $x$  and  $p$ :

$$\Delta x \Delta p \geq \frac{1}{2} |\langle [x, p] \rangle| \quad (\text{II.8})$$

$$\geq \frac{1}{2} \left| \left\langle x \frac{\hbar}{i} \frac{\partial}{\partial x} - \frac{\hbar}{i} \left( 1 + \frac{\partial}{\partial x} \right) \right\rangle \right| \quad (\text{II.9})$$

$$\geq \frac{1}{2} |\langle i\hbar \rangle| \quad (\text{II.10})$$

$$\geq \frac{\hbar}{2} \quad (\text{II.11})$$

## III. PURE STATES AND MIXTURES: DENSITY MATRIX

Suppose you have an experiment. The beam is 50% spin up and 50% spin down. The state

$$\frac{1}{\sqrt{2}} (\uparrow + \downarrow) \quad (\text{III.1})$$



is a pure state. It is a linear combination of states but we know the state exactly. Another possibility is literally 50% of the electrons and 50% are in the down state. How do we differentiate these two cases? We could use

$$\langle S_z \rangle = \frac{\hbar}{2} \sigma_z \quad (\text{III.2})$$

where

$$\sigma = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \quad (\text{III.3})$$

In the case of a pure state we calculate this the expectation value by

$$\left\langle \frac{1}{\sqrt{2}} (\uparrow + \downarrow) \left| S_z \right| \frac{1}{\sqrt{2}} (\uparrow + \downarrow) \right\rangle = \frac{\hbar}{4} (0) \quad (\text{III.4})$$

$$= 0 \quad (\text{III.5})$$

In the second case we use

$$\frac{1}{2} \langle \uparrow | S_z | \uparrow \rangle + \frac{1}{2} \langle \downarrow | S_z | \downarrow \rangle = 0 \quad (\text{III.6})$$

Next we do the same for  $S_x$ . For the first case:

$$\left\langle \frac{1}{\sqrt{2}} (\uparrow + \downarrow) \left| S_x \right| \frac{1}{\sqrt{2}} (\uparrow + \downarrow) \right\rangle = \frac{1}{2} \frac{\hbar}{2} \langle 2 \rangle = \frac{\hbar}{2} \quad (\text{III.7})$$

For the second case

$$\frac{1}{2} \langle \uparrow | S_x | \uparrow \rangle + \frac{1}{2} \langle \downarrow | S_x | \downarrow \rangle = 0 \quad (\text{III.8})$$

Hence the two states are distinguishable since we can measure the spin in the  $x$  direction and see the difference.

Lecture 5 - Jan 13, 2011

Every state we have seen thus far has been a pure state. We say that the pure state is coherent while mixed states are incoherent.

The density matrix is used to handle both pure and mixed states. For a mixed state we say the probability(not amplitude) of being in state  $|\alpha_i\rangle$  is equal to  $\omega_i$  and  $\sum_i \omega_i = 1$ . Therefore the expectation value for a mixed state is written as

$$\langle A \rangle = \sum_i \omega_i \langle \alpha_i | A | \alpha_i \rangle \quad (\text{III.9})$$

Important point: there are two averaging procedures in this equation. One is the usual quantum mechanical average procedure ( $\langle \alpha_i | A | \alpha_i \rangle$ ). e.g.

$$\langle x \rangle = \int \psi^*(x) x \psi(x) dx \quad (\text{III.10})$$

$$= \int P(x) x dx \quad (\text{III.11})$$

The other is the classical averaging of multiplying the probability of being in a state by the value of being in that state. It's important to realize that  $|\alpha_i\rangle$  need not be orthogonal but they must be normalized. For example you may have the states 50%  $|\uparrow\rangle$  and 50%  $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ . For a mixed state  $\langle A \rangle = \sum_i \omega_i \langle \alpha_i | A | \alpha_i \rangle$  can be written as follows

$$\langle A \rangle = \text{Tr}(\rho A); \quad \text{where } \rho = \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| \quad (\text{III.12})$$

Recall that

$$\text{Tr}(B) = \sum_j \langle j | B | j \rangle \quad (\text{III.13})$$

Proof of the relation shown above:

$$\text{Tr}(\rho A) = \sum_j \langle j | \rho A | j \rangle \quad (\text{III.14})$$

$$= \sum_j \langle j | \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| A | j \rangle \quad (\text{III.15})$$

$$= \sum_j \sum_i \omega_i \langle j | \alpha_i \rangle \langle \alpha_i | A | j \rangle \quad (\text{III.16})$$

$$= \sum_i \omega_i \langle \alpha_i | A \sum_j | j \rangle \langle j | \alpha_i \rangle \quad (\text{III.17})$$

$$= \sum_i \omega_i \langle \alpha_i | A | \alpha_i \rangle \quad (\text{III.18})$$

The operator  $\rho$  is called the density matrix operator which is defined as

$$\rho = \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| \quad (\text{III.19})$$

Remember that you can write any state  $|\alpha_i\rangle$  as

$$|\alpha_i\rangle = \sum_j C_j |\alpha_j\rangle \quad (\text{III.20})$$

where here  $j$  is labeling the basis state and  $i$  is labeling state state in the mixture. We can now expand the density matrix as

$$\rho = \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| \quad (\text{III.21})$$

$$= \sum_i \sum_j \sum_k \omega_i C_j^i C_k^{i\dagger} |j\rangle \langle k| \quad (\text{III.22})$$

$$= \sum_{j,k} \rho_{j,k} |j\rangle \langle k| \quad (\text{III.23})$$

where  $\rho_{j,k} = \sum_i \omega_i C_j^i C_k^{i\dagger}$ . Traces are basis-independent quantities (since  $\text{Tr}(ABC) = \text{Tr}(BCA)$ ). In particular  $\text{Tr}(\rho A)$  is independent of basis. Next consider the trace of  $\rho$ :

$$\text{Tr}(\rho) = \sum_j \langle j | \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| h \rangle \quad (\text{III.24})$$

$$= \sum_j \sum_i \omega_i \langle j | \alpha_i \rangle \langle \alpha_i | j \rangle \quad (\text{III.25})$$

$$= \sum_i \sum_j \omega_i C_j^i \sum_k C_k^{i\dagger} \langle k | j \rangle \quad (\text{III.26})$$

$$= \sum_i \sum_j \omega_i C_j^i C_j^{i\dagger} \quad (\text{III.27})$$

$$= \sum_i \omega_i \quad (\text{III.28})$$

$$= 1 \quad (\text{III.29})$$

If we have a pure state the density matrix is just the projection operator

$$\rho = \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| \quad (\text{III.30})$$

$$= |\alpha_i\rangle \langle \alpha_i| \quad (\text{III.31})$$

Hence in for a pure state

$$\rho^2 = \rho \quad (\text{III.32})$$

For a mixed state

$$\rho^2 \neq \rho \quad (\text{III.33})$$

Proof: We can go to basis which diagonalizes  $\rho$  and then we have

$$\rho = \begin{pmatrix} \omega_1 & 0 & 0 \\ 0 & \omega_2 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \quad (\text{III.34})$$

but for a mixed state all the  $\omega_i < 1$  and hence the square of them is less than 1. For example find  $\rho$  for case the pure state  $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}(|\uparrow_z\rangle + |\downarrow_z\rangle)$ . This can be done in several ways

$$\rho = \sum_i \omega_i |\alpha_i\rangle \langle \alpha_i| \quad (\text{III.35})$$

$$= \left| \frac{1}{\sqrt{2}} (\uparrow + \downarrow) \right\rangle \left\langle \frac{1}{\sqrt{2}} (\uparrow + \downarrow) \right| \quad (\text{III.36})$$

$$= \frac{1}{2} (|\uparrow\rangle \langle \uparrow| + |\uparrow\rangle \langle \downarrow| + |\downarrow\rangle \langle \uparrow| + |\downarrow\rangle \langle \downarrow|) \quad (\text{III.37})$$

$$(\text{III.38})$$

$$\rho_{j,k} = \sum_i \omega_i C_j^i C_k^{i\dagger} \quad (\text{III.39})$$

$$= C_j C_k^\dagger \quad (\text{III.40})$$

but  $C_1 C_1^\dagger = C_1 C_2^\dagger = C_2 C_1^\dagger = C_2 C_2^\dagger = \frac{1}{2}$  hence

$$\rho_{j,k} = \frac{1}{2} \quad (\text{III.41})$$

We use this result to find some expectation values:

$$\langle S_z \rangle = \text{Tr}(\rho S_z) \quad (\text{III.42})$$

$$\frac{1}{2} \frac{\hbar}{2} \text{Tr} \left\{ \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \quad (\text{III.43})$$

$$= \frac{\hbar}{4} \text{Tr} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \quad (\text{III.44})$$

$$= 0 \quad (\text{III.45})$$

and

$$\langle S_x \rangle = \text{Tr}(\rho S_x) \quad (\text{III.46})$$

$$\frac{1}{2} \frac{\hbar}{2} \text{Tr} \left\{ \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} \quad (\text{III.47})$$

$$= \frac{\hbar}{4} \text{Tr} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad (\text{III.48})$$

$$= \frac{\hbar}{2} \quad (\text{III.49})$$

Assignment: to be handed in on Monday

1. Find  $\rho$  for case B (50%  $\uparrow$  and 50%  $\downarrow$ )
2. Evaluate  $\text{Tr}(\rho S_z)$  and  $\text{Tr} \{ \rho S_x \}$

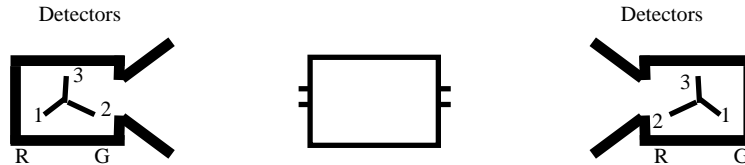


FIG. 1. The EPR experiment

Lecture 6 - January 20th, 2012

Consider the EPR setup shown in figure 1. The experiment has two observations.

1. 100% of the time if the two detectors are pointing in the same directions then opposite colours flash. 100% anti-correlation of the colours if the pointers are pointing in the same direction
2. If we pay no attention to the direction of the pointers then there is no correlation (completely random)

Classical understanding of the experiment says if we consider observation 1 then the particles know prior to the experiment what they will choose. This can be thought of as the particles having genes. This is shown in table I. Consider the second row of table I. In total there are 9 possible pointer positions: 11, 12, 13, 23, ... (always true). For

TABLE I. The gene table of the EPR experiment

1	2	3	1	2	3
G	G	G	R	R	R
G	G	R	R	R	G
G	R	G	R	G	R
R	G	G	G	R	R
R	G	R	G	R	G
G	R	R	R	G	G
R	R	G	G	G	R
R	R	R	G	G	G

the second gene 11, 22, 33, 12, 21 gives us anti correlation (e.g.  $G \Rightarrow R$ ) while 13, 31, 32, 23 gives us perfect correlation (e.g.  $G \rightarrow G$ ). Looking at this gene we see that  $\frac{5}{9}$  of the time we get anti correlation. But there is nothing special about this gene. The only important feature of this gene is that one of the colours is different. In other words we'd get anti-correlation  $\frac{5}{9}$  of the time for genes 2, 3, 4, 5, 6, 7. The conclusion is that for 6 out of the 8 genes we get  $\frac{5}{9}$  of the time. For genes 1 and 8 (the remaining two) we have perfect anti-correlation. The final conclusion is:

$$P(\text{anti-correlation}) > \frac{5}{9} \quad (\text{III.50})$$

i.e. Bell's theorem says that classically there is anti-correlation greater than  $\frac{5}{9}$  of the time. The experiment violates Bell's theorem!

We now consider the quantum calculation. We consider the state of an entangled positron electron pair emitted by a decaying  $\pi^0$  meson. This state is

$$\chi = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (\text{III.51})$$

Comments:

1. This is a pure state.
- 2.

$$J_z \chi = 0 \quad (\text{III.52})$$

3.

$$J^2 \chi = 0 \quad (\text{III.53})$$

4.

$$S_1^z S_2^z \chi = -\frac{\hbar^2}{4} \chi \quad (\text{III.54})$$

5. Define the correlator:

$$C(\mathcal{O}_1, \mathcal{O}_2) \equiv \frac{\langle \mathcal{O}_1 \mathcal{O}_2 \rangle}{\sqrt{\langle \mathcal{O}_1^2 \rangle \langle \mathcal{O}_2^2 \rangle}} \quad (\text{III.55})$$

Note if  $\mathcal{O}_1 = \mathcal{O}_2 \Rightarrow C = 1$ .

6. It's easy to see (or show) that we get perfect anti-correlation

$$C(S_1^z S_2^z) = -1 \quad (\text{III.56})$$

7. Further one can show that

$$C(S_1^x S_2^x) = C(S_1^y S_2^y) = -1 \quad (\text{III.57})$$

The state we are considering is an example of an entangled state. The state cannot be written as a simple product. This confirms observation 1 since the particles always have perfect anti-correlation. Next we need to show that quantum mechanics can produce observation 2. Consider the explicit pointer directions shown in figure 2:

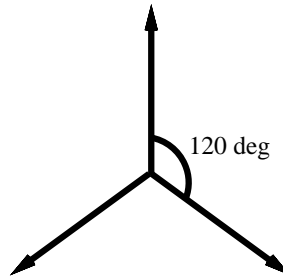


FIG. 2. The EPR pointer directions

$$n_1 = \hat{z} \quad (\text{III.58})$$

$$n_2 = \frac{\sqrt{3}}{2} \hat{x} - \frac{1}{2} \hat{z} \quad (\text{III.59})$$

$$n_3 = \frac{\sqrt{3}}{2} \hat{x} - \frac{1}{2} \hat{z} \quad (\text{III.60})$$

We measure the correlation of the spins dotted into one of the pointer directions:

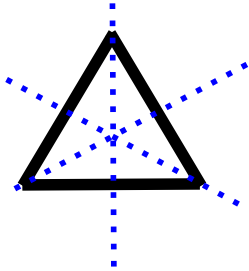
$$\sum_{ij} \langle \chi | \mathbf{S}_1 \cdot \hat{n}_i \mathbf{S}_2 \cdot \hat{n}_j | \chi \rangle = \langle \chi | \mathbf{S}_1 \cdot \left( \sum_i \hat{n}_i \right) \mathbf{S}_2 \cdot \left( \sum_j \hat{n}_j \right) | \chi \rangle \quad (\text{III.61})$$

$$= 0 \quad (\text{III.62})$$

## IV. GROUP THEORY FOR QUANTUM MECHANICS

### A. Fundamentals

The uses of studying group theory is that you can study the effects of symmetry. A symmetry is if we can perform some transformation and the system doesn't change. For example if we have a triangle



Then there are 6 symmetry transformations. Three reflection symmetries, 2 rotations ( $120^\circ$  and  $240^\circ$ ), as well as the identity transformation.

Symmetries lead to conservation laws

$$\langle \alpha | A | b \rangle \rightarrow \langle \alpha' | A' | b' \rangle = \langle \alpha | U^{-1} A' U | b \rangle \quad (\text{IV.1})$$

If

$$\langle \alpha | A | b \rangle = \langle \alpha' | A' | b' \rangle \quad (\text{IV.2})$$

then we have an invariance.  $U^{-1}AU = A$  if  $[A, U] = 0$ . For example consider the time translation operator,  $U(t) = e^{-iHt/\hbar}$ . Operators that commute with  $U$  will not change with time. For example

$$[H, U] = 0 \Rightarrow \text{Energy conservation} \quad (\text{IV.3})$$

Conservation of energy is a result of time translation invariance. Next consider the spatial transformation operator

$$T(x) = e^{-ixp/\hbar} \quad (\text{IV.4})$$

Commutation with this operator implies momentum conservation. Invariance with respect to rotations leads to angular momentum conservation. Invariance gauge transformation leads to charge conservation.

$$U(1) \rightarrow \text{Charge conservation} \quad (\text{IV.5})$$

$$SU(2) \rightarrow \text{Weak charge conservation} \quad (\text{IV.6})$$

$$SU(3) \rightarrow \text{Colour conservation} \quad (\text{IV.7})$$

Lecture 8 - January 27th, 2012

Suppose  $\mathcal{R}$  is the rotation operator and  $\mathcal{R}$  leaves the Hamiltonian invariant. For example

$$\mathcal{R} | \ell m \rangle \quad (\text{IV.8})$$

leaves all the  $m$  states invariant. For example all the states with a given  $\ell$  invariant ( $2p_x, 2p_y, 2p_z$ ) are degenerate.

The mathematics of symmetry is Group Theory. A group  $\mathcal{G}$  is a set with a rule for assigning to every ordered pair a third element satisfying the following:

1. Closure: If  $f, g \in \mathcal{G}$  then  $h = fg \in \mathcal{G}$
2. Associativity: For  $f, g, h \in \mathcal{G}$ ,  $f(gh) = (fg)h$
3. Identity: There is an identity element  $e$  such that  $ef = fe = f$  (where  $f$  is every element in the set)

4. Inverse: Every element  $f \in \mathcal{G}$  has an inverse which we call  $f^{-1}$  such that  $ff^{-1} = f^{-1}f = e$

A group really is a “multiplication table” satisfying all these properties. The table specifies  $g_1g_2 \forall g_1, g_2 \in \mathcal{G}$ . If the group elements are discrete, then we can write the multiplication table.

