Theoretical Physics
Prof. Ruiz, UNC Asheville, doctorphys on YouTube
Chapter L Notes. The Dirac Equation

L1. Review of Spin and the Pauli Equation.

Sophus Lie (1842-1899)
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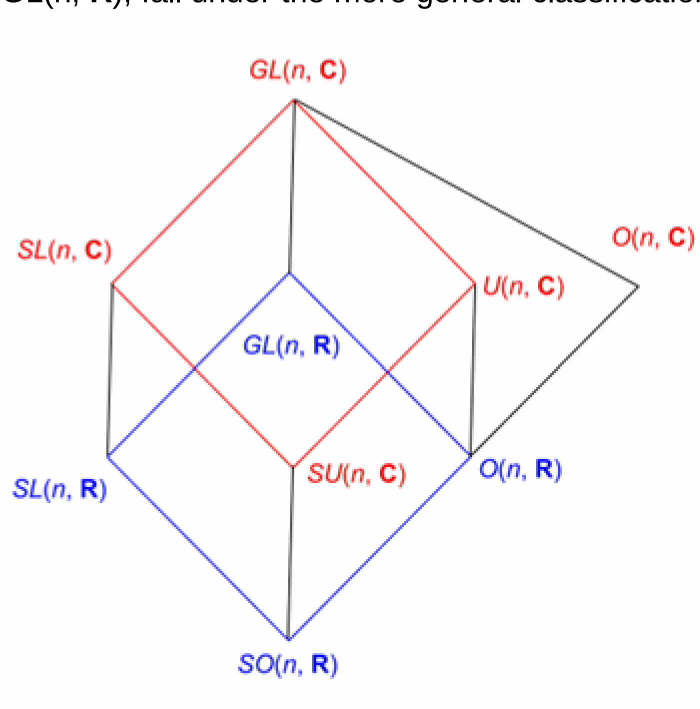
The groups we have studied so far are subgroups of the general linear group of n x n matrices over the complex field: GL(n,**C**).

The groups are linear because matrices act on vectors as linear operators. A linear matrix operator A acts on vectors u and v as follows

$$A(\alpha u + \beta v) = \alpha A u + \beta A v \,,$$

where the α and β are scalars (in this case complex numbers). Since real numbers and complex numbers are continuous, GL(n, **C**) and GL(n, **R**), fall under the more general classification of Lie groups.



Lie Algebras:

$$\left[L_j, L_k\right] = i\hbar \varepsilon_{jkl} L_l$$

$$\left[\sigma_j, \sigma_k\right] = 2i \varepsilon_{jkl} \sigma_l$$

These relate to the Lie groups.

This leads to the spin operators of the electron.

$$\left[\frac{\hbar\sigma_j}{2}, \frac{\hbar\sigma_k}{2}\right] = i\hbar \varepsilon_{jkl} \frac{\hbar\sigma_l}{2}$$

Let's review incorporating spin by hand to arrive at the Pauli equation.

We have seen Schrödinger equation in one dimension.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=i\hbar\frac{\partial\psi}{\partial t}$$

If the potential energy does not depend on time, then we have seen the solution has the general form $\psi(x,t)=\psi(x)e^{-i\omega t}$ with

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x).$$

Remember that $E=\hbar\omega$ and we call also write

$$\psi(x,t)=\psi(x)e^{-iEt/\hbar}.$$

We have seen that the Pauli equation is arrived at by replacing the Schrödinger wave function with a spinor wave function.

$$-\frac{\hbar^2}{2m}\nabla^2\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}+V\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}=E\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$$

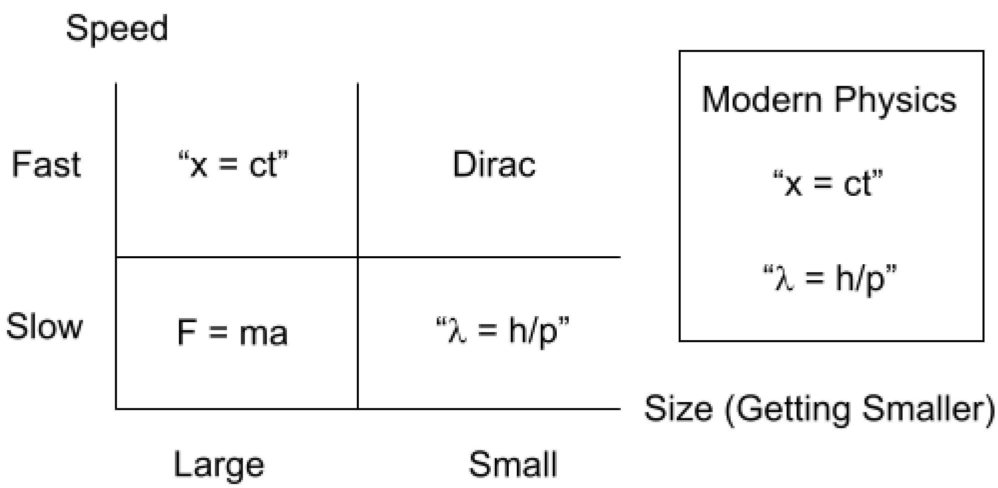
We can also write this out explicitly showing the matrix operators:

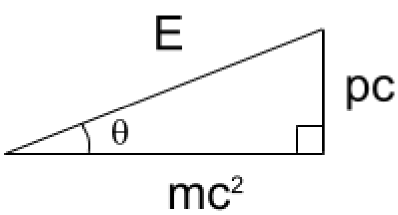
$$-\frac{\hbar^2}{2m}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\frac{d^2}{dx^2}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}+\begin{bmatrix}V_{11} & V_{12}\\ V_{21} & V_{22}\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}=E\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$$

In general, V is a 2 x 2 Hermitian matrix.

L2. The Klein-Gordon Equation.

We are in search of an equation for the fast and small. This equation will have both "c" and "h" in it.





$$E^2 = m^2c^4 + p^2c^2$$

Recall our prescriptions

$$E \rightarrow i\hbar\frac{\partial}{\partial t} \quad \text{and} \quad \vec{p} \rightarrow -i\hbar\nabla ,$$

which some like to write as

$$E \rightarrow i\hbar\frac{\partial}{\partial t} \quad \text{and} \quad \vec{p} \rightarrow \frac{\hbar}{i}\nabla .$$

Then $\left[\frac{p^2}{2m} + V\right]\psi = E\psi$ gives the non-relativistic Schrödinger equation.

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Let's use $E \rightarrow i\hbar \dfrac{\partial}{\partial t}$ and $\vec{p} \rightarrow \dfrac{\hbar}{i} \nabla$ with the relativistic energy equation

$E^2 = m^2c^4 + p^2c^2$ instead of the classical $\left[\dfrac{p^2}{2m} + V \right] \psi = E\psi$.

The relativistic version is

$$i\hbar \frac{\partial}{\partial t} i\hbar \frac{\partial}{\partial t} \psi = m^2c^4\psi + \left[\frac{\hbar}{i} \right]^2 \nabla \cdot \nabla c^2 \psi$$

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = m^2c^4\psi - \hbar^2 c^2 \nabla^2 \psi$$

Note the relativistic equation has both "c" and "h" in it. Divide by $\hbar^2 c^2$ to clean things up.

$$-\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \frac{m^2c^2}{\hbar^2} \psi - \nabla^2 \psi$$

Now get all the derivatives to the left side.

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \frac{m^2c^2}{\hbar^2} \psi$$

Note how "c" appears with the time and a relative minus sign occurs when comparing space to time. This is a characteristic of relativity and reminiscent of

$$x^2 - c^2t^2 .$$

We can write our relativistic equation more compactly using the d'Alembertian operator. The d'Alembertian is defined as

$$\Box \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 .$$

Sometimes you see $\Box^2$ written instead of $\Box$.

Then

$$\nabla^2 \psi - \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = \frac{m^2 c^2}{\hbar^2}\psi \quad \text{becomes} \quad (\Box + \frac{m^2 c^2}{\hbar^2})\psi = 0 .$$

To incorporate potential energy, you can let

$E \rightarrow i\hbar \dfrac{\partial}{\partial t} + V_0$, but you can also do

$$\vec{p} \rightarrow \frac{\hbar}{i}\nabla + \vec{V} .$$

The first is a scalar potential and the second is a vector potential. Schrödinger tried the Coulomb scalar potential energy since for the hydrogen atom that is all you have. He obtained the wrong energy levels for the hydrogen atom in 1925. So he reverted to the classical form for the energy and was successful in getting the correct energies.

PL1 (Practice Problem). Review of Intro Physics - Potential Energy. Calculate the scalar potential energy that Schrödinger used for the Coulomb electric force field $\vec{F}(r) = -\dfrac{e^2}{4\pi\varepsilon_0}\hat{r}$ between a proton and electron. The charge of the proton is +e (positive) and that for the electron is –e (negative). Do you remember how potential energy is related to force? If you forgot, remember it from Gravity near Earth: $\vec{F} = -mg\hat{k}$. Show that the work you do in picking up a mass from the ground to a height z is $W = mgz$. If you let it go, you get this energy back in the form of kinetic energy when the mass reaches the floor. $F(z) = -\frac{dV}{dz}$. So for $F(r)$, use $F(r) = -\frac{dV}{dr}$. Note that there is freedom in your choice of zero reference point: $V = mgz + const$. For the inverse-square-law force, the reference is taken to be infinity, i.e., $V(\infty) = 0$. So find the $V(r)$ that goes with $F(r) = -\frac{e^2}{4\pi\varepsilon_0}$.