	$e$	$g_1$	$g_2$	$\dots$
$e$	$e$	$g_1$	$g_2$	$\dots$
$g_1$	$g_1$	$g_2g_1$	$\dots$	$\dots$
$g_2$	$g_2$	$\vdots$	$\ddots$	$\ddots$
$\vdots$	$\vdots$	$\vdots$	$\dots$	$\ddots$

A representation of  $\mathcal{G}$  is a mapping of the elements of  $\mathcal{G}$  onto a set of linear operators with the following properties.

1. Let  $D$  be the representation

$$D(e) = I \quad (\text{IV.9})$$

where  $I$  is the identity operators in the space where the linear operator act.

2.

$$D(g_1)D(g_2) = D(g_1g_2) \quad (\text{IV.10})$$

In other words the group multiplication law is mapped onto the natural multiplication in the linear space on which the operators act.

When we write

$$D(g)|\alpha\rangle \quad (\text{IV.11})$$

We mean that  $D$  is the representation,  $g$  is the group element, and  $|\alpha\rangle$  is the state.

Consider for example the group  $Z_3$ .

**Def 1.** A group is **finite** if it has a finite number of elements. Otherwise it's infinite.

**Def 2.** The number of elements in a finite group is called the **order** of the group.

$Z_3$  is of order 3:

	$e$	$a$	$b$
$e$	$e$	$a$	$b$
$a$	$a$	$b$	$e$
$b$	$b$	$e$	$a$

Note that  $Z_3$  is commutative ( $g_1g_2 = g_2g_1$ ).

**Def 3.** Commutative groups are called **Abelian** groups

A representation of  $Z_3$  is

$$\begin{aligned} D(e) &= 1 \\ D(a) &= e^{2\pi i/3} \\ D(b) &= e^{4\pi i/3} \end{aligned}$$

The dimension of the representation is the dimension of the space on which the representation acts. This representation is two dimensional. This representation clearly represents the table since

$$D(a)D(b) = e^{2\pi i/3}e^{4\pi i/3} = e^{2\pi i} = 1 \quad (\text{IV.12})$$

The rest of the relations are easy to show. Another representation for the same group is

$$D(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad D(a) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad D(b) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

This is a 3 dimensional representation. This representation has a special name. This is called the **regular** representation. The trick to construct the regular representation is as follows.

1. First we identify the orthonormal basis on which the presentation acts with group elements.

$$|e_1\rangle \equiv |e\rangle, |e_2\rangle \equiv |a\rangle, |e_3\rangle \equiv |b\rangle \quad (\text{IV.13})$$

2. Now we can construct the representation with

$$[D(g)]_{i,j} = \langle e_i | D(g) | e_j \rangle \quad (\text{IV.14})$$

The dimension of any regular representation is equal the number of group elements.

As an example we check  $D(a)$ :

$$\langle e_1 | D(a) | e_1 \rangle = \langle e | a \rangle \quad (\text{IV.15})$$

$$= 0 \quad (\text{IV.16})$$

$$\langle e_1 | D(a) | e_2 \rangle = \langle e | b \rangle \quad (\text{IV.17})$$

$$= 0 \quad (\text{IV.18})$$

$$\langle e_1 | D(a) | e_3 \rangle = 1 \quad (\text{IV.19})$$

Do the rest in bundles:

$$\langle e_2 | D(a) | e_{1,2,3} \rangle = \begin{cases} 1 & \text{for } e_2 \\ 0 & \text{for } e_1 \text{ and } e_3 \end{cases} \quad (\text{IV.20})$$

Assignments:

Construct the multiplication table for  $Z_2$

1. Find the 1 dimensional representation
2. Find the 2D representation
3. Is 2 the regular representation

Lecture 9 - January 30th, 2012

Recall the trick to find the regular representation. The reason it works is because the following

$$[D(g_1 g_2)]_{i,j} = [D(g_1) D(g_2)] \quad (\text{IV.21})$$

$$= \langle e_i | D(g_1) D(g_2) | e_j \rangle \quad (\text{IV.22})$$

$$= \sum_k \langle e_i | D(g_1) | e_k \rangle \langle e_k | D(g_2) | e_j \rangle \quad (\text{IV.23})$$

$$= \sum_k D_{i,k}(g_1) D_{k,j}(g_2) \quad (\text{IV.24})$$

We can transform the basis. A transformation on the states implies a transformation on the operators:

$$D(g) \rightarrow D'(g) = S^{-1} D(g) S \quad (\text{IV.25})$$

The transformed operators ( $D'(g)$ ) will have the same multiplication table so we say that  $D'$  and  $D$  are **equivalent** because they only differ by a trivial change of basis.

**Def 4.** A representation is **reducible** if it has an **invariant** subspace. This means that the action  $D(g)$  on any vector in the **subspace** is still in the subspace.



Every group has a trivial representation,  $D(g) = 1$ . e.g. for  $Z_2$ ,

$$D(e) = 1; \quad D(a) = 1 \quad (1D) \quad (IV.26)$$

One can have a two dimensional representation:

$$D(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad D(a) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad (2D) \quad (IV.27)$$

A third dimensional representation of  $Z_2$  is

$$D(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad D(a) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (IV.28)$$

Any action onto a vector  $\begin{pmatrix} 0 \\ a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ a' \\ b' \end{pmatrix}$  stays inside the subspace. The same goes for the vector  $\begin{pmatrix} c \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} c' \\ 0 \\ 0 \end{pmatrix}$ .

A representation is **irreducible** if it is not reducible. A representation is **completely reducible** if it is equivalent to a representation whose matrix elements have the following form:

$$\begin{pmatrix} D_1(g) & 0 & \dots \\ 0 & D_2(g) & \vdots \\ \vdots & \dots & \ddots \end{pmatrix} \quad (IV.29)$$

where  $D_i(g)$  is irreducible. This is called **block diagonal** form. A representation in block diagonal form is said to be the **direct sum** of the sub representations  $D_j(g)$ :

$$D_1 \oplus D_2 \oplus \dots \quad (IV.30)$$

e.g. Take our 3-D representation to  $Z_3$  and apply the similarity transformation

$$S = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & w^2 & w \\ 1 & w & w^2 \end{pmatrix} \quad (IV.31)$$

where  $w \equiv e^{2\pi i/3}$ . With this process we find

$$D'(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad D'(a) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & w & 0 \\ 0 & 0 & w^2 \end{pmatrix}; \quad D'(b) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & w^2 & 0 \\ 0 & 0 & w \end{pmatrix} \quad (IV.32)$$

If we act on any of the three vectors

$$\begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}; \quad \begin{pmatrix} 0 \\ b \\ 0 \end{pmatrix}; \quad \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} \quad (IV.33)$$

The vectors will stay in the subspace hence this is an irreducible representation.

In Quantum Mechanics the  $D(g)$  are unitary transformations. They map the Hilbert space to an equivalent one. They reflect the symmetry of the problem if

$$[D(g), H] = 0 \quad (IV.34)$$

This means we can always choose the energy eigenstates to transform like irreducible representations of the group. For example:  $Y_{00}$  doesn't rotate so it transforms under the trivial representation.  $Y_{10}$  transform according to a 3 dimensional representation (since  $|1, m\rangle$  can only transform to  $|1, m'\rangle$ ). Furthermore the  $Y_{2m}$  transforms according to

a 5 dimensional representation.

Consider the parity (reflection in a mirror) transformation,  $\mathcal{P}$

$$\mathcal{P}^2 = e \quad (\text{IV.35})$$

Hence

$$\begin{array}{c|cc} & e & \mathcal{P} \\ \hline e & e & \mathcal{P} \\ \mathcal{P} & \mathcal{P} & e \end{array}$$

There is a trivial representation for this group,  $D(g) = 1$  and a non-trivial representation,  $D(e) = 1$  and  $D(\mathcal{P}) = -1$ . If

$$[D(g), H] = 0 \quad (\text{IV.36})$$

e.g. 1D parity,  $x \rightarrow -x$ . Consider the harmonic oscillator potential. This does not mean that all the eigenfunctions are even. However it does mean that the even wavefunctions will transform trivially (they are already even) and the odd functions will transform according to the non-trivial representation.

Note if two groups have a different physical origin, e.g. Parity and rotations by  $\pi$  but have the same multiplication table we say the two groups are **isomorphic**.

Assignment (not to hand in): Construct the multiplication table for  $S_3$  (the group of permutations of 3 objects). For notational purposes call the elements,  $e, a, b, x, y, z$

Lecture 10th - February 1st, 2012

Consider the regular representation of  $Z_2$

$$D(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad D(a) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{IV.37})$$

We can think of this  $D(a)$  as reflection in the  $y = x$  line (thinking of it as a 2D space).

- This suggests the similarity transformation that will reduce this reducible representation
- What about rotating by 45%? Try

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad (\text{IV.38})$$

$$D(a) \rightarrow D'(a) = S^{-1}D(a)S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{IV.39})$$

and

$$D(a) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{IV.40})$$

Consider the group  $S_3$ . The elements are listed below. The notation is as follows the element  $(3, 1, 2)$  is element 1 goes to position 2, element 2 goes to position 3 and element 3 goes to position 1.

$$\begin{aligned} e &= (1, 2, 3) \\ a &= (2, 3, 1) \\ b &= (3, 1, 2) \\ x &= (1, 3, 2) \\ y &= (3, 2, 1) \\ z &= (2, 1, 3) \end{aligned}$$

Can think of these as the symmetry group of the equilateral triangle.

$$\begin{aligned} e &\rightarrow \text{Identity} \\ a, b &\rightarrow \text{Rotation} \\ x, y, z &\rightarrow \text{Reflection} \end{aligned}$$

The multiplication table of this group is as follows

	$e$	$a$	$b$	$x$	$y$	$z$
$e$	$a$	$b$	$e$	$z$	$x$	$y$
$b$	$b$	$e$	$a$	$y$	$z$	$x$
$x$	$x$	$y$	$z$	$e$	$a$	$b$
$y$	$y$	$z$	$x$	$b$	$e$	$a$
$z$	$z$	$x$	$y$	$a$	$b$	$e$

We lost commutativity and hence this is a non-Abelian group. Notice that the top left corner of the table is closed within itself. Hence we say that  $\{e, a, b\}$  forms a **subgroup**. In fact this is the same group as  $Z_3$ . Therefore this subgroup is isomorphic with  $Z_3$ . A two-dimensional representation of  $S_3$  is

$$\begin{aligned} D(e) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; & D(a) &= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}; & D(b) &= \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\ D(z) &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; & D(x) &= \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}; & D(y) &= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \end{aligned}$$

Since this is irreducible there is not similarity transformation that will diagonalize all the matrices in the representation. It is necessary that at least some of the irreps (irreducible representations) are matrices so that the non-commutativity (non-Abelian) can hold (numbers always commute!). Here's a 3D rep (reducible representation) of  $S_3$

$$\begin{aligned} D(e) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; & D(a) &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}; & D(b) &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \\ D(z) &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; & D(x) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; & D(y) &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \end{aligned}$$

This particular representation (NOT the regular representation) is important because it is the **defining** representation for the group (we call this the **fundamental** representation). It actually implements the permutation on the states. Note that a subscript on a representation given as

$$D_n \tag{IV.41}$$

means the dimensionality of the representation. However a subscript in denoting the group:

$$S_m \tag{IV.42}$$

means the number of objects the group is acting on. Consider the following where  $|1\rangle$  denotes the states which are the objects

$$D_3(a) |1\rangle = \sum_{k=1}^3 |k\rangle [D_3(a)]_{k,1} = |2\rangle \tag{IV.43}$$

$$D_3(a) |2\rangle = |3\rangle = \sum_k |k\rangle [D_3(a)]_{k,2} \tag{IV.44}$$

$$D_3(a) |3\rangle = |1\rangle = \sum_k |k\rangle [D_3(a)]_{k,3} \quad (\text{IV.45})$$

This 3D representation decomposes into a direct sum of the irreducible representations

$$D_3 = D_1 \oplus D_2 \quad (\text{IV.46})$$

The regular representation of  $Z_2 \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}$  is reducible as

$$D_2 = D_1 \oplus D_1 \quad (\text{IV.47})$$

Consider the following theorems

- All of the irreducible representations of a finite Abelian group are 1D. e.g.  $Z_3, 3D \rightarrow 1 \oplus 1 \oplus 1$ .
- If a Hermitian operator  $H$ , commutes with all the elements  $D(g)$  of a representation of a group  $G$ , then you can choose the eigenstates of  $H$  to transform according to irreducible representations of  $G$ .
  - If an irrep appears only once in the Hilbert space every state in the irrep is an eigenstate of with the same eigenvalue.

Lecture 11th, February 2nd, 2012

We have finished finite (point) groups. One can consider having shapes with more and more sides. Start with a triangle then square... all the way to a circle. A circle is invariant under any rotation. This is an example of a continuous group.

A rotation in 2-d can be represented by

$$\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad (\text{IV.48})$$

Because the parameter  $\theta$  is continuous, the group is said to be continuous. We need to check that this is a group. This transformation clearly has an identity. Proof that it's closed:

$$\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} = \begin{pmatrix} \cos \theta \cos \phi - \sin \theta \sin \phi & \cos \theta \sin \phi + \sin \theta \cos \phi \\ -(\cos \theta \sin \phi + \sin \theta \cos \phi) & \sin \theta \sin \phi + \cos \theta \cos \phi \end{pmatrix} \quad (\text{IV.49})$$

$$= \begin{pmatrix} \cos(\theta + \phi) & \sin(\theta + \phi) \\ -\sin(\theta + \phi) & \cos(\theta + \phi) \end{pmatrix} \quad (\text{IV.50})$$

This group clearly also has an inverse (if  $\theta = -\phi$ ) you get the identity. This group is clearly Abelian (if we rotate one way or another way the order doesn't matter). This group is called  $SO(2)$ .  $S$  denotes special,  $O$  denotes orthogonal, and 2 denotes 2D.

Consider multiplication by the complex numbers,  $e^{i\theta}$ . There is clearly an identity ( $\theta = 0$ ). The other properties are

$$e^{i\theta} e^{i\phi} = e^{i(\theta+\phi)}$$

$$e^{i\theta} e^{-i\theta} = 1$$

This group rotates numbers in the complex plane. This group is called  $U(1)$  where  $U$  denotes unitary ( $U^{-1} = U^\dagger$ ) and 1 denotes 1D.  $U(1)$  and  $SO(2)$  are clearly isomorphic (see figure 3). They have the same multiplication table, parameterized by 1 real number.

## B. Lie Groups

Consider rotations in 3D, we could characterize these rotations with 3 parameters, e.g.  $\{\theta_x, \theta_y, \theta_z\}$  where each define a rotation about  $x, y, z$  respectively. Alternatively we can use the 3 Euler angles. The group members of

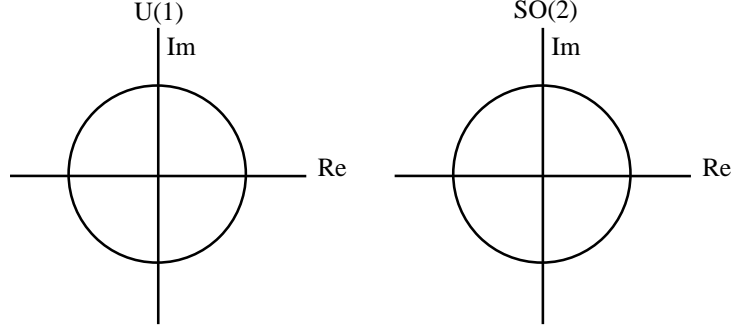


FIG. 3.  $SO(2)$  and  $U(1)$  are isomorphic

rotations in 3 dimensions can be written as the set  $\{g(\alpha)\}$  where  $\alpha$  is a “vector” of 3 parameters. If the product  $g(\alpha'') = g(\alpha)g(\alpha')$  then the group is a **Lie group** if  $\alpha'' = \Gamma(\alpha, \alpha')$  where  $\Gamma$  is an analytic function. The group elements depend smoothly on the set of parameters. By smooth we mean there is some notion of “closeness” on the group such that if two-elements of a group are “close together” in the space of the group the parameters that describe the elements are close. Another way to say this in a fancy-shmancy way is to say is that the group is a **manifold**. A manifold looks like  $\mathcal{R}_n$  locally. Thus in the neighborhood of the identity the group elements can be described by a function of  $n$  real parameters. We now parameterize the group by

$$\alpha_a, \quad a = 1, 2, \dots, n \tag{IV.51}$$

$$g(\alpha) \Big|_{\alpha=0} = e \tag{IV.52}$$

Then if we find a representation we will parameterize the representation in a way such that

$$D(\alpha) \Big|_{\alpha=0} = I \tag{IV.53}$$

In some neighborhood of the identity we can Taylor expand (since it’s analytic)  $D(\alpha)$

$$D(\delta\alpha) = I + i\delta\alpha_a X_a \tag{IV.54}$$

here we are using Einstein summation convention. The  $\delta\alpha_a$  are infinitesimal and the

$$X_a = -i \frac{\partial}{\partial \alpha_a} D(a) \Big|_{\alpha=0} \tag{IV.55}$$

The  $X_a$  are matrices for  $a = 1, 2, \dots, n$  (as many of them as the dimension of the group). These are called **generators** of the group.

On the first test, the first question will be to show that

$$H\psi = E\psi \tag{IV.56}$$

Recall our previous discussion. The  $D(\delta\alpha)$  form a group so we can multiply two elements

$$(I + i\delta\alpha_a X_a)(I + i\delta\beta_b X_b) \tag{IV.57}$$

In particular we do this. We can write  $\delta\alpha_a = \frac{\alpha_a}{k}$  where  $k$  is large. Consider the following group element

$$\lim_{k \rightarrow \infty} \left( I + i \frac{\alpha_a}{k} X_a \right)^k = e^{i\alpha_a X_a} \tag{IV.58}$$

Note the summation in the exponents. This is equal to the exponential by a definition of the exponential (not the Taylor expansion). Hence any finite representation can be written as an exponential.

### C. Lie Algebra

Now in any particular **direction** the group multiplication is uncomplicated because we can parametrize our element with  $\lambda$

$$U(\lambda) = e^{i\lambda\alpha_a X_a} \quad (\text{IV.59})$$

$$U(\lambda_1)U(\lambda_2) = U(\lambda_1 + \lambda_2) = e^{i(\lambda_1 + \lambda_2)\alpha_a X_a} \quad (\text{IV.60})$$

However it is complicated if we go into different directions.

$$e^{i\alpha_a X_a} e^{i\beta_b X_b} \neq e^{i(\alpha_a + \beta_b) X_a} \quad (\text{IV.61})$$

but we have closure in the group and therefore

$$e^{i\alpha_a X_a} e^{i\beta_b X_b} = e^{i\gamma_c X_c} \quad (\text{IV.62})$$

In other words the product is equal to some group element. We find that to next to lowest order, i.e. expanding both sides of the equation above to next to lowest order

$$\boxed{\gamma_c = \alpha_c + \beta_c - \frac{1}{2}\alpha_a \beta_b f_{abc}} \quad (\text{IV.63})$$

where

$$[X_a, X_b] = i f_{abc} X_c \quad (\text{IV.64})$$

where the  $f_{abc}$  are called the **structure constants** of the group and  $[X_a, X_b] = i f_{abc} X_c$  is called the Lie Algebra for the Lie Group. For unitary transformations the  $f_{abc}$  are real.

The worry is that this is true to next to lowest order but we'll need more to characterize group multiplication at each order. The remarkable thing is that the  $f_{abc}$  completely characterizes the group. The matrix generators satisfy the Jacobi identity

$$[X_a, [X_b, X_c]] = 0 \quad (\text{IV.65})$$

This is true for all cyclic permutations as well. The adjoint representation of an algebra is given by

$$[T_a]_{bc} = -i f_{abc} \quad (\text{IV.66})$$

i.e. the  $bc$ 'th element of the  $a$ 'th generator matrix is equal to  $-i f_{abc}$ .

The unitary group of order  $n$ ,  $U(n)$  is the group associated with  $n \times n$  unitary matrices. The matrices operate on  $n - d$  complex vectors.

$$U^\dagger U = I \quad (\text{IV.67})$$

To parameterize a complex  $n \times n$  matrix we require  $2n^2$  numbers. The unitarity condition requires  $n^2$  constraints on the matrix and therefore we are left with  $n^2$  free parameters. Therefore there are  $n^2$  generators.

$SU(n)$  is a subclass of  $U(n)$ . The  $S$  stands for special which means that the determinant of  $U$  is  $+1$ . In other words

$$\det U = |e^{i\theta}| \quad (\text{IV.68})$$

Because  $U^\dagger U = I$  it implies that

$$(I - i\delta\alpha X^\dagger)(I + i\delta\alpha X) = I \quad (\text{IV.69})$$

$$\Rightarrow i\delta\alpha (X^\dagger - X) = 0 \quad (\text{IV.70})$$

$$X = X^\dagger \quad (\text{IV.71})$$

In other words the generators are Hermitian. Now we use a general property of matrices:

$$\det A = \exp \text{Tr}(\ln A) \quad (\text{IV.72})$$

Consider

$$\det(I + \epsilon) = 1 + \text{Tr}\epsilon \quad (\text{IV.73})$$

If we use that  $\det U = 1$  we have that

$$\text{Tr}X = 0 \quad (\text{IV.74})$$

Thus the generators in  $SU(n)$  are traceless and Hermitian.

Lecture 13 - February 8, 2012

$U(n)$  is a unitary group. If we have  $SU(n)$  then  $|\det U| = 1$ .  $U(n)$  has  $n^2$  generators while  $SU(n)$  has  $n^2 - 1$ .  $U(n)$  and  $SU(n)$  have subgroups  $O(n)$  and  $SO(n)$ . These are just the real versions of  $U(n)$  and  $SU(n)$ . These transformations act on real vectors and are said to correspond to the **isometries** in n-D (this means that they don't change the shape of objects). The  $n^2$  parameters of  $U(n)$  go down to  $\frac{n(n-1)}{2}$  for  $O(n)$  ( $O$  stands for the orthogonal group). If

$$|\det U| = 1 \quad (\text{IV.75})$$

for  $O(n)$  then we have  $\det U = \pm 1$  and this group is called  $SO(n)$ . The unitarity condition for the orthogonal group is just

$$O^T O = O O^T = 1 \quad (\text{IV.76})$$

Note that we often see this notation

$$U(n) = SU(n) \otimes U(1) \quad (\text{IV.77})$$

It means that  $U(n)$  is made up of  $SU(n)$  and  $U(1)$ .

Consider some particular groups.

$$U(1) : e^{i\alpha Q} \quad (\text{IV.78})$$

where  $Q$  is the charge operator. If we construct a Hamiltonian invariant under this  $U(1)$  then it implies that we have charge conservation. We can generalize the above in the following way

$$U(1) : e^{i\alpha(x)Q} \quad (\text{IV.79})$$

The parameter controlling the phase change depends on  $x$ . In other words it depends on position in space. Hamiltonians can be constructed that are invariant under  $U(1) = e^{i\alpha(x)Q}$ . This is called a local or gauge symmetry. In order to construct such a Hamiltonian we require a gauge field (which predicts the existence of the photon). History didn't work this way for electromagnetism (the gauge symmetry was found after). Physicists later constructed gauge Hamiltonians and group was used to predict  $W^+$ ,  $W^-$ ,  $Z$ , and  $g$ .

Consider the  $SU(2)$  group. It acts on  $2 - D$  complex vectors. The defining representation is  $2 - D$ . In other words two by two matrices. There are  $n^2 - 1$  generators and since  $n = 2$  we have 3 generators. There are three directions you can go on the group manifold. Recall that the generators are traceless and hermitian. This can be encoded by writing a general representation as

$$\begin{pmatrix} a & b^* \\ b & -a \end{pmatrix} \quad (\text{IV.80})$$

There are three parameters here:  $a, \text{Re}(b), \text{Im}(b)$ . A non-unique but suitable representation are the set of generators

$$J_i = \frac{\sigma_i}{2} \quad (\text{IV.81})$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{IV.82})$$

and we know the structure constants since

$$[J_i, J_j] = i\epsilon_{ijk} J_k \quad (\text{IV.83})$$

where  $\epsilon_{ijk}$  is the Levi-Cevita symbol. Here we have  $\epsilon_{ijk} = f_{ijk}$ .

**Def 5.** A **Casimir operator** is an operator which commutes with all of the generators.

For  $SU(2)$  we need a Casimir such that

$$[J_1, J_1] = [J_2, J_2] = [J_3, J_3] = 0 \quad (\text{IV.84})$$

One such operator is  $J^2$ . The importance of a Casimir operator is that we can construct simultaneous eigenstates of  $J^2$  and  $J_i$ . It's easy to show that (try at home) that

$$[J_3, J_\pm] = \pm J_\pm \quad (\text{IV.85})$$

where  $J_\pm = J_1 \pm J_2$ . We define eigenstates  $|j, m\rangle$  such that

$$J^2 |j, m\rangle = j(j+1) |j, m\rangle \quad (\text{IV.86})$$

and

$$J_3 |j, m\rangle = m |j, m\rangle \quad (\text{IV.87})$$

Recall from quantum mechanics that  $J_+$  and  $J_-$  generate different states within a multiplet. In other words

$$J_3 J_\pm |j, m\rangle = (m \pm 1) J_\pm |j, m\rangle \quad (\text{IV.88})$$

Furthermore

$$J^2 J_\pm |j, m\rangle = j(j+1) J_\pm |j, m\rangle \quad (\text{IV.89})$$

and

$$J_\pm |j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)} |j, m \pm 1\rangle \quad (\text{IV.90})$$

We use these results to form a two dimensional representation of  $SU(2)$  by choosing

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{IV.91})$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (\text{IV.92})$$

We can now find the matrix elements of  $J_3$ :

$$\left\langle \frac{1}{2}, \frac{1}{2} \left| J_3 \right| \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{1}{2} \quad (\text{IV.93})$$

$$\left\langle \frac{1}{2}, -\frac{1}{2} \left| J_3 \right| \frac{1}{2}, \frac{1}{2} \right\rangle = 0 \quad (\text{IV.94})$$

$$\left\langle \frac{1}{2}, \frac{1}{2} \left| J_3 \right| \frac{1}{2}, -\frac{1}{2} \right\rangle = 0 \quad (\text{IV.95})$$

$$\left\langle \frac{1}{2}, -\frac{1}{2} \left| J_e \right| \frac{1}{2}, -\frac{1}{2} \right\rangle = -\frac{1}{2} \quad (\text{IV.96})$$

Hence

$$J_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{IV.97})$$

Now we find the matrix elements of  $J_+$ . Define  $\uparrow$  and  $\downarrow$  as usual. We use the following

$$J_+ |\downarrow\rangle = \sqrt{\left(\frac{1}{2} + \frac{1}{2}\right)} (1) = 1 \quad (\text{IV.98})$$



$$\langle \uparrow | J_+ | \uparrow \rangle = 0 \quad (\text{IV.99})$$

$$\langle \uparrow | J_+ | \downarrow \rangle = 1 \quad (\text{IV.100})$$

$$\langle \downarrow | J_+ | \uparrow \rangle = 0 \quad (\text{IV.101})$$

$$\langle \downarrow | J_+ | \downarrow \rangle = 0 \quad (\text{IV.102})$$

$$J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad (\text{IV.103})$$

For  $J_- = J_+^\dagger$  we get

$$J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (\text{IV.104})$$

It's now easy to find  $J_1$  and  $J_2$  using  $J_\pm = J_1 \pm iJ_2$ :

$$J_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad J_2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (\text{IV.105})$$

So we recover  $J_i = \frac{\sigma_i}{2}$ .

Lecture 14, February 10th 2012

We can construct a 2-D representation of  $SU(2)$ . The  $SU(2)$  generators are  $\frac{\sigma_i}{2}$  and therefore the  $SU(2)$  group elements are

$$U = e^{i\theta_i \sigma_i / 2} \quad (\text{IV.106})$$

(here we use summation notation), where  $\theta_i$  are continuous parameters. Note that in  $U = e^{i\theta_i \sigma_i / 2}$  is implicit but it turns out that in  $SU(2)$  we can construct the explicit matrix. For convenience we write  $\theta_i \equiv 2\omega n_i$  where  $n_i$  is a normal vector (determines how much of  $\theta_i$  is in the direction  $\hat{n}_i$ . With this change in notation we write

$$U = e^{i\omega \hat{n} \cdot \boldsymbol{\sigma}} = I + i\omega \hat{n} \cdot \boldsymbol{\sigma} - \frac{\omega^2 (\hat{n} \cdot \boldsymbol{\sigma})}{2} + \dots \quad (\text{IV.107})$$

To simplify this quantity we work out the following

$$(\hat{n} \cdot \boldsymbol{\sigma})^2 = (n_1 \sigma_1 + n_2 \sigma_2 + n_3 \sigma_3)^2 \quad (\text{IV.108})$$

$$= n_1^2 + n_2^2 + n_3^2 + n_1 n_2 \sigma_1 \sigma_2 + n_1 n_3 \sigma_1 \sigma_3 + n_2 n_3 \sigma_2 \sigma_3 + n_1 n_2 \sigma_2 \sigma_1 + n_1 n_3 \sigma_3 \sigma_1 + n_2 n_3 \sigma_3 \sigma_2 \quad (\text{IV.109})$$

$$= I \quad (\text{IV.110})$$

where we used  $\{\sigma_i, \sigma_j\}$ ,  $i \neq j$ . We can now simplify  $U$ :

$$U = I + i\omega \hat{n} \cdot \boldsymbol{\sigma} - \frac{\omega^2}{2} - i\omega^3 \frac{\hat{n} \cdot \boldsymbol{\sigma}}{2} + \dots \quad (\text{IV.111})$$

$$= \left\{ 1 - \frac{\omega^2}{2} + \frac{\omega^4}{4!} \dots \right\} + i \left\{ \omega - \frac{\omega^3}{3!} + \frac{\omega^5}{5!} + \dots \right\} \hat{n} \cdot \boldsymbol{\sigma} \quad (\text{IV.112})$$

$$= \cos \omega + i \sin \omega (\hat{n} \cdot \boldsymbol{\sigma}) \quad (\text{IV.113})$$

$$= \cos \left( \frac{\theta}{2} \right) + i \hat{n} \cdot \boldsymbol{\sigma} \sin \left( \frac{\theta}{2} \right) \quad (\text{IV.114})$$

Now we work out the matrix

$$\hat{n} \cdot \boldsymbol{\sigma} = n_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + n_2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + n_3 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{IV.115})$$

$$= \begin{pmatrix} n_3 & n_1 - in_2 \\ n_1 + in_2 & -n_3 \end{pmatrix} \equiv \begin{pmatrix} n_3 & n_- \\ n_+ & -n_3 \end{pmatrix} \quad (\text{IV.116})$$

Thus we have explicitly:

$$\begin{pmatrix} \cos \left( \frac{\theta}{2} \right) + n_3 i \sin \left( \frac{\theta}{2} \right) & in_- \sin \left( \frac{\theta}{2} \right) \\ in_+ \sin \left( \frac{\theta}{2} \right) & \cos \left( \frac{\theta}{2} \right) - in_3 \sin \left( \frac{\theta}{2} \right) \end{pmatrix} \quad (\text{IV.117})$$

**D. SU (3)**

$SU(3)$  is the group of Special unitary transformations acting on 3D complex “vectors”. For  $SU(n)$  there are  $n^2 - 1$  generators and therefore for  $SU(2)$  there are 8 generators:

$$\{X_1, X_2, \dots, X_8\} \tag{IV.118}$$

One possible choice for these generators  $X_i = \frac{\lambda_i}{2}$  where the  $\lambda_i$  are the Gell-man matrices:

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}; & \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}; & \lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & 1 & 0 \end{pmatrix}; & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \end{aligned}$$

These matrices obey

$$\text{Tr}(\lambda_i \lambda_j) = 2\delta_{ij} \tag{IV.119}$$

They obey the Lie algebra relation

$$[X_i, X_j] = f_{ijk} x_k \tag{IV.120}$$

However the  $f_{ijk}$  are not simple as in  $SU(2)$ .

Nature has an **approximate**  $SU(3)$  global symmetry, flavour:

$$\begin{pmatrix} u \\ d \\ s \end{pmatrix} \tag{IV.121}$$

but nature also has an **exact**  $SU(3)$  local (gauge) symmetry, colour:

$$\begin{pmatrix} q^1 \\ q^2 \\ q^3 \end{pmatrix} \tag{IV.122}$$

Lecture 15, February 13th, 2012

Recall that for  $SU(2)$ :

$$\cos \frac{\theta}{2} + i(\hat{n} \cdot \boldsymbol{\sigma}) \sin \frac{\theta}{2} \tag{IV.123}$$

The algebra is defined by

$$\left[ \frac{\sigma_i}{2}, \frac{\sigma_j}{2} \right] = i\epsilon_{ijk} \frac{\sigma_k}{2} \tag{IV.124}$$

The defining representation is 2D. Consider  $SO(3)$ :

$$[L_i, L_j] = i\epsilon_{ijk} L_k \tag{IV.125}$$

and the defining representation is 3D.  $SU(2)$  and  $SO(3)$  have the same Lie Algebra and they are locally isomorphic. For this to be true the group manifold must have the same dimension (3D). For  $SU(2)$

$$\begin{aligned} \theta = 0 &\rightarrow I \\ \theta = 2\pi &\rightarrow -I \end{aligned}$$

If you have some angle  $\theta$  then  $\theta$  and  $\theta + 2\pi$  gives minus the original transformation. This doesn't occur in  $SO(3)$  (we know that since we are familiar with orbital angular momentum).

In fancy shamncy words we say: The groups are locally isomorphic but the global topology of the two groups is different. In group theory language we say

$$SO(3) \rightarrow \frac{SU(2)}{Z_2} \quad (\text{IV.126})$$

## V. ACCIDENTAL DEGENERACIES

Accidental degeneracies mean there are degeneracies in the spectrum in a QM system that are unexpected. However there is no such thing as a true accident so this is just a misnomer. We will consider Hydrogen. Consider the Hamiltonian:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} \quad (\text{V.1})$$

We see that this is rotationally invariant (nothing in this problem is picking out a direction). I.e.

$$[SO(3)(g), H] = 0 \quad (\text{V.2})$$

where  $SO(3)(g)$  is a rotation matrix. Therefore the eigenstates of  $H$  transform according to irreducible representations of  $SO(3)$ . Also note invariance is  $O(3)$  which includes Parity transformations ( $\det = -1$ ). Therefore eigenstates of the Hamiltonian will also be irreducible representations of Parity. The  $1s$  forms a 1D irrep of  $SO(3)$ ,  $2P$  is a 3D irrep of  $SO(3)$ ,  $3d$  forms a 5D irrep of  $SO(3)$ . This again is sloppy language the better way to say this is to say that the states transform among each other under  $SO(3)$  if states transform among each other they are transformed by an irrep (i.e. block matrix). These are the expected degeneracies.