PL2 (Practice Problem). Force as Gradient of Scalar Potential Field. Note that you can formally write $\vec{F} = -\nabla V$. Find the force field for the potential $V = xy + z^2$.

The equation

$$(\Box + \frac{m^2c^2}{\hbar^2})\psi = 0$$

has proven useful for particles with spin 0. It is called the Klein-Gordon equation. Klein and Gordon proposed using this equation for the hydrogen atom in 1927 by adding the potential energy. But as we mentioned earlier, you get the wrong energy spectrum. Pauli and Weisskopf showed in 1934 that the Klein-Gordon equation describes particles with spin 0.

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L3. The Dirac Equation.

Paul Adrien Maurice Dirac (1902-1984)
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$$E\psi = \left[\sqrt{p^2c^2 + m^2c^4}\right]\psi$$

A first-order differential equation in space and time?

$$i\hbar\frac{\partial\psi}{\partial t} = c\left[\sqrt{-\hbar^2\nabla^2 + m^2c^2}\right]\psi$$

What? Taking the square root of a "differential equation" or at least a differential operator?

$$\sqrt{p^2c^2 + m^2c^4} = c(\alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z + \beta mc)$$

PL3 (Practice Problem). Square both sides and show that there is no solution for the alphas and beta to make this work. You get nowhere with regular algebra.

Dirac proceeds anyway. He insists that $p^2c^2 + m^2c^4$ must equal

$$c^2(\alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z + \beta mc)(\alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z + \beta mc).$$

Well, you have to indeed have $\alpha_1{}^2 = \alpha_2{}^2 = \alpha_3{}^2 = \beta^2 = 1$. But also,

$$\alpha_j\alpha_k + \alpha_k\alpha_j = \{\alpha_j, \alpha_k\} = 0 \text{ for } j \neq k \text{ and } \{\alpha_j, \beta\} = 0.$$

Dirac interpreted these as MATRIX EQUATIONS to make it work!

$$\{\alpha_j, \alpha_k\} = 2I\delta_{jk} \qquad \{\alpha_j, \beta\} = 0 \qquad \beta^2 = I$$

The Pauli matrices can get you this far:

$$\{\sigma_j, \sigma_k\} = 2I\delta_{jk}$$

but we can't find a β matrix. Remember that the three Pauli matrices and the identify matrix are basis matrices for all the 2 x 2 SU(2) matrices. But the β matrix cannot be the identity since $\{\alpha_j, \beta\} = 0$ will not be true. So we go to 4 x 4 matrices to make it work. We use the Pauli matrices as our guide. The following are the Dirac matrices.

$$\alpha_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad \alpha_2 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix} \quad \alpha_3 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

PL4 (Practice Problem). Show a few of the following results.

$$\alpha_1{}^2 = \alpha_2{}^2 = \alpha_3{}^2 = \beta^2 = I$$

$\alpha_1 a_2 + \alpha_2 a_1 = 0$, $\alpha_1 a_3 + \alpha_3 a_1 = 0$, $\alpha_2 a_3 + \alpha_3 a_2 = 0$, and

$$\alpha_j \beta + \beta \alpha_j = 0$$

$$\left[\sqrt{p^2c^2 + m^2c^4}\right]\psi = c(\alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z + \beta mc)\psi$$

The Dirac Equation is $c(\vec{\alpha}\cdot\vec{p}+\beta mc)\psi = E\psi$, where $\vec{p}\rightarrow -i\hbar\nabla$.

L4. Spin and Antimatter.

Matter and Antimatter

Paul Adrien Maurice Dirac (1902-1984)

The Dirac Equation:

$$c(\vec{\alpha}\cdot\vec{p}+\beta mc)\psi = E\psi$$

For a particle at rest, there is no momentum. So we have

$$\beta mc^2\psi = E\psi$$

Let's solve this.

$$mc^2\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}\psi = \begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}E\psi$$

Since our operator is diagonalized, we have our eigenvalues: +1, +1, –1, –1, each multiplied by mc^2. The four corresponding eigenstates are

$$\psi_1 \sim \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad \psi_2 \sim \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \quad \psi_3 \sim \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \quad \psi_4 \sim \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

ψ_1 and ψ_2 represent the electron with spin up and spin down.

ψ_3 and ψ_4 represent the antielectron (positron) with spin up and spin down.

L5. Dirac Matrices Shortcuts

PL5 (Practice Problem). Show that one can write as a shortcut the following.

$$\alpha_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \equiv \begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix}$$

$$\alpha_2 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix} \equiv \begin{bmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{bmatrix}$$

$$\alpha_3 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \equiv \begin{bmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{bmatrix}$$

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \equiv \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$

Watch this. We can multiply the matrices in "2 x 2 chunks." Why does this work?

$$\begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix}\begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$