However in practice we see that the  $2s$  is also degenerate which  $2p$  and  $3s, 3p$  are all degenerate with  $3d$ , etc. These degeneracies are called accidental. There is way more degeneracy then we expect. There must be more symmetry then we naively think. Since symmetries produce conservation laws there must be some conservation law we are not seeing. Before we look at quantum mechanics can we see something in the classical problem? The classical problem is the Kepler problem where

$$E = \frac{p^2}{2m} - \frac{GmM}{r} \quad (\text{V.3})$$

When we solve this problem we find the orbits are elliptical. The orbitals are shown in figure 4. We also notice that

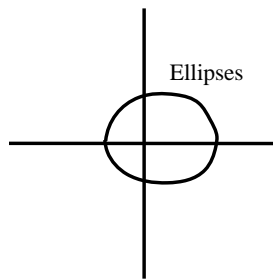


FIG. 4. The elliptical orbit of the Kepler problem

the angular momentum is conserved and hence the orbit is planar. We summarize the interesting points below:

1. Orbits are ellipses
2. Angular momentum is conserved
3. Orbit is planar

## 4. Orbit closes (no precession)

The major axis points in the same direction are all times and has the same magnitude. We are getting hints of another conserved quantity. If the potential was not  $\frac{1}{r}$  but  $\frac{1}{r^{1+\epsilon}}$  the orbit does not close! In fact in the real solar system the orbit does **not** close. They almost do but they in fact don't. The most famous example of this is Mercury. Where the parahelien precesses. The orbit of Mercury precesses because

1. There are other planets which also exert a force on Mercury (classical Newtonian effect)
2. Einstein's theory of General Relativity modifies the  $\frac{1}{r}$  potential

Now back to quantum mechanics, we define a new quantity called

$$\mathbf{M} = \frac{\mathbf{p} \times \mathbf{L}}{\mu} - \frac{e^2}{r} \mathbf{r} \quad (\text{V.4})$$

This quantity is a conserved quantity. To show that this is conserved we need to show that  $[\mathbf{M}, H] = 0$ . However there is a problem,  $\mathbf{p}$  and  $\mathbf{L}$  don't commute and  $\mathbf{M}$  is not Hermitian. To make this Hermitian we do the following:

$$\mathbf{M} = \frac{1}{2\mu} (\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{e^2}{r} \mathbf{r} \quad (\text{V.5})$$

In assignment 9 we will show that  $[\mathbf{M}, H] = 0$ . We will also show that  $\mathbf{L} \cdot \mathbf{M} = \mathbf{M} \cdot \mathbf{L} = 0$  as well as  $M^2 = \frac{2H}{\mu} (L^2 + \hbar^2) + e^4$ .

Lecture 16, February 15th, 2012

The vector  $\mathbf{M}$  is always perpendicular to  $\mathbf{L}$ . This is shown in figure 5. We have the commutation relations

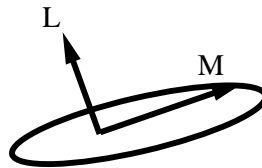


FIG. 5. The direction of the vector  $\mathbf{M}$

$$[L_i, L_j] = i\epsilon_{ijk} \hbar L_k \quad (\text{V.6})$$

$$[L_i, M_j] = i\hbar \epsilon_{ijk} M_k \quad (\text{V.7})$$

$$[M_i, M_j] = 2i \frac{\hbar}{\mu} H L_k \epsilon_{ijk} \quad (\text{V.8})$$

Notice that  $[L_i, L_j]$  closes. It is just  $SO(3)$ . Further note that  $[L_i, M_j]$  and  $[L_i, L_j]$  close. However  $[M_i, M_j]$  doesn't close! Since  $H$  is there. However

$$[H, \mathbf{M}] \quad (\text{V.9})$$

$$[H, \mathbf{L}] \quad (\text{V.10})$$

So if we restrict ourselves to subspace that corresponds to a particular eigenvalue of  $H$  we can replace  $H$  by the eigenvalue  $E$ . If you replace  $H$  by a number then the relations all stay within  $M, L$ ! Therefore in the subspace we have closure. This implies that we have a Lie Algebra in the subspace. Thus we can write the commutator (it's understood that we are staying in this subspace for which this is true)

$$[M_i, M_j] = -\frac{2i\hbar}{\mu} E L_k \epsilon_{ijk} \quad (\text{V.11})$$

Therefore the algebra of all the  $L_i$  and  $M_i$  close. For convenience we rescale  $\mathbf{M}$

$$\mathbf{M}' = \left(-\frac{\mu}{2E}\right)^{1/2} \mathbf{M} \quad (\text{V.12})$$

Remember that for bound state spectrum we have  $E < 0$ . Now  $\mathbf{r} = (r_1, r_2, r_3)$  and  $\mathbf{p} = (p_1, p_2, p_3)$  satisfy

$$[r_i, p_j] = i\hbar\delta_{ij} \quad (\text{V.13})$$

where  $i, j = 1, 2, 3$ . Lets extend  $i, j$  to  $\{1, 2, 3, 4\}$ . In other words add  $r_4, p_4$ . We define

$$L_{ij} = r_i p_j - r_j p_i \quad (\text{V.14})$$

For example In this notation

$$L_{23} = r_2 p_3 - r_3 p_2 = L_x \quad (\text{V.15})$$

We call

$$M'_i = L_{i4} = r_i p_4 - r_4 p_i \quad (\text{V.16})$$

If we do this and still use  $[r_i, p_j] = i\hbar\delta_{ij}$  then you retrieve all the commutation relations of  $L_i$  and  $M_i$ . Note that  $r_4$  and  $p_4$  are **NOT** time and energy.  $r_4$  and  $p_4$  are artificial constructs. This is not 4D.

$$[L_i, L_j] = i\hbar\epsilon_{ijk} L_k \quad (\text{V.17})$$

is the Lie Algebra of  $SO(3)$ .  $(L_{23}, L_{31}, L_{12}) = (L_x, L_y, L_z)$  but  $(L_{14}, L_{24}, L_{34}) = (M_1, M_2, M_3)$ . We know that  $SO(3)$  is a subgroup and we also know that there are 6 generators. We also know that in  $SO(n)$  there are  $\frac{n(n-1)}{2}$  generators. In fact we have the Lie Algebra of  $SO(4)$ . We have rotations in 4D (but it's not real 4D, just 3 real dimensions and 1 artificial). We can construct the generators

$$L_{nm} = |n\rangle \langle m| - |m\rangle \langle n| \quad (\text{V.18})$$

Thus

$$L_{12} = |1\rangle \langle 2| - |2\rangle \langle 1| \quad (\text{V.19})$$

Warning:  $L_{12}$  is not a matrix element. This is the operator. Using the basis

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}; \dots \quad (\text{V.20})$$

we have

By finding the matrix elements we have

$$L_{12} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{V.21})$$

We now find the commutator

$$[L_{23}, L_{31}] = (|2\rangle \langle 3| - |3\rangle \langle 2|)(|3\rangle \langle 1| - |1\rangle \langle 3|) - (|3\rangle \langle 1| - |1\rangle \langle 3|)(|2\rangle \langle 3| - |3\rangle \langle 2|) \quad (\text{V.22})$$

$$= |2\rangle \langle 1| - |1\rangle \langle 2| \quad (\text{V.23})$$

$$= -L_{12} \quad (\text{V.24})$$

$$= -L_z \quad (\text{V.25})$$

$$e^{i\theta L_{12}} = 1 + \theta L_{12} + \theta^2 \frac{L_{12}^2}{2!} + \theta^3 \frac{L_{12}^3}{3!} \quad (\text{V.26})$$

$$= 1 + \begin{pmatrix} 0 & \theta & 0 & 0 \\ -\theta & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \frac{\theta^2}{2} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \frac{\theta^3}{3!} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \dots \quad (\text{V.27})$$

$$= \begin{pmatrix} \cos \theta & \sin \theta & 0 & 0 \\ -\sin \theta & \cos \theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{V.28})$$

In a fancy shancy way we can say

$$SO(4) = \frac{SU(2) \otimes SU(2)}{Z_2}$$

We can define

$$\mathbf{I} = \frac{1}{2} (\mathbf{L} + \mathbf{M}), \quad \mathbf{K} = \frac{1}{2} (\mathbf{L} - \mathbf{M}) \quad (\text{V.29})$$

Thus we get

$$[I_i, I_j] = i\hbar \epsilon_{ijk} I_k \quad (\text{V.30})$$

$$[K_i, K_j] = i\hbar \epsilon_{ijk} K_k \quad (\text{V.31})$$

and

$$[\mathbf{I}, \mathbf{K}] = [\mathbf{I}, H] = [\mathbf{K}, H] = 0 \quad (\text{V.32})$$

We have two casimir operators

$$I^2 = i(i+1)\hbar^2; \quad K^2 = k(k+1)\hbar^2 \quad (\text{V.33})$$

where  $i, k = 0, \frac{1}{2}, 1, \dots$ . There are two Casimir Invariants

$$C = I^2 + K^2 = \frac{1}{2} (L^2 + M'^2); \quad C' = I^2 - K^2 = \mathbf{L} \cdot \mathbf{M}' = 0 \quad (\text{V.34})$$

Hence

$$I^2 = K^2 \quad (\text{V.35})$$

which implies that  $i = k$ . Therefor the eigenvalue of

$$C = I^2 + K^2 = 2I^2 = 2k(k+1)\hbar^2 \quad (\text{V.36})$$

where  $k = 0, \frac{1}{2}, 1, \dots$ . We just said

$$C = \frac{1}{2} (L^2 + M'^2) \quad (\text{V.37})$$

$$= \frac{1}{2} \left( L^2 - \frac{\mu}{2E} M^2 \right) \quad (\text{V.38})$$

$$= \frac{1}{2} \left( L^2 - \frac{\mu}{2E} (L^2 + \hbar^2) + e^4 \right) \quad (\text{V.39})$$

$$= \frac{1}{2} \left( -\hbar^2 - \frac{\mu}{4E} e^4 \right) \quad (\text{V.40})$$

$$= -\frac{\mu e^4}{4E} - \frac{\hbar^2}{2} \quad (\text{V.41})$$

but  $C$  also has values of  $2k(k+1)\hbar^2$ ,  $k = 0, \frac{1}{2}, 1, \dots$ . Therefore

$$2k(k+1)\hbar^2 = -\frac{\mu e^4}{4E} - \frac{\hbar^2}{2} \quad (\text{V.42})$$

$$\hbar^2 \left( 2k^2 + 2k + \frac{1}{2} \right) = -\frac{\mu e^4}{4E} \quad (\text{V.43})$$

$$\hbar^2 (2k+1)^2 = -\frac{\mu e^4}{2E} \quad (\text{V.44})$$

$$E = -\frac{1}{2} \mu \frac{e^4}{\hbar^2 (2k+1)^2} \quad (\text{V.45})$$

where  $2k+1 = n$  where  $n$  is an integer. So we can finally write

$$E = -\frac{1}{2} \frac{\mu e^4}{\hbar^2 n^2} \quad (\text{V.46})$$

where the degeneracy is  $n^2$ .

Lecture 17 - February 27th ,2012

Test 1 consists of (the marks are in brackets)

1. Hydrogen eigenstates (6)
2. EPR (4)
3. Density matrix (6)
4. Groups (18)

- Know your definitions

The test is in TEL 0005, from 9:30-11:30.

## VI. DIRAC EQUATION

This is the subject of relativistic quantum mechanics. We first consider the Lorentz group. In  $SO(3)$ , the quantity  $r^2 = x^2 + y^2 + z^2$  is invariant under rotations. In other words

$$Rr^2 = r'^2 = x'^2 + y'^2 + z'^2 = r^2 \quad (\text{VI.1})$$

In special relativity the invariant quantity is the length of the 4-vector  $(ct, x, y, z)$ . In other words

$$c^2 t^2 - x^2 - y^2 - z^2 = c^2 t'^2 - x'^2 - y'^2 - z'^2 \quad (\text{VI.2})$$

This quantity measures the space-time distance between space-time events. Notation:

$$x^\mu = (t, \mathbf{r}) = (t, x, y, z) = (t, r^i) \quad (\text{VI.3})$$

where from now on we use units such that  $c = 1$ . We also have

$$x_\mu = (t, -\mathbf{r}) = (t, -x, -y, -z) = (t, -r^i) \quad (\text{VI.4})$$

We call  $x^\mu$  a contravariant quantity (i.e. a quantity which transforms as the position 4-vector) and we call  $x_\mu$  a covariant quantity (quantity that transforms like the derivative of a 4-vector,  $\frac{\partial}{\partial x^\mu}$ ). Therefore we have

$$x^2 = x^\mu x_\mu \quad (\text{VI.5})$$

where here Einstein summation notation is used. We can also write

$$x^2 = x^\mu x_\mu = g_{\mu\nu} x^\mu x^\nu \quad (\text{VI.6})$$

where  $g^{\mu\nu}$  is called the **metric tensor**. In special relativity we have

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (\text{VI.7})$$

In general relativity  $g^{\mu\nu}$  becomes a dynamical quantity (it satisfies (Einstein) field equations) and may have time dependence. A Lorentz transformation (LT) is a transformation that leaves the length of 4 – *vectors* invariant. We write this as

$$X'^\mu = \Lambda^\mu_\nu X^\nu \quad (\text{VI.8})$$

or

$$X^\mu = (\Lambda^{-1})^\mu_\nu X'^\nu \quad (\text{VI.9})$$

we require that

$$X'^2 = X^2 \quad (\text{VI.10})$$

but we have

$$X'^2 = X'^\mu g_{\mu\nu} X'^\nu = \Lambda^\mu_\alpha X^\alpha g_{\mu\nu} \Lambda^\nu_\beta X^\beta \quad (\text{VI.11})$$

$$X^2 = g_{\alpha\beta} X^\alpha X^\beta \quad (\text{VI.12})$$

Hence we demand that

$$g_{\alpha\beta} = \Lambda^\mu_\alpha g_{\mu\nu} \Lambda^\nu_\beta \quad (\text{VI.13})$$

To rewrite this consider

$$g_{\mu\nu} \Lambda^\nu_\beta = g_{\mu\beta} \quad (\text{VI.14})$$

and

$$\Lambda^\nu_\alpha g_{\mu\nu} = \Lambda^\nu_\alpha g_{\mu\nu} = \Lambda^T g \quad (\text{VI.15})$$

Therefore our condition can be written in matrix notation as

$$g = \Lambda^T g \Lambda \quad (\text{VI.16})$$

We will specialize to **proper LT** (LT without parity inversion). We will also specialize to **orthochronous LT** (LT without time reversal). These are the physical transformations. Hence we can be in the neighborhood of the identity:

$$\Lambda = 1 + \epsilon\lambda \quad (\text{VI.17})$$

We insert this into our condition

$$g = (1 + \epsilon\lambda^T) g (1 + \epsilon\lambda) \quad (\text{VI.18})$$

$$g = g + \epsilon(\lambda^T g + g\lambda) + \epsilon^2 \lambda^T g \lambda \quad (\text{VI.19})$$

To first order we have  $\lambda^T g + g\lambda = 0$ . Alternatively we can write

$$\Lambda^T = -g\lambda g \quad (\text{VI.20})$$



since  $g^2 = 1$ . Consider the matrix:

$$\lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} & \lambda_{24} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} & \lambda_{34} \\ \lambda_{41} & \lambda_{42} & \lambda_{43} & \lambda_{44} \end{pmatrix} \quad (\text{VI.21})$$

Then using the equation above we have

$$\lambda = \begin{pmatrix} \lambda_{11} & \lambda_{21} & \lambda_{31} & \lambda_{41} \\ \lambda_{12} & \lambda_{22} & \lambda_{32} & \lambda_{42} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{43} \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} \end{pmatrix} = \begin{pmatrix} -\lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} \\ \lambda_{21} & -\lambda_{22} & -\lambda_{23} & -\lambda_{24} \\ \lambda_{31} & -\lambda_{32} & -\lambda_{33} & -\lambda_{34} \\ \lambda_{41} & -\lambda_{42} & -\lambda_{43} & -\lambda_{44} \end{pmatrix} \quad (\text{VI.22})$$

Clearly we have  $\lambda_{ii} = -\lambda_{ii}$  and hence each of these is zero. Furthermore  $\lambda_{12} = \lambda_{21}, \lambda_{13} = \lambda_{31}, \lambda_{14} = \lambda_{41}$ . The rest of the relations are  $\lambda_{23} = -\lambda_{32}, \lambda_{42} = -\lambda_{24}, \dots$ . Initially we required 16 parameters to specify this matrix. However these conditions show that there  $16 - 4 - 3 - 3 = 6$  free parameters. The number of generators of the group are equal to the number of free parameters. Hence there are 6 generators of the LT group. To specify the generators we use the conventions that  $(1, 2, 3, 4) \rightarrow (0, 1, 2, 3)$  and we called the generators  $\omega_{\mu\nu}$  where  $\mu, \nu = \{0, 1, 2, 3\}$ . Note: DO NOT confuse  $\mu, \nu$  with matrix indices, they are labeling a generator.

$$\begin{aligned} \omega_{10} &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; & \omega_{20} &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; & \omega_{30} &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \\ \omega_{12} &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; & \omega_{23} &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}; & \omega_{13} &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \end{aligned}$$

This can be written as

$$(\omega_{\mu\nu})_{\beta}^{\alpha} = -\frac{1}{2}\epsilon_{\mu\nu\lambda\sigma}\epsilon_{\beta}^{\lambda\sigma\alpha} \quad (\text{VI.23})$$

where  $\epsilon_{\mu\nu\lambda\sigma}$  is the 4D Levi-Cevita Symbol. One can show that

$$\omega_{01} = \omega_{10}, \omega_{21} = -\omega_{12} \quad (\text{VI.24})$$

The most general infinitesimal LT can be written

$$\Lambda = 1 + \xi_i \omega_{i0} + \frac{1}{2} \theta_i \epsilon_{ijk} \omega_{jk} \quad (\text{VI.25})$$

This group contains 6 parameters  $\theta_i, i = 1, 2, 3$  and  $\xi_i, i = 1, 2, 3$ . Therefore a finite LT can be written

$$\Lambda = \exp \left( \xi_i \omega_{i0} + \frac{1}{2} \theta_i \epsilon_{ijk} \omega_{jk} \right) \quad (\text{VI.26})$$

This is called the Lorentz group, denoted by  $SO(1, 3)$ .

Lecture 18 - March 2nd, 2012

Consider the LT for  $\xi_i = \theta_i = 0$  for all  $i$  except for  $\theta_3$ .

$$\Lambda(\theta_3) = \exp \left( \frac{1}{2} \theta_3 \epsilon_{3jk} \omega_{jk} \right) \quad (\text{VI.27})$$

$$= \exp \left( \frac{1}{2} \{-\omega_{21} \theta_3 + \omega_{12} \theta_3\} \right) \quad (\text{VI.28})$$

$$= \exp \left( \frac{1}{2} \{-2\theta_3 \omega_{21}\} \right) \quad (\text{VI.29})$$

$$= \exp(\omega_{12} \theta_3) \quad (\text{VI.30})$$

we have

$$\omega_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{VI.31})$$

$$(\omega_{12})^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{VI.32})$$

Since this is diagonal this is easy

$$(\omega_{12})^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -\omega_{12} \quad (\text{VI.33})$$

$$(\omega_{12})^4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{VI.34})$$

and then the sequence repeats,i.e.  $\omega_{12}^5 = \omega_{12}$  etc. We can now find  $\Lambda$  explicitly:

$$\Lambda(\theta_3) = I + \theta_{12} + \frac{\theta_2}{2}\omega_{12}^2 + \frac{\theta^3}{3!}\omega_{12}^3 + \dots \quad (\text{VI.35})$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 - \frac{\theta^2}{2} & -\theta + \frac{\theta^3}{3!} + \dots & 0 \\ 0 & \theta + \frac{\theta^3}{3!} + \dots & 1 - \frac{\theta^2}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{VI.36})$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta & 0 \\ 0 & \sin \theta & \cos \theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{VI.37})$$

We see that  $\theta_3$  gives a rotation about the 3 axis. Since there is nothing special about  $\theta_3$ ,  $\theta_1$  and  $\theta_2$  give us rotations about the  $x$  and  $y$  axes. If we set all the  $\xi_i = 0$  then we have the group  $\text{SO}(3)$ . Now lets set all parameters to zero except  $\xi_1$ .

$$\Lambda(\xi_1) = \exp(\xi_1 \omega_{10}) \quad (\text{VI.38})$$

Recall that

$$\omega_{10} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Hence we have

$$\omega_{10}^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and hence

$$\omega_{10}^3 = \omega_{10}$$

Hence we have

$$\Lambda(\xi) = I + \xi\omega_{10} + \frac{\xi^2}{2}(\omega_{10})^2 + \frac{\xi^3}{3!}(\omega_{10})^3 + \dots \quad (\text{VI.39})$$

$$= \begin{pmatrix} 1 + \frac{\xi^2}{2} + \dots & \xi + \frac{\xi^3}{3} + \dots & 0 & 0 \\ \xi + \frac{\xi^3}{3} + \dots & 1 + \frac{\xi^2}{2} + \dots & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{VI.40})$$

$$= \begin{pmatrix} \cosh \xi & \sinh \xi & 0 & 0 \\ \sinh \xi & \cosh \xi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{VI.41})$$

Hence under the action of the Lorentz Transformation,  $\Lambda(\xi_1)$  we see that

$$\begin{pmatrix} t' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cosh \xi & \sinh \xi & 0 & 0 \\ \sinh \xi & \cosh \xi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} t \\ x \\ y \\ z \end{pmatrix} \quad (\text{VI.42})$$

Explicitly we have

$$\begin{aligned} t' &= \cosh \xi t + \sinh \xi x \\ x' &= \sinh \xi t + \cosh \xi x \\ y' &= y \\ z' &= z \end{aligned}$$

If we define  $\xi = \tanh^{-1} v$  which is called the rapidity. This gives

$$\begin{aligned} v &= \tanh \xi \\ v^2 &= \tanh^2 \xi \\ &= 1 - \operatorname{sech}^2 \xi \\ &= 1 - \frac{1}{\cosh^2 \xi} \\ \cosh^2 \xi &= \frac{1}{1 - v^2} \end{aligned}$$

We define  $\gamma = \cosh \xi$ . We can write

$$\tanh \xi = \frac{\sinh \xi}{\cosh \xi} = \frac{v/c}{\sqrt{1 - v^2/c^2}}$$

and we get

$$\begin{aligned} t' &= \gamma(1 + \beta x) \\ x' &= \gamma(1 + \beta ct) \end{aligned}$$

We see that we have a subgroup of **boosts**. So all together the Lorentz group has 3 rotations and 3 boosts. If we choose a more familiar parameterization

$$U(\theta) \approx 1 + \frac{i}{2} \theta_{\mu\nu} J^{\mu\nu} \quad (\text{VI.43})$$

where we relate these  $J_{\mu\nu}$ 's to our angular momentum operators by

$$J_i = \frac{1}{2} \epsilon_{ijk} J_{jk} \quad (\text{VI.44})$$

and we define

$$K_i = J_i^0 \quad (\text{VI.45})$$

This gives

$$[J_i, J_j] = i\epsilon_{ijk} J_k \quad (\text{VI.46})$$

$$[J_i, K_j] = i\epsilon_{ijk} K_k \quad (\text{VI.47})$$

$$[K_i, K_j] = -i\epsilon_{ijk} J_k \quad (\text{VI.48})$$

This forms the algebra of  $SO(3, 1)$

Lecture 19 - March 5th, 2012

We have finished with the Lorentz group. Now we move on to the Dirac equation. The Schrodinger equation is given by

$$\left( \frac{p^2}{2m} + V \right) \psi = E\psi \quad (\text{VI.49})$$

$$(K + V) \psi = E\psi \quad (\text{VI.50})$$

where  $K$  is the kinetic energy operator,  $V$  is the potential energy operator and  $E$  is the energy operator. This equation is Galilean covariant but obviously not Lorentz covariant. This is because  $E = \frac{p^2}{2m} + V$  is not the relativistic Energy-momentum (dispersion) relation. The relativistic energy-momentum relation is what we get from constructing a Lorentz-invariant quantity. This quantity is  $p^2$ , where  $p^\mu$  is the Lorentz 4-vector equal to  $p^\mu = (p^0, \mathbf{p}) = (E, \mathbf{p})$ .

$$p^2 = p^\mu p_\mu = g_{\mu\nu} p^\mu p^\nu \quad (\text{VI.51})$$

$$p^2 = E^2 - \mathbf{p}^2 = m^2 \Rightarrow E^2 = p^2 + m^2 \quad (\text{VI.52})$$

Thus

$$E = (m^2 + p^2)^{1/2} \quad (\text{VI.53})$$

If we demand the correct dispersion relation then we would have

$$i\hbar \frac{\partial}{\partial t} \psi = (m^2 - \hbar^2 \nabla^2)^{1/2} \psi \quad (\text{VI.54})$$

$$= m \left( 1 - \frac{\nabla^2}{2m} - \frac{\nabla^4}{8m^4} + \dots \right) \quad (\text{VI.55})$$

Even though this equation works many problems are encountered using this method and this route was not historically taken. Alternatively we can not taken the square root:

$$E^2 = m^2 + p^2 \quad (\text{VI.56})$$

where  $E^2 = (i\hbar \frac{\partial}{\partial t})^2 = -\hbar \frac{\partial^2}{\partial t^2}$ . Recall that  $p^2 = -\hbar \frac{\partial^2}{\partial x^2}$ . We now introduce useful notation that says

$$\square = g_{\mu\nu} \square^\mu \square^\nu \quad (\text{VI.57})$$

with this we have

$$(\square + m^2) \psi = 0 \quad (\text{VI.58})$$

This is called the Klien Gordan equation. Solutions to this equation take the form

$$\phi_n^\pm = N e^{i(\mathbf{k} \cdot \mathbf{r} - E_n t)} \quad (\text{VI.59})$$

where  $E_n = \sqrt{m^2 + k_n^2}$ . However there two problems with this solution

- Some states turn out to have a negative norm.
- This generates states with negative energy

The origin of the negative energy can be traced back to the fact that we have the square of the energy. Is there an equation that is first order in time AND first order in space so that one can have manifest Lorentz symmetry? This is a fancy way of saying symmetry between time and space. With this in mind Dirac wrote

$$i\hbar \frac{\partial}{\partial t} \psi = H\psi = (\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m) \psi \quad (\text{VI.60})$$

where  $\alpha$  and  $\beta$  are at this point two unknowns. However we do know that

$$E^2 = p^2 + m^2 \quad (\text{VI.61})$$

(we demand this to be true). We now implement this on our equation

$$\left( i\hbar \frac{\partial}{\partial t} \right)^2 \psi = (\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m)^2 \psi \quad (\text{VI.62})$$

$$= (p^2 + m^2) \psi \quad (\text{VI.63})$$

This requires

$$(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m)^2 = p^2 + m^2 \quad (\text{VI.64})$$

$$(\alpha_i p_i + \beta m)^2 = p^2 + m^2 \quad (\text{VI.65})$$

$$\alpha_i p_i \alpha_j p_j + \alpha_i \beta p_i m + \beta \alpha_i p_i m + \beta^2 m^2 = p^2 + m^2 \quad (\text{VI.66})$$

$$(\text{VI.67})$$

This tells us that  $\alpha$  and  $\beta$  can't be just numbers because in order to get the two terms first order in  $p$  to be zero we require that

$$\alpha_i \beta + \beta \alpha_i \equiv \{\alpha_i, \beta\} = 0 \quad (\text{VI.68})$$

Continuing we can write the left hand side as

$$\alpha_i^2 p_i^2 + \frac{1}{2} \{\alpha_j, \alpha_i\} p_i p_j + \{\alpha_j, \beta\} m p_j + \beta^2 m^2 \quad (\text{VI.69})$$

Now demanding that this equal  $p^2 + m^2$  we must have

$$\alpha_i^2 = 1; \quad \{\alpha_i, \alpha_j\} = 2\delta_{ij}; \quad \{\alpha_i, \beta\} = 0; \quad \beta^2 = 1$$

We have the following Lemmas:

1.  $\beta$  and  $\alpha_i$  are traceless:

$$\alpha_i \beta + \beta \alpha_i = 0 \quad (\text{VI.70})$$

$$\alpha_i \beta = -\beta \alpha_i \quad (\text{VI.71})$$

$$\beta \alpha_i \beta = -\beta^2 \alpha_i \quad (\text{VI.72})$$

$$\beta \alpha_i \beta = -\alpha_i^2 \quad (\text{VI.73})$$

$$\text{Tr}(\beta \alpha_i) = -\text{Tr}(\alpha_i) \quad (\text{VI.74})$$

$$\text{Tr}(\alpha_i) = -\text{Tr}(\alpha) \quad (\text{VI.75})$$

Hence the  $\alpha_i$  are traceless (it's similar to prove that  $\beta$  is traceless) but also we have  $\alpha_i^2 = 1$  and  $\beta^2 = 1$ .

2. Now we can diagonalize the  $\alpha_i$  and  $\beta$ . If we have a diagonal matrix that the square is equal to the identity we have

$$\begin{pmatrix} x & & & \\ & x & & \\ & & x & \\ & & & x \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{VI.76})$$

This requires that we have eigenvalues of  $\pm 1$ .

3. The matrices are  $n \times n$  where  $n$  is even (since the eigenvalues must add to 0 and they are  $\pm 1$ )

The dimensionality of the matrices is even. Is it possible for  $n$  to equal 2? There are  $n^2$  independent Hermitian matrices ( $n^2$  parameters). However the identity is not traceless so it can't be a candidate for  $\alpha_i$  or  $\beta$ . Thus subtracting the identity gives  $n^2 - 1$  matrices. Thus we have  $n^2 - 1 = 3$  possible independent matrices. However we need at least 4 matrices to have one for all of  $\alpha_i, \beta$ .  $n = 4$  gives  $n^2 - 1 = 15$  matrices which is more than enough.

**Conclusion:** We can find  $4 \times 4$  independent Hermitian matrices that satisfy all our requirements. Since  $n = 4$  gives many matrices we can choose which we want to use. We make the choice:

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad (\text{VI.77})$$

where each of these entries is a 2 by 2 entry.

Lecture 20, March 7th, 2012

As it stands this equation doesn't look manifestly covariant (though it is). We define

$$\gamma^\mu = (\beta, \beta\alpha^i) \quad (\text{VI.78})$$

where  $\gamma^0 = \beta$  and  $\gamma^i = \beta\alpha_i$ . Thus

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \quad (\text{VI.79})$$

This gives the anticommutation relation:

$$\{\gamma^\mu, \gamma^\nu\} = g^{\mu\nu} \quad (\text{VI.80})$$

This gives

$$\left( i\gamma^\mu \frac{d}{dx^\nu} - m \right) \psi = 0 \quad (\text{VI.81})$$

Note that  $\psi$  has the form  $\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$ , but it is not a four-vector! It is a four-spinor. We will learn later how  $\psi$  transforms

under rotations and boosts (i.e. LT).

Recall that the Klein-Gordon equation had problems. One problem was there were states with negative norm and the other problem was that it had states of negative energy. We shouldn't have negative states because if there were then electrons would fall to these negative energy states emitting energy which we don't observe.

Consider the following

$$i\frac{\partial}{\partial t}\psi_b = H\psi_b \Rightarrow \psi_a^\dagger i\frac{\partial}{\partial t}\psi_b = \psi_a^\dagger H\psi_b \quad (\text{VI.82})$$

and

$$-i\frac{\partial}{\partial t}\psi_a^\dagger = (H\psi_a)^\dagger \Rightarrow -i\frac{\partial}{\partial t}\psi_a^\dagger\psi_b = (H\psi_a)^\dagger\psi_b \quad (\text{VI.83})$$

subtracting these equations gives

$$i\frac{\partial}{\partial t}(\psi_a^\dagger\psi_b) - i\psi_a^\dagger\alpha_i \left[ \overrightarrow{\nabla}_i + \overleftarrow{\nabla}_i \right] \psi_b \quad (\text{VI.84})$$

where the arrows denote direction over which they act. This gives

$$i\frac{\partial}{\partial t}(\psi_a^\dagger\psi_b) + i\nabla_i(\psi_a^\dagger\alpha_i\psi_b) = 0 \quad (\text{VI.85})$$

$$i \frac{\partial}{\partial x^\mu} [\psi_a^\dagger \gamma^0 \gamma^\mu \psi_b] = 0 \quad (\text{VI.86})$$

If we define  $\psi^\dagger \gamma^0 \equiv \bar{\psi}$  we have

$$i \frac{\partial}{\partial x^\mu} [\bar{\psi}_a \gamma^\mu \psi_b] = 0 \quad (\text{VI.87})$$

Comparing with the known equation  $\frac{\partial}{\partial x^\mu} J^\mu = 0$ , this is just the continuity equation! Recall in electromagnetism we have

$$\mathbf{J}^\mu = (\rho, \mathbf{J}) \quad (\text{VI.88})$$

In electromagnetism we have

$$\frac{\partial}{\partial t} \rho = -\nabla \cdot \mathbf{J} \quad (\text{VI.89})$$

Integrating over some volume

$$\frac{\partial}{\partial t} \int \rho dV = - \int_V \nabla \cdot \mathbf{J} dV \quad (\text{VI.90})$$

$$\frac{\partial}{\partial t} Q = - \int_S \mathbf{J} \cdot d\mathbf{A} \quad (\text{VI.91})$$

Back to Quantum mechanics. If charge was conserved before what is conserved now? What is this object

$$\bar{\psi} \gamma^\mu \psi \quad ? \quad (\text{VI.92})$$

This is the probability current. Since this satisfies the continuity equation probability is conserved. Therefore norm is conserved. The Dirac equation can be written in covariant form as

$$\left( i \gamma^\mu \frac{\partial}{\partial x^\mu} - m \right) \psi = 0 \quad (\text{VI.93})$$

This is the free Dirac equation (no potential), written in covariant form. To make it non-free we need to add a potential. However the idea of a potential is non relativistic. The way we add interactions is by adding a four-potential:

$$\left[ \gamma^\mu \left( i \frac{\partial}{\partial x^\mu} - e A_\mu \right) - m \right] \psi = 0 \quad (\text{VI.94})$$

where  $A^\mu = (\phi, \mathbf{A})$ . Note that the Dirac equation is mainly good for electromagnetism. We try free-Dirac equation solutions of the form  $\psi_p^\pm(\mathbf{r}, t) = N_p e^{\mathbf{p} \cdot \mathbf{r} \mp E_p t} \begin{pmatrix} \chi \\ \eta \end{pmatrix}$ .  $\chi$  and  $\eta$  are  $2 \times 1$  column vectors.  $\pm$  refer to positive and negative energy solutions  $E_p > 0$ . We substitute the positive energy solution into the free-Dirac equation:

$$\left( i \gamma^\mu \frac{\partial}{\partial x^\mu} - m \right) N_p e^{\mathbf{p} \cdot \mathbf{r} - E_p t} \begin{pmatrix} \chi \\ \eta \end{pmatrix} \quad (\text{VI.95})$$

Lecture 21 -  
Missed a lecture

Lecture 22 - March 12th, 2012  
We have the Dirac equation

$$\left( i \gamma^\mu \frac{\partial}{\partial x^\mu} - m \right) \psi = 0 \quad (\text{VI.96})$$

We try the solution  $\psi^+(\mathbf{r}, t) = N e^{-ip \cdot x} \begin{pmatrix} \chi \\ \eta \end{pmatrix}$  (not  $\psi^\dagger$  but  $\psi^+$ , where  $p \cdot x = p^\mu x_\mu = p^0 x_0 - \mathbf{p} \cdot \mathbf{x} = Et - \mathbf{p} \cdot \mathbf{x}$ . We found a solution terms of arbitrary  $\chi$  but we require

$$\eta = \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{E + m} \chi \quad (\text{VI.97})$$

For normalization we require

$$\int \psi^\dagger \psi d^3r = \int (\chi^\dagger \eta^\dagger) \begin{pmatrix} \chi \\ \eta \end{pmatrix} N^2 \quad (\text{VI.98})$$

$$= N^2 (\chi^\dagger \eta^2) \begin{pmatrix} \chi \\ \eta \end{pmatrix} L^3 \quad (\text{VI.99})$$

$$= N^2 L^3 (\chi^\dagger \chi + \eta^\dagger \eta) \quad (\text{VI.100})$$

$$= N^2 L^3 \left( \chi^\dagger \chi + \chi^\dagger \frac{(\boldsymbol{\sigma} \cdot \mathbf{p})^2}{(E + m)^2} \chi \right) \quad (\text{VI.101})$$

but  $(\boldsymbol{\sigma} \cdot \mathbf{p})^2 = p^2$  (see notes from previous lecture). Thus we have  $\frac{(\boldsymbol{\sigma} \cdot \mathbf{p})^2}{(E + m)^2} = \frac{p^2}{(E + m)^2}$ . Inserting in this result gives

$$\int d^3r \psi^\dagger \psi = N^2 L^3 \left( \chi^\dagger \chi + \chi \chi^\dagger \frac{p^2}{(E + m)^2} \chi \right) \quad (\text{VI.102})$$

Since  $\chi$  is just a number we have

$$\int d^3r \psi^\dagger \psi = N^2 L^3 \chi^\dagger \chi \left( \frac{(E + m)^2 + p^2}{(E + m)^2} \right) \quad (\text{VI.103})$$

$$= N^2 L^3 \chi^\dagger \chi \left( \frac{2E^2 + 2Em}{(E + m)^2} \right) \quad (\text{VI.104})$$

$$= N^2 L^3 \frac{2E}{E + m} \chi^\dagger \chi \quad (\text{VI.105})$$

We will choose  $\chi^\dagger \chi = 1$ . Thus we require

$$N = \left( \frac{E + m}{2EL^3} \right)^{1/2} \quad (\text{VI.106})$$

It is conventional to choose

$$u(p, s) = \sqrt{E + m} \begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{E + m} \end{pmatrix} \chi^s \quad (\text{VI.107})$$

where  $\chi^{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\chi^{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . Note that more explicitly we have

$$u(p, s) = \sqrt{E + m} \begin{pmatrix} \chi^s & 0 & 0 & 0 \\ 0 & \chi^s & 0 & 0 \\ 0 & 0 & \frac{\chi^s}{E + m} p_z & \frac{\chi^s}{E + m} (p_x - ip_y) \\ 0 & 0 & \frac{\chi^s}{E + m} (p_x + ip_y) & -\frac{\chi^s}{E + m} p_z \end{pmatrix} \quad (\text{VI.108})$$

Putting this together we have

$$\psi_{p,s}^+ = \frac{1}{\sqrt{2EL^3}} u(p, s) e^{-p \cdot x} \quad (\text{VI.109})$$



similarly we have

$$\psi_{-p,-s}^-(x) = \frac{1}{\sqrt{2EL^3}} v(\mathbf{p}, s) e^{ip \cdot x} \quad (\text{VI.110})$$

where  $v(\mathbf{p}, s) = \sqrt{E+m} \begin{pmatrix} \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{E+m} \\ 1 \end{pmatrix} (-i\sigma_2 \chi^s)$ . Notice that the zero momentum solutions take the form of

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \text{ and } \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}.$$

Consider the following operation

$$\psi \rightarrow \psi^c = C\beta\psi^* \quad (\text{VI.111})$$

where  $C = -i\alpha_2 = \begin{pmatrix} 0 & -\sigma_2 \\ -i\sigma_2 & 0 \end{pmatrix}$  and we have  $C^2 = -1$ . Other properties of  $C$  are

$$\begin{aligned} C &= i\gamma^2\gamma^0 \\ C &= -C^{-1} \\ C &= -C^\dagger \\ C &= C^T \\ C\alpha C^{-1} &= -\alpha^* \\ C\gamma^\mu C^{-1} &= \gamma^{\mu T} \end{aligned}$$

Consider the Dirac equation

$$i\frac{\partial}{\partial t}\psi = (\alpha_i(-i\nabla_i - eA^i) + eA^0 + \beta m)\psi \quad (\text{VI.112})$$

with  $A^\mu$  as the vector potential and in non-manifestly covariant form.

$$-i\frac{\partial}{\partial t}\psi = (\alpha_i^*(i\nabla_i - eA^i) + eA^0 + \beta m)\psi^* \quad (\text{VI.113})$$

$$-i\frac{\partial}{\partial t}\psi^* = (\alpha_i(i\nabla_i - eA^i) + eA^0 - \beta m)\psi^c \quad (\text{VI.114})$$

$$i\frac{\partial}{\partial t}\psi^* = (\alpha_i(-i\nabla_i + eA^i) - eA^0 + \beta m)\psi^c \quad (\text{VI.115})$$

This is the original Dirac equation but  $e \rightarrow -e$ .  $\psi^c$  satisfies the Dirac equation but with **opposite charge**. We also find that  $C\beta u^*(\mathbf{p}, s) = v(\mathbf{p}, s)$ . Therefore we have  $C\beta\psi_{-p,-s}^{-*} = \psi_{p,s}^+(x)$ .

$\psi_{-p,-s}^{-c}$  describes an antiparticle with positive energy with momentum and spin. Dirac's interpretation (which was eventually overtaken by QFT) is that electrons satisfy the Pauli exclusion principle so he says that the world has all the negative energy states filled. Dirac says that  $\psi^{-c}$  correspond to holes in the negative energy sea. Pair creation can be thought of as knocking out an electron in a negative electron state into the positive energy states.

Lecture 23, March 16th, 2012

### A. Non-relativistic limit of the Dirac equation

One reason to do this is to make contact with the Schrodinger equation and the Pauli equation. The Pauli equation is just the Schrodinger equation with two component spinors.

This will give us intuition on what a 4-spinor is. Recall that we have

$$\psi_+ = \frac{1}{\sqrt{2EL^3}} u(\mathbf{p}, s) e^{-ip \cdot x} \quad (\text{VI.116})$$

where  $u(\mathbf{p}, s) = \sqrt{E+m} \begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{E+m} \chi^s \end{pmatrix}$ . Consider the  $v \rightarrow 0$  limit. In this limit we have  $\mathbf{p} \rightarrow 0$  and  $p = (m, \mathbf{0})$ . Hence

$$\psi^+(s = \frac{1}{2}) = \frac{1}{\sqrt{2mL^3}} u(0, s) e^{-imt} = \frac{1}{\sqrt{2mL^3}} \sqrt{2m} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-imt} \quad (\text{VI.117})$$

$$= \frac{1}{\sqrt{L^3}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-imt} \quad (\text{VI.118})$$

while we have

$$\psi^+(s = -\frac{1}{2}) = \frac{1}{\sqrt{L^3}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-imt} \quad (\text{VI.119})$$

Similarly the negative energy solutions are

$$\psi^-(s = \frac{1}{2}) = \frac{1}{\sqrt{2mL^3}} \sqrt{2m} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{imt} = \frac{1}{\sqrt{L^3}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{imt} \quad (\text{VI.120})$$

$$\psi^-(s = -\frac{1}{2}) = \frac{1}{\sqrt{L^3}} \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix} e^{imt} \quad (\text{VI.121})$$

This is the spinors at rest. To gain more insight on the problem we need to boost these spinors. We don't yet know how to do this since we only know the transformations in the fundamental representation. However in 1950 Folby and Wouthuysen came up with a technique to the non-relativistic reduction properly. They showed that you could expand the spinors in a  $\frac{p}{m}$  expansion.

We call  $\chi$  the large components of this expansion and  $\eta$  the small components (this is clear by the results above, for electrons the  $\eta$  components,  $\frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{E+m}$  are 0). What Folby and Wouthuysen found was to find a way to write the spinors in terms of  $\chi$ 's in terms of Pauli spinors.

This trick is difficult. We start with a practice problem. Consider you have the following Hamiltonian  $H = \sigma_x B_x + \sigma_z B_z$  (a  $H$  that just involves pauli matrices). The Hamiltonian is a  $2 \times 2$  matrix. This Hamiltonian would describe Pauli spinors interacting with the magnetic field. Also consider the unitary transformation

$$U = e^{i\sigma_y \theta/2} = \cos \frac{\theta}{2} + i\sigma_y \sin \frac{\theta}{2} \quad (\text{VI.122})$$

$$H' = U H U^{-1} = e^{i\sigma_y \theta/2} H e^{-i\sigma_y \theta/2} \quad (\text{VI.123})$$

$$= \left( \cos \frac{\theta}{2} + i\sigma_y \sin \frac{\theta}{2} \right) H \left( \cos \frac{\theta}{2} - \sigma_y \sin \frac{\theta}{2} \right) \quad (\text{VI.124})$$

$$= \cos^2 \frac{\theta}{2} (\sigma_x B_x + \sigma_z B_z) + i \sin \frac{\theta}{2} \cos \frac{\theta}{2} ([\sigma_y, \sigma_x] B_x + [\sigma_y, \sigma_z] B_z) + \sin^2 \frac{\theta}{2} (\sigma_y \sigma_x \sigma_y B_x + \sigma_y \sigma_z \sigma_y B_z) \quad (\text{VI.125})$$

$$= \sigma_x (\cos \theta B_x - \sin \theta B_z) + \sigma_z (\cos \theta B_z + \sin \theta B_x) \quad (\text{VI.126})$$

If  $\tan \theta = \frac{B_x}{B_z}$  then the coefficient of  $\sigma_x$  is zero. Hence we have diagonalized  $H$ . We have decoupled the upper and lower components.

We now do a more difficult problem (however still not the full problem). Consider the free Dirac equation (no vector potential).

$$H = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m \quad (\text{VI.127})$$

Here we want to decouple the large and small components of the Dirac equation (due to low velocity limit). Recall that

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

Hence in block diagonal form we have

$$H = \begin{pmatrix} 0 & \boldsymbol{\sigma} \cdot \mathbf{p} \\ \boldsymbol{\sigma} \cdot \mathbf{p} & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} m \quad (\text{VI.128})$$

It turns out that  $e^{is}$  where  $is = \beta \boldsymbol{\alpha} \cdot \mathbf{p} \theta(\mathbf{p})$  does the trick. This can be written as

$$e^{is} = \cos(|\mathbf{p}| \theta) + \beta \frac{\boldsymbol{\alpha} \cdot \mathbf{p}}{|\mathbf{p}|} \sin(|\mathbf{p}| \theta) \quad (\text{VI.129})$$

If we transform  $H$  then we have

$$H' = U H U^{-1} \quad (\text{VI.130})$$

$$= \beta (m \cos 2(|\mathbf{p}| \theta) + |\mathbf{p}| \sin(|\mathbf{p}| \theta)) \quad (\text{VI.131})$$

if we choose  $\tan(|\mathbf{p}| \theta) = \frac{|\mathbf{p}|}{m}$  then we have

$$H' = \beta \sqrt{m^2 + \mathbf{p}^2} \quad (\text{VI.132})$$

$$= \begin{pmatrix} E & & & \\ & E & & \\ & & -E & \\ & & & -E \end{pmatrix} \quad (\text{VI.133})$$

Lecture 24 - March 19th, 2012

We are not responsible for the Foldy-Wouthuysen online but we are responsible for the toy example, Dirac free example, and the March 19th (today) example.

We now continue with FW. The general case is

$$H = \boldsymbol{\alpha} \cdot (\mathbf{p} - e\mathbf{A}) + \beta m + e\phi \quad (\text{VI.134})$$

where  $A^0 = \phi$  and  $A^i = \mathbf{A}$ . So far we were able to completely decouple large and small components of the Dirac equation but only in the free case (i.e.  $A^\mu = 0$ ). In the general case this is impossible to all orders in  $\frac{|\mathbf{p}|}{m}$  (this tells us how relativistic the system is). However Foldy-Wouthuysen tells us how to decouple to any desired finite order in  $\frac{|\mathbf{p}|}{m}$ . Recall we are interested in decoupling so that we have an equation which is Schrodinger-like for the Pauli 2-spinor  $\chi$ . We could continue with a systematic expansion through FW (which is done in the posted notes). Instead of developing a general systematic approach, we will use hindsight to efficiently get to the next level of desired accuracy.

First lets define two quantities:

$$T = E - m \quad (\text{VI.135})$$

(roughly speaking this is the kinetic energy). Further we define

$$V^\mu = eA^\mu \quad (\text{VI.136})$$

(just to simplify notation). We can now write the Dirac equation in first order with a Hamiltonian by

$$T \begin{pmatrix} \chi \\ \eta \end{pmatrix} = (-m + V^0 + \boldsymbol{\alpha} \cdot (\mathbf{p} - \mathbf{V}) + \beta m) \begin{pmatrix} \chi \\ \eta \end{pmatrix} = H \begin{pmatrix} \chi \\ \eta \end{pmatrix} \quad (\text{VI.137})$$

Consider

$$U = U^\dagger = A\beta + \frac{\lambda}{m}\boldsymbol{\alpha} \cdot \mathbf{p} \quad (\text{VI.138})$$

where  $A = \sqrt{1 - \frac{\lambda^2 p^2}{m^2}}$  with  $\lambda$  as an undetermined parameter.

$$\begin{aligned} UU^\dagger &= \left( A\beta + \frac{\lambda}{m}\boldsymbol{\alpha} \cdot \mathbf{p} \right) \left( A\beta + \frac{\lambda}{m}\boldsymbol{\alpha} \cdot \mathbf{p} \right) \\ &= A^2\beta^2\lambda\frac{A}{m}(\boldsymbol{\alpha} \cdot \mathbf{p}\beta + \beta\boldsymbol{\alpha} \cdot \mathbf{p}) + \frac{\lambda^2}{m^2}(\boldsymbol{\alpha} \cdot \mathbf{p})^2 \\ &= A^2\beta^2 + \frac{\lambda A p_i}{m} \left( \overbrace{\alpha_i\beta + \beta\alpha_i} \right) + \frac{\lambda^2}{m^2} p_i p_j \frac{1}{2} \left( \overbrace{\alpha_i\alpha_j + \alpha_j\alpha_i}^{\delta_{ij}} \right) \end{aligned} \quad (\text{VI.139})$$

$$= A^2 + \frac{\lambda^2 p^2}{m^2} \quad (\text{VI.140})$$

$$= 1 \quad (\text{VI.141})$$

Hence  $U$  is unitary. We have

$$T \begin{pmatrix} \chi \\ \eta \end{pmatrix} = H \begin{pmatrix} \chi \\ \eta \end{pmatrix} \quad (\text{VI.142})$$

$$UT \begin{pmatrix} \chi \\ \eta \end{pmatrix} UHU^{-1}U \begin{pmatrix} \chi \\ \eta \end{pmatrix} \quad (\text{VI.143})$$

$$T \begin{pmatrix} \chi' \\ \eta' \end{pmatrix} = H' \begin{pmatrix} \chi' \\ \eta' \end{pmatrix} \quad (\text{VI.144})$$

Note that we used  $T' = U(E - m)U^{-1} = T$  We now find  $H' = UHU^{-1}$

$$U(-m)U^{-1} = -m \quad (\text{VI.145})$$

We go on now

$$UV^0U^{-1} = AV^0A + \frac{\beta\lambda}{m}(AV^0\boldsymbol{\alpha} \cdot \mathbf{p} - \boldsymbol{\alpha} \cdot \mathbf{p}V^0A) + \frac{\lambda^2}{m^2}\boldsymbol{\alpha} \cdot \mathbf{p}V^0\boldsymbol{\alpha} \cdot \mathbf{p} \quad (\text{VI.146})$$

The third term is

$$U\boldsymbol{\alpha} \cdot (\mathbf{p} - \mathbf{V})U^{-1} = -A\boldsymbol{\alpha} \cdot (\mathbf{p} - \mathbf{V})A + \frac{\beta\lambda}{m}(A\boldsymbol{\alpha} \cdot (\mathbf{p} - \mathbf{V})\boldsymbol{\alpha} \cdot \mathbf{p}) \quad (\text{VI.147})$$

and the last term is

$$UmpU^{-1} = m\beta A^2 + 2\lambda A\boldsymbol{\alpha} \cdot \mathbf{p} - \beta\frac{\lambda^2 p^2}{2m^2} \quad (\text{VI.148})$$

Remember our goal is to limit off-diagonal terms. To lowest order the off-diagonal terms all come from the  $\boldsymbol{\alpha} \cdot (\mathbf{p} - \mathbf{V})$  term.

$$H'_{off-diag} = -\boldsymbol{\alpha} \cdot (\mathbf{p} - \mathbf{V}) + 2\lambda\boldsymbol{\alpha} \cdot \mathbf{p} \quad (\text{VI.149})$$

We now tune  $\lambda$  to  $\lambda = \frac{1}{2}$ . Our new off diagonal part of the Hamiltonian is

$$H'_{off-diag} = \boldsymbol{\alpha} \cdot \mathbf{V} \quad (\text{VI.150})$$

The coupled equations become

$$T\chi' = H'_{11}\chi + \boldsymbol{\alpha} \cdot \mathbf{V}\eta' \quad (\text{VI.151})$$

$$T\eta' = \boldsymbol{\sigma} \cdot \mathbf{V}\chi' - 2m\eta' \quad (\text{VI.152})$$

The key step is to say that  $T\eta'$  is must smaller then  $2m\eta'$  (since we are in the nonrelativistic limit). This allows us to write

$$\eta' = \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{2m}\chi' \quad (\text{VI.153})$$

We have decoupled these equations to some order. The error we are making is higher-order in  $\frac{|\mathbf{p}|}{m}$ . Now the equations are decoupled and we have one equation:

$$T\chi' = H'_{11}\chi' + \frac{\boldsymbol{\sigma} \cdot \mathbf{V}\boldsymbol{\sigma} \cdot \mathbf{V}}{2m}\chi' \quad (\text{VI.154})$$

where

$$H'_{11} = V^0 - \frac{p^2}{8m^2}V^0 - V^0\frac{p^2}{8m^2} + \frac{\boldsymbol{\sigma} \cdot \mathbf{p}V^0\boldsymbol{\sigma} \cdot \mathbf{p}}{4m^2} + \frac{1}{2m}(\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V}\boldsymbol{\sigma} \cdot \mathbf{p}) + \boldsymbol{\sigma} \cdot \mathbf{p}\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V})) - \frac{p^4}{8m^3} - \frac{p^2}{2m} \quad (\text{VI.155})$$

One can simplify this equation and you find that (and we put  $e\phi = V^0$  and  $e\mathbf{A} = \mathbf{V}$ )

$$H'_{11} + \frac{V^2}{2m} = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + e\phi - \frac{e}{2m}\boldsymbol{\sigma} \cdot \mathbf{B} - \frac{p^4}{8m^3} + e\frac{(\nabla^2\phi)}{8m^2} + \frac{e}{8m^2}\boldsymbol{\sigma} \cdot ([\nabla\phi] \times \mathbf{p}) \quad (\text{VI.156})$$

Lecture 25 - March 21st, 2012

Recall we are doing the non-relativistic reduction of the Dirac equation. However we are not doing a full reduction as we are keeping important relativistic effects. We are doing it systematically so that we keep all relativistic effects to some order in  $\frac{|\mathbf{p}|}{m}$ . Foldy-Wootherhuysen shows how you to do this in general. We will just do this to lowest order. However in practice for hydrogen our results will be highly accurate, namely up to  $\alpha^4$ .

Recall we were taking the Dirac equation and applying a unitary transformation

$$U = A\beta + \frac{\lambda}{m}\boldsymbol{\alpha} \cdot \mathbf{p} \quad , \quad (\text{VI.157})$$

where  $A = \sqrt{1 - \frac{\lambda^2 p^2}{m^2}}$ . This transformation let us to this coupled system

$$T\chi' = H'_{11}\chi' + \boldsymbol{\sigma} \cdot \mathbf{V}\eta' \quad (\text{VI.158})$$

$$T\eta' = \boldsymbol{\sigma} \cdot \mathbf{V}\chi' - 2m\eta' \quad (\text{VI.159})$$

If we have  $T \ll 2m$  then

$$T\chi' = H'_{11}\chi' + \frac{\boldsymbol{\sigma} \cdot \mathbf{V}\boldsymbol{\sigma} \cdot \mathbf{V}}{2m}\chi' \quad , \quad (\text{VI.160})$$

where

$$H'_{11} = V^0 - \frac{p^2}{8m^2}V^0 - V^0\frac{p^2}{8m^2} + \frac{\boldsymbol{\sigma} \cdot \mathbf{p}V^0\boldsymbol{\sigma} \cdot \mathbf{p}}{4m^2} + \frac{1}{2m}(\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V}(\boldsymbol{\sigma} \cdot \mathbf{p})) + \boldsymbol{\sigma} \cdot \mathbf{p}\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V})) - \frac{p^4}{8m^3} - \frac{p^2}{2m} \quad (\text{VI.161})$$

We simplify this term by term

$$\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V})\boldsymbol{\sigma} \cdot \mathbf{p} + \boldsymbol{\sigma} \cdot \mathbf{p}(\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V})) = 2p^2 - \boldsymbol{\sigma} \cdot \mathbf{p}\boldsymbol{\sigma} \cdot \mathbf{V} - \boldsymbol{\sigma} \cdot \mathbf{V}\boldsymbol{\sigma} \cdot \mathbf{p} \quad (\text{VI.162})$$

$$= 2p^2 - \mathbf{p} \cdot \mathbf{V} - \mathbf{V} \cdot \mathbf{p} - i\boldsymbol{\sigma} \cdot (\mathbf{p} \times \mathbf{V}) - i\boldsymbol{\sigma} \cdot (\mathbf{V} \times \mathbf{p}) \quad (\text{VI.163})$$

$$= (\mathbf{p} - \mathbf{V})^2 + p^2 - V^2 - \boldsymbol{\sigma} \cdot [\nabla \times \mathbf{V}] \quad (\text{VI.164})$$

where we have used  $\mathbf{A} \times \mathbf{B} = \epsilon_{ijk}A_jB_k$  and square brackets, [ ] means that the operators inside act only inside. Our potential could have been any vector potential. We note choose the electromagnetic force:

$$\mathbf{V} = e\mathbf{A} \quad (\text{VI.165})$$

This gives (with  $\mathbf{B} = \nabla \times \mathbf{A}$ )

$$\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V}) \boldsymbol{\sigma} \cdot \mathbf{p} + \boldsymbol{\sigma} \cdot \mathbf{p} (\boldsymbol{\sigma} \cdot (\mathbf{p} - \mathbf{V})) = (\mathbf{p} - \mathbf{V})^2 + p^2 - V^2 - e\boldsymbol{\sigma} \cdot \mathbf{B} \quad (\text{VI.166})$$

This shows you that the electric interacts with the magnetic field with the expression  $e\boldsymbol{\sigma} \cdot \mathbf{B}$ ! Thus this actually predicts that the electron has a magnetic moment. Continuouing with the reduction we have

$$p^2 V^0 + V^0 p^2 = [p^0 V^0] + 2 [\mathbf{p} B^0] \cdot \mathbf{p} + 2V^0 p^2 \quad (\text{VI.167})$$

and

$$\boldsymbol{\sigma} \cdot \mathbf{p} V^0 \boldsymbol{\sigma} \cdot \mathbf{p} = \boldsymbol{\sigma} \cdot [\mathbf{p} V^0] \boldsymbol{\sigma} \cdot \mathbf{p} + V^0 p^2 \quad (\text{VI.168})$$

$$= \boldsymbol{\sigma} \cdot [\mathbf{p} V^0] \boldsymbol{\sigma} \cdot \mathbf{p} + V^0 p^2 \quad (\text{VI.169})$$

$$= [\mathbf{p} V^0] \mathbf{p} + i\boldsymbol{\sigma} \cdot ([\mathbf{p} V^0] \times \mathbf{p}) + V^0 p^2 \quad (\text{VI.170})$$

so we see that

$$-\frac{1}{8m^2} (p^2 V^0 + V^0 p^2) + \frac{\boldsymbol{\sigma} \cdot \mathbf{p} V^0 \boldsymbol{\sigma} \cdot \mathbf{p}}{4m^2} = -\frac{[p^2 V^0]}{8m} + \frac{i\boldsymbol{\sigma} \cdot ([\mathbf{p} V^0] \times \mathbf{p})}{4m^2} \quad (\text{VI.171})$$

If we now input in

$$\mathbf{p} = -i\nabla$$

$$\mathbf{V} = e\mathbf{A}$$

$$V^0 = e\phi$$

then we have

$$H'_{11} + \frac{V^2}{2m} = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + e\phi - \frac{e}{2m} \boldsymbol{\sigma} \cdot \mathbf{B} - \frac{p^4}{8m^3} + e \frac{[\nabla^2 \phi]}{8m^2} + \frac{e}{8m^2} \boldsymbol{\sigma} \cdot ([\nabla \phi] \times \mathbf{p}) \quad (\text{VI.172})$$

if we assume that  $\phi$  is spherically symmetric then we have  $\phi = \phi(r)$  and thus  $\nabla \phi = \frac{\mathbf{r}}{r} \frac{d\phi}{dr}$  then we finally have

$$H_{11} = \overbrace{\frac{(\mathbf{p} - e\mathbf{A})^2}{2m}}^{(1)} + \overbrace{e\phi}^{(2)} - \overbrace{\frac{p^4}{8m^3}}^{(1)} - \overbrace{\frac{e}{2m} \boldsymbol{\sigma} \cdot \mathbf{B}}^{(4)} + e \overbrace{\frac{[\nabla^2 \phi]}{8m^2}}^{(5)} + \overbrace{\frac{3}{4m^2 r} \frac{d\phi}{dr} \boldsymbol{\sigma} \cdot \mathbf{L}}^{(6)} \quad (\text{VI.173})$$

The first term can be rearranged: (we assume that  $A^2$  is small)

$$\frac{(\mathbf{p} - e\mathbf{A})^2}{2m} = \frac{p^2}{2m} - \frac{e}{2m} (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) \quad (\text{VI.174})$$

$$= \frac{p^2}{2m} + \frac{ie}{2m} (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) \quad (\text{VI.175})$$

$$= \frac{p^2}{2m} + \frac{ie}{m} \mathbf{A} \cdot \nabla \quad (\text{VI.176})$$

$$= \frac{p^2}{2m} - \frac{ie}{2m} (\mathbf{r} \times \mathbf{B}) \cdot \nabla \quad (\text{VI.177})$$

$$= \frac{p^2}{2m} + \frac{ie}{2m} \mathbf{B} \cdot (\mathbf{r} \times \nabla) \quad (\text{VI.178})$$

$$= \frac{p^2}{2m} - \frac{e}{2m} \mathbf{B} \cdot \mathbf{L} \quad (\text{VI.179})$$

$\frac{p^2}{2m}$  is the kinetic energy and  $\frac{e}{2m} \mathbf{B} \cdot \mathbf{L}$  is the Zeeman term. Thus we have obtains a field-orbit coupling term without explicitly putting it in again! Now consider the second term. This is the non-relativistic potential. This is just the Coloumb potential for hydrogen

$$e\phi = -\frac{e^2}{r} \quad (\text{VI.180})$$

The third term

$$\frac{p^4}{8m^3} \quad (\text{VI.181})$$

is just the next order relativistic correction to the kinetic energy. Now consider the fourth term:

$$-\frac{e}{2m} \boldsymbol{\sigma} \cdot \mathbf{B} = -\frac{e}{m} \mathbf{S} \cdot \mathbf{B} \quad (\text{VI.182})$$

$$= -\frac{e}{m} \mathbf{S} \cdot \mathbf{B} \quad (\text{VI.183})$$

This is a prediction that the gyromagnetic ratio of the electron is equal to 2 ( $g = 2$ )! The full Zeeman effect can be written  $-\frac{e}{2m} \mathbf{B} \cdot (\mathbf{L} + 2\mathbf{S})$ . Now consider the fifth term:

$$e \frac{[\nabla^2 \phi^2]}{8m^2} = -\frac{e^2}{8m^2} \nabla \cdot \mathbf{E} \quad (\text{VI.184})$$

$$= -\frac{e^2}{8m} \delta(\mathbf{R}) \quad (\text{VI.185})$$

(with  $\phi = -\frac{e^2}{r}$ ). This term is called “Zetterbeuwegung”. The sixth term is

$$\frac{e}{4m^2 r} \frac{d\phi}{dr} \mathbf{S} \cdot \mathbf{L} \quad (\text{VI.186})$$

This is spin-orbit coupling which is because the electron sees  $(\phi, 0, 0, 0) \xrightarrow{LT} (\phi', \mathbf{A}')$  under a Lorentz transformation.

Lecture 26 - March 23rd, 2012  
Missed this lecture.

Lecture 27 - March 25th, 2012

## B. Covariance of the Dirac equation

We are trying to prove that

$$\{\gamma^\mu (p_\mu - eA_\mu) - m\} \psi = 0 \quad (\text{VI.187})$$

$$\Rightarrow \{\gamma^\mu (p'_\mu - eA'_\mu) - m\} \psi' = 0 \quad (\text{VI.188})$$

Contravariant vectors transform as

$$p'^\mu = \Lambda^\mu_\nu p^\nu \quad (\text{VI.189})$$

and the covariant vectors transform as

$$p'_\mu = (\Lambda^{-1})^\mu_\nu p_\nu \quad (\text{VI.190})$$

We have

$$p^2 = p'^\mu p'_\mu = p^\mu p_\mu \quad (\text{VI.191})$$

We insert in

$$\psi' = S\psi \quad (\text{VI.192})$$

$S$  is the spinor representation of the Lorentz group. After inserting  $\Lambda$  and  $S$  into preed equation we get

$$S^{-1}(\Lambda) \gamma^\mu S(\Lambda) = \Lambda^\mu_\nu \gamma^\nu \quad (\text{VI.193})$$

For Lie groups, to find the generators we only have to satisfy this equation to infinitesimal order and then its true to all orders

$$\Lambda = 1 + \epsilon_i \omega_{i0} + \frac{1}{2} \theta_i \epsilon_{ijk} \omega_{jk} \quad (\text{VI.194})$$

we have 6 parameters  $(\epsilon_i, \theta_i)$  and 6 generators  $\omega_{i0}, \omega_{jk}$  (note these are NOT indices but labels!). Whatever  $S(\Lambda)$  is in infinitesimal form it will look like

$$S(\Lambda) = 1 + \epsilon_i B_i + \frac{1}{2} \theta_i \epsilon_{ijk} R_{jk} \quad (\text{VI.195})$$

where  $\epsilon_i$  and  $\epsilon_{ijk}$  are the same parameters as for  $\Lambda$ . At this point we don't know what the generators of the spinor representation are,  $B_i, R_{jk}$ . We insert infinitesimal forms into  $S^{-1} \gamma^\mu S = \Lambda_\nu^\mu \gamma^\nu$ . Last time we finished class at (he left this as an exercise)

$$- [B_i, \gamma^\mu] = (\omega_{i0})_\nu^\mu \gamma^\nu \quad (\text{VI.196})$$

$$- [R_{jk}, \gamma^\mu] = (\omega_{jk})_\nu^\mu \gamma^\nu \quad (\text{VI.197})$$

The new exercise is to verify that

$$B_i = \frac{1}{2} \gamma^0 \gamma^i \leftarrow \text{Boosts} \quad (\text{VI.198})$$

$$R_{jk} = \frac{1}{2} \gamma^j \gamma^k \leftarrow \text{Rotations} \quad (\text{VI.199})$$

This appears non-covariant. This can be written in covariant form

$$\sigma^{\mu\nu} = \frac{i}{2} [\gamma^\mu, \gamma^\nu] \quad (\text{VI.200})$$

where  $\sigma^{0i} = 2iB_i$  and  $\sigma^{ij} = 2iR_{ij}$  (these are not the Pauli matrices! We are just using  $\sigma$  as some matrix). Note however that this is not a convenient form of the generators.  $B_i$  are the generators of boosts for spinors and  $R_{jk}$  are the generators for rotations for spinors. Let's introduce some more notation.

$$\Sigma_j \equiv \sigma_j = \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix} \quad (\text{VI.201})$$

and

$$\gamma^5 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{VI.202})$$

We now have (using the  $\alpha$  matrix we had before)

$$B_i = \frac{1}{2} \alpha_i \quad (\text{VI.203})$$

$$R_{jk} = \frac{i}{2} \epsilon_{jkl} \gamma^5 \alpha_\ell \quad (\text{VI.204})$$

A boost in Dirac-space is

$$S(\Lambda_\xi) = 1 + \frac{\xi \cdot \boldsymbol{\alpha}}{2} + \frac{1}{2} \left( \frac{\xi \cdot \boldsymbol{\alpha}}{2} \right)^2 + \dots \quad (\text{VI.205})$$

$$= \cosh \left( \frac{\xi}{2} \right) + \hat{\xi} \cdot \boldsymbol{\alpha} \sinh \left( \frac{\xi}{2} \right) \quad (\text{VI.206})$$

$$\quad (\text{VI.207})$$

where  $\xi$  is the rapidity,  $\tanh(\xi) = \frac{v}{c}$ ,  $\frac{E}{m} = \cosh(\xi)$ ,  $\cosh(\frac{\xi}{2}) = \sqrt{\frac{E+m}{2m}}$ , and  $\sinh(\frac{\xi}{2}) = \sqrt{\frac{E+m}{2m}} \left( \frac{p}{E+m} \right)$ . For a spinor at rest we have

$$\psi_{0,s}(x) = \frac{e^{-imt}}{\sqrt{L^3}} \begin{pmatrix} \chi^s \\ 0 \end{pmatrix} = \frac{e^{-imt}}{\sqrt{2mL^3}} u(0, s) \quad (\text{VI.208})$$



remember that

$$\boldsymbol{\alpha} \equiv \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad (\text{VI.209})$$

and therefore

$$\cosh \frac{\xi}{2} + \hat{\xi} \cdot \boldsymbol{\alpha} \sinh \frac{\xi}{2} = \begin{pmatrix} \cosh \frac{\xi}{2} & \hat{\xi} \cdot \boldsymbol{\alpha} \sinh \frac{\xi}{2} \\ \hat{\xi} \cdot \boldsymbol{\alpha} \sinh \frac{\xi}{2} & \cosh \frac{\xi}{2} \end{pmatrix} \quad (\text{VI.210})$$

Lets apply  $S(\Lambda_\xi)$  to  $\begin{pmatrix} X^s \\ 0 \end{pmatrix}$ .

$$S(\Lambda_\xi) \begin{pmatrix} X^s \\ 0 \end{pmatrix} = \left\{ \cosh \left( \frac{\xi}{2} \right) + \hat{\xi} \cdot \boldsymbol{\alpha} \sinh \left( \frac{\xi}{2} \right) \right\} \begin{pmatrix} X^s \\ 0 \end{pmatrix} \quad (\text{VI.211})$$

$$= \begin{pmatrix} \cosh \left( \frac{\xi}{2} \right) X^s \\ \sinh \frac{\xi}{2} \boldsymbol{\sigma} \cdot \hat{\xi} \chi^s \end{pmatrix} \quad (\text{VI.212})$$

$$= \sqrt{\frac{E+m}{2m}} \begin{pmatrix} 1 \\ \hat{\xi} \cdot \boldsymbol{\sigma} \left( \frac{\mathbf{p}}{E+m} \right) \end{pmatrix} \chi^s \quad (\text{VI.213})$$

$$= \sqrt{\frac{E+m}{2m}} \begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{E+m} \end{pmatrix} \chi^s \quad (\text{VI.214})$$

we have retrieved that solutions for arbitrary momentum. Now consider rotations in Dirac space.

$$S(\Lambda_\theta) = e^{-(i/2)\boldsymbol{\gamma}^5 \boldsymbol{\theta} \cdot \boldsymbol{\alpha}} \quad (\text{VI.215})$$

$$= \cos \frac{\theta}{2} - i\boldsymbol{\gamma}^5 \hat{\boldsymbol{\theta}} \cdot \boldsymbol{\alpha} \sin \frac{\theta}{2} \quad (\text{VI.216})$$

Consider the rotation below

$$S(\Lambda_\theta)u(\mathbf{p}, s) \quad (\text{VI.217})$$

Recall from our study of  $SU(2)$  we know how Pauli spinors transform under rotations.

$$\chi^{s'} = S(\theta)\chi^s = \left( \cos \frac{\theta}{2} - i\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\theta}} \sin \frac{\theta}{2} \right) \chi^s \quad (\text{VI.218})$$

Let's pick to rotate about the  $\hat{z}$  axis. Back to our rotation in Dirac space we have

$$S(\Lambda_\theta)u(\mathbf{p}, s) = \sqrt{E+m} \begin{pmatrix} 1 \\ \frac{S(\theta)\boldsymbol{\sigma} \cdot \mathbf{p} S^\dagger(\theta)}{E+m} \end{pmatrix} \chi^{s'} \quad (\text{VI.219})$$

(check this at home) where if we are specializing to rotations in the  $z$  axis we have

$$S(\theta) = \cos \frac{\theta}{2} + i\sigma_z \sin \frac{\theta}{2} \quad (\text{VI.220})$$

To simplify  $S(\Lambda_\theta)u(\mathbf{p}, s)$  we need to simplify the following

$$S(\theta)\boldsymbol{\sigma} \cdot \mathbf{p} S^\dagger(\theta) = \left( \cos \frac{\theta}{2} - i\sigma_z \sin \frac{\theta}{2} \right) \boldsymbol{\sigma} \cdot \mathbf{p} \left( \cos \frac{\theta}{2} + \sigma_z \sin \frac{\theta}{2} \right) \quad (\text{VI.221})$$

$$= \cos^2 \frac{\theta}{2} \boldsymbol{\sigma} \cdot \mathbf{p} - i \sin \frac{\theta}{2} \cos \frac{\theta}{2} (\sigma_z \boldsymbol{\sigma} \cdot \mathbf{p} - \boldsymbol{\sigma} \cdot \mathbf{p} \sigma_z) + \sin^2 \frac{\theta}{2} \sigma_z \boldsymbol{\sigma} \cdot \mathbf{p} \sigma_z \quad (\text{VI.222})$$

$$= \boldsymbol{\sigma} \cdot \mathbf{p}' \quad (\text{VI.223})$$

where  $\mathbf{p}' = (p_z \cos \theta - p_y \sin \theta, p_y \cos \theta + p_x \sin \theta, p_z)$ . Note that we skipped about a half page of steps in the last step. This is also left as an exercise.

Lecture 28 - March 28th, 2012

For the test:

- Some qualitative questions
- In accidental degeneracy prove some commutation relation or identities
  - Nothing too long, but take a good look at the assignment with  $\mathbf{M}$
- Short-ish proofs from the Dirac equation, similar to as done in the notes
- Formula sheet will be posted

## VII. HYDROGEN

One can obtain exact solutions to the hydrogen Dirac problem. The Dirac equation takes the form

$$\left[ \gamma^\mu \left( i \frac{\partial}{\partial x^\mu} - e A_\mu \right) - \mu \right] \psi = 0 \quad (\text{VII.1})$$

where  $A_\mu = (e\phi, \mathbf{0})$  with  $eA_\mu = \frac{-e^2}{r}$ . We have chosen the rest frame of the proton. It no longer looks covariant. That's okay as long as you stay in that frame. In this case the Dirac equation becomes (exercise) (where we have used  $\beta = \gamma^0$  and  $\beta^2 = I$ ).

$$E\psi = \left[ -i\alpha_i \frac{\partial}{\partial x^i} + \beta m - \frac{e^2}{r} \right] \psi \quad (\text{VII.2})$$

One should ask where is the time dependence? It is in  $\gamma^0 i \frac{\partial}{\partial t}$ .  $V = V(\mathbf{r})$ , thus just like the Schrodinger equation

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-iEt/\hbar} \quad (\text{VII.3})$$

The time dependence in the wave function is just a phase rotation ( $\psi^\dagger \psi$  doesn't change with time). Derivative term just gives the energy term on the left, where  $E$  is the constant (an eigenvalue). Now we have

$$\begin{aligned} \mathbf{L} &= \mathbf{r} \times \mathbf{p} = -i\hbar (\mathbf{r} \times \nabla) \\ \mathbf{S} &= \frac{1}{2} \gamma^5 \boldsymbol{\alpha} \end{aligned}$$

$$[L^i, H] = [-i\epsilon_{ijk} r_j \partial_k, -i\alpha_\ell \partial_\ell] = \epsilon_{ijk} \alpha_j \partial_k \neq 0 \quad (\text{VII.4})$$

This is another exercise. Note that one should memorize  $L^i = -i\epsilon_{ijk} r_j \partial_k$ , useful expression. That means that  $\mathbf{L}$  is **not** conserved! ( $\mathbf{L}$  is not a good quantum number).

$$[S^i, H] = \frac{1}{2} [\gamma^5 c \alpha_i, -i\alpha_j \partial_j] = -\epsilon_{ijk} \alpha_j \partial_k \neq 0 \quad (\text{VII.5})$$

(exercise) This is bad news! We lost all our good quantum numbers. However the good news is that the commutator

$$[L^i + S^i, H] = 0 \quad (\text{VII.6})$$

Hence the total angular momentum is conserved.  $\mathbf{J}$  is a good quantum number.

$$S^2 = S^i S^i = \frac{1}{4} \boldsymbol{\alpha} \cdot \boldsymbol{\alpha} = \frac{3}{4} \quad (\text{VII.7})$$

( The magnitude of  $|\mathbf{S}|$  is constant. This tells us we can label states by good quantum numbers,  $J^2, J_z, S^2, L^2$ . All these operators commute with  $H$  and therefore we can have simultaneous eigenfunctions of  $J^2, J_z, S^2, L^2$ . Now we write the 4-spinor as

$$\psi(\mathbf{r}) = \begin{pmatrix} F(\mathbf{r}) \\ G(\mathbf{r}) \end{pmatrix} \quad (\text{VII.8})$$

We introduce the following new object  $y_{jm}(\hat{r})$ .

$$y_{jm}(\mathbf{r}) = \left\langle \ell, m - \frac{1}{2} \right| \otimes \left\langle \frac{1}{2}, \frac{1}{2} \right| \otimes |j, m\rangle Y_{\ell, m - \frac{1}{2}} \uparrow + \left\langle \ell, m + \frac{1}{2} \right| \otimes \left\langle \frac{1}{2}, -\frac{1}{2} \right| \otimes |j, m\rangle Y_{\ell, m + \frac{1}{2}}(\mathbf{r}) \downarrow \quad (\text{VII.9})$$

Equivalently one often uses the notation:

$$y_{jm}(\mathbf{r}) = \left\langle \ell, m - \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right| j, m \rangle Y_{\ell, m - \frac{1}{2}} \uparrow + \left\langle \ell, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right| j, m \rangle Y_{\ell, m + \frac{1}{2}}(\mathbf{r}) \downarrow \quad (\text{VII.10})$$

These are just the Clebsh-Gordan coefficients. It is useful to define an operator,

$$K = (\boldsymbol{\sigma} \cdot \mathbf{L} + 1) \quad (\text{VII.11})$$

since

$$K_{\ell, m}^{\pm} = \pm k y_{j, m}^{\pm} \quad (\text{VII.12})$$

where

$$k = \begin{cases} j + \frac{1}{2} & \text{if } j = \ell - \frac{1}{2} \\ -(j + \frac{1}{2}) & \text{if } j = \ell + \frac{1}{2} \end{cases} \quad (\text{VII.13})$$

We can write the solution as

$$\psi_{j, m}^k(\mathbf{r}) = \begin{pmatrix} f_j^k(r) y_{j, m}^k(\hat{r}) \\ i g_i^k(r) y_{j, m}^{-k}(\hat{r}) \end{pmatrix} \quad (\text{VII.14})$$

Note that this needs to be verified. At this point we have solved the angular problem. This is equivalent to  $\psi(\mathbf{r}) = R(r)Y_{\ell, m}(\theta, \phi)$  but **not** the radial problem. Notice the angular part is solved with the familiar spherical harmonics.

Lecture 29 - March 30th, 2012

To check this solutions we need the following simplifications to our expressions (prove these)

$$-i\boldsymbol{\sigma} \cdot \nabla = -i\boldsymbol{\alpha} \cdot \hat{r} \frac{\partial}{\partial r} + i\boldsymbol{\sigma} \cdot \hat{r} \frac{\boldsymbol{\sigma} \cdot \mathbf{L}}{r} \quad (\text{VII.15})$$

$$\boldsymbol{\sigma} \cdot \mathbf{L} y_{j, m}^k(\hat{r}) = -(k+1) y_{j, m}^k(\hat{r}) \quad (\text{VII.16})$$

$$\boldsymbol{\sigma} \cdot \hat{r} y_{j, m}^k(\hat{r}) = y_{j, m}^{-k}(\hat{r}) \quad (\text{VII.17})$$

$$-i\boldsymbol{\sigma} \cdot \nabla y_{j, m}^k(\hat{r}) = i \frac{\partial y_{j, m}^{-k}(\hat{r})}{\partial r} + i \frac{(k+1)}{r} y_{j, m}^{-k}(\hat{r}) \quad (\text{VII.18})$$

Separation of variables is successful and we find find two coupled linear 1st order homogenous equations

$$E f^k(r) = \left( m - \frac{e^2}{r} \right) f^k(r) - \frac{g^k(r)}{dr} - \frac{1-k}{r} g^k(r) \quad (\text{VII.19})$$

$$E g^k(r) = \left( -m - \frac{e^2}{r} \right) g^k(r) + \frac{df^k(r)}{dr} + \frac{1+k}{r} f^k(r) \quad (\text{VII.20})$$

To solve these solutions we rescale our solutions (just as in the S.E. solutions)

$$\begin{aligned} f_R &= \frac{f}{r}, & g_R &= \frac{g}{r} \\ \rho &= \sqrt{m^2 - E^2} r \\ \epsilon &= \sqrt{\frac{m-E}{m+E}} \end{aligned}$$

In natural units we call  $e^2 = \alpha$ . This gives two equations:

$$\frac{df_R}{d\rho} + \frac{k}{\rho} f_R - \left( \frac{1}{\epsilon} + \frac{\alpha}{\rho} \right) g_R = 0 \quad (\text{VII.21})$$

$$\frac{dg_R}{d\rho} - \frac{k}{\rho} g_R - \left( \epsilon - \frac{e^2}{\rho} \right) f_R = 0 \quad (\text{VII.22})$$

We solve with a power series:

$$f_R = \rho^\nu \sum_{n=0}^{\infty} A_n \rho^n e^{-\rho} \quad (\text{VII.23})$$

$$g_R = \rho^\nu \sum_{n=0}^{\infty} B_n \rho^n e^{-\rho} \quad (\text{VII.24})$$

Substitute forms in. There is a non trivial solution if  $\nu = \sqrt{k^2 - m^2}$ . These differential equations have a continuous set of solutions. However to enforce normalizability we must force the solutions to terminate the infinite series so that solutions are well behaved. This discrete subset are our physical solutions. We can force termination by demanding

$$2\nu + 2N - \frac{\alpha}{\epsilon} (1 - \epsilon^2) = 0 \quad (\text{VII.25})$$

where  $N$  is an integer. As always this is where the quantization of  $E$  comes from (comes from the quantization of  $\epsilon$ ). Amazingly one can solve this problem in terms of confluent hypergeometric function.

$$E_{n,j} = m \left[ 1 - \frac{\alpha^2}{n^2 + 2(n - (j + \frac{1}{2})) \left( \sqrt{(j + \frac{1}{2})^2 - \alpha^2} - (j + \frac{1}{2}) \right)} \right]^{1/2} \quad (\text{VII.26})$$

where we have now translated from  $k \rightarrow j$ . We can expand terms of  $\alpha$  (since in Hydrogen  $\frac{p}{m}$  is of order  $\alpha$ ,  $\frac{p}{m} \tilde{\alpha}$ ).

$$E_{n,j} = m - \frac{m\alpha^2}{2n^2} - \frac{m\alpha^4}{2n^4} \left( \frac{n}{n + \frac{1}{2}} - \frac{3}{4} \right) \quad (\text{VII.27})$$

Note that we have lost a lot of our degeneracies. What about real hydrogen? there also have a proton with a spin,



. This produces a magnetic moment,

$$\boldsymbol{\mu} = \frac{ge}{2m} \mathbf{S} \quad (\text{VII.28})$$

This creates a spin-spin interaction which splits the  $1S_{1/2}$  state into two states. The triplet and single states. This is the famous  $21cm$  line. The energy difference is very simple and its given by

$$E = m\sqrt{1 - \alpha^2} \quad (\text{VII.29})$$

This is exact in the Dirac equation. The  $1s_{1/2}$  state from the Dirac equation is

$$\psi_{\frac{1}{2}, s=+\frac{1}{2}} = A_0 \rho^{\gamma-1} e^{-\rho} \begin{pmatrix} 1 \\ 0 \\ -\frac{1-\gamma}{\alpha} \cos \theta \\ -\frac{1-\gamma}{\alpha} \sin \theta e^{i\phi} \end{pmatrix} \quad (\text{VII.30})$$

where  $\gamma = (1 - \alpha^2)^{1/2}$ . Notice that even the ground state has angular dependence! We also have

$$\psi_{\frac{1}{2}, s=-\frac{1}{2}} = A_0 \rho^{\gamma-1} e^{-\rho} \begin{pmatrix} 0 \\ 1 \\ -\frac{1-\gamma}{\alpha} \sin e^{-i\phi} \\ -\frac{1-\gamma}{\alpha} \cos \theta \end{pmatrix} \quad (\text{VII.31})$$

We can write this in more convenient notation:

$$\begin{pmatrix} \cos \theta \\ \sin \theta e^{i\phi} \end{pmatrix} = \frac{\hat{z}}{\hat{x} + i\hat{y}} \quad (\text{VII.32})$$

and

$$\boldsymbol{\sigma} \cdot \mathbf{r} = \begin{pmatrix} \hat{z} & \hat{x} - i\hat{y} \\ \hat{x} + i\hat{y} & -\hat{z} \end{pmatrix} \quad (\text{VII.33})$$

Hence

$$\boldsymbol{\sigma} \cdot \hat{\mathbf{r}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \theta \\ \sin e^{i\phi} \end{pmatrix} \quad (\text{VII.34})$$

This gives

$$\psi_{\frac{1}{2}, s=\frac{1}{2}} = A_0 \rho^{\gamma-1} e^{-\rho} \left( \boldsymbol{\sigma} \cdot \hat{\mathbf{r}} \left( \frac{1-\gamma}{\alpha} \right) \chi^{1/2} \right) \quad (\text{VII.35})$